Supplementary Material (ESI) for Dalton Transactions

Catalytic hydrosilylation of olefins with organolanthanides : a DFT study. Part I : Hydrosilylation of propene by SiH_4

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Cp_2SmH and alkylsilanes

Cp_2SmH

Sm	-0.012028	-0.360917	-0.032744
C	2.651518	0.166910	0.400364
C	2.628053	-1.035725	-0.347190
C	2.153089	-0.727706	-1.648215
C	1.896905	0.667000	-1.707315
C	2.201572	1.220440	-0.439044
C	-2.676905	0.192820	0.357255
C	-2.204661	1.238468	-0.479754
C	-1.885825	0.676625	-1.740853
C	-2.155637	-0.715416	-1.679663
C	-2.653000	-1.013341	-0.384672
H	2.995320	0.268995	1.424094
H	2.924893	-2.013303	0.009195
H	2.049911	-1.428719	-2.469134
H	1.563384	1.217923	-2.578639
H	2.150921	2.271424	-0.175649
H	-3.035485	0.302623	1.375108
H	-2.148484	2.290123	-0.220217
H	-1.534462	1.220687	-2.609468
H	-2.046267	-1.421049	-2.495806
H	-2.964166	-1.986614	-0.028729
H	-0.026518	-2.217018	0.902785

E = -422.333039019
G = -422.201852

Reactions of Cp_2SmH with propene : cf. [15]

Reactions with $MeSiH_3$

$MeSiH_3$

H	0.082327	-0.069948	-0.046652
Si	-0.009324	0.048153	1.442242
C	1.710836	0.208583	2.210415
H	-0.712818	-1.165761	1.962534
H	-0.848214	1.244991	1.763120
H	2.223030	1.096913	1.829621
H	1.641903	0.294030	3.298731
H	2.323125	-0.666545	1.974361

E = -45.6053273639
G = -45.569288

$Cp_2SmH + MeSiH_3$: Si(α)-H(β) activation

$Cp_2SmH + MeSiH_3 \rightarrow Cp_2SmSiH_2Me + H_2$

Transition state

C	0.146184	1.405960	-2.035253
C	1.433604	0.874953	-1.757656
C	1.439723	-0.488737	-2.149956
C	0.153499	-0.803581	-2.653687
C	-0.645937	0.370074	-2.586560
Sm	-0.244937	-0.385151	0.006781
C	-1.454239	-2.409675	1.410038
C	-1.650614	-1.253838	2.208917
C	-2.544859	-0.391036	1.522762
C	-2.891722	-1.005648	0.295767
C	-2.214457	-2.253929	0.224899
Si	1.426218	1.109440	1.971659
H	2.544142	1.989153	1.496897
C	1.347390	1.159789	3.866297
H	0.150424	1.788548	1.419352
H	1.562816	-0.553719	1.284682
H	1.407070	-1.538549	0.692660
H	-0.153714	-1.758881	-3.063870
H	-1.667521	0.464938	-2.936153
H	-0.164754	2.433598	-1.884132
H	2.279902	1.428242	-1.368354
H	2.283929	-1.163782	-2.091411
H	-2.304291	-2.980874	-0.574193
H	-0.847519	-3.267488	1.670854
H	-1.239739	-1.090270	3.197973
H	-2.922966	0.556982	1.888715
H	-3.585720	-0.615191	-0.439511
H	1.313387	2.190108	4.231890
H	0.467482	0.629386	4.239526
H	2.236444	0.678930	4.286352

E = -467.933625619
G = -467.747535

Cp_2SmSiH_2Me

C	-2.405491	-0.982129	-0.839758
C	-2.703376	0.013717	0.127023
C	-2.371361	1.277142	-0.427954
C	-1.860549	1.063232	-1.730492
C	-1.882452	-0.333085	-1.986505
Sm	0.013207	-0.018494	-0.024789
C	0.648062	-0.921484	2.462017
C	0.165141	-2.064697	1.775440
C	1.106161	-2.399223	0.768687
C	2.172701	-1.464878	0.840841
C	1.892679	-0.552237	1.888072
Si	1.296593	2.690173	0.280661
H	1.140240	3.171169	1.716056
C	0.796073	4.212459	-0.792270
H	2.812322	2.628207	0.163871
H	3.067926	-1.469180	0.228302
H	2.526486	0.264591	2.208713
H	0.171270	-0.436650	3.306627
H	-0.744038	-2.608694	2.002402
H	1.045389	-3.251394	0.100622
H	-1.537496	1.836067	-2.417588
H	-1.599187	-0.815539	-2.916171
H	-2.584673	-2.045612	-0.734264
H	-3.159370	-0.157469	1.095512
H	-2.501537	2.240088	0.050908
H	1.355218	5.107784	-0.504119
H	0.988574	4.023078	-1.853909
H	-0.271495	4.431570	-0.683767

E = -466.760391005
G = -466.589548

H_2
E = -1.17751649843
G = -1.178858

$Cp_2SmH + MeSiH_3$: Si(β)-H(α) activation

$Cp_2SmH + MeSiH_3 \rightarrow Cp_2SmH + MeSiH_3$

Transition state

C	-2.320700	-0.838019	-1.276761
C	-2.717299	-0.501000	0.043526
C	-2.607323	0.906000	0.186749
C	-2.150035	1.438881	-1.046086
C	-1.974833	0.361315	-1.951058
Sm	-0.038607	0.005772	-0.040046
C	0.853453	-0.570649	2.487622
C	0.248553	-1.768160	2.027920
C	1.050980	-2.289182	0.980534
C	2.155675	-1.417569	0.798486
C	2.033236	-0.355208	1.729647
C	3.537981	1.800481	-1.311923
Si	1.729116	1.962712	-1.855540
H	1.666011	1.747434	-3.358395
H	1.364441	3.437877	-1.837735
H	2.970164	-1.557991	0.098380
H	2.737187	0.456897	1.864117
H	0.501451	0.045722	3.307614
H	-0.646967	-2.225743	2.431489
H	0.877754	-3.218060	0.448350
H	-1.994346	2.487525	-1.268928
H	-1.660336	0.444743	-2.984367
H	-2.330915	-1.832424	-1.709241
H	-3.079945	-1.191647	0.795768
H	-2.872390	1.478023	1.069177
H	1.177918	0.349109	-1.789372
H	0.891771	1.927520	-0.370611
H	4.153923	2.457490	-1.933604
H	3.668880	2.098436	-0.268243
H	3.902499	0.776930	-1.432649

E = -467.942979485
G = -467.754530

$Cp_2SmH + MeSiH_3$: Si(α)-C(β) activation

$Cp_2SmH + MeSiH_3 \rightarrow Cp_2SmSiH_3 + CH_4$

Transition state

Sm	-0.103284	-0.253826	-0.014221
Si	-2.696218	-1.255055	0.026791
H	-3.486491	-1.567135	1.253997
H	-2.537100	0.328351	-0.022777
H	-3.496027	-1.641198	-1.172829
H	0.020227	-2.297868	0.053961
C	-1.276003	-3.029056	0.070885
H	-2.377489	-3.292215	0.084201
H	-0.926962	-3.529064	0.977931
H	-0.937238	-3.565660	-0.818844
C	1.710355	0.160603	1.982315
C	0.938076	1.353519	1.943769
C	-0.364925	1.044647	2.400485
C	-0.404757	-0.339532	2.715835
C	0.882909	-0.883379	2.464957
C	1.701598	0.043066	-2.039128
C	0.881081	-1.036640	-2.449761
C	-0.411520	-0.520078	-2.731483
C	-0.381613	0.882022	-2.507763
C	0.920071	1.229939	-2.075780
H	2.761434	0.075330	1.731143
H	1.296909	2.334761	1.654974
H	-1.181465	1.747633	2.518107
H	-1.247282	-0.868129	3.145558
H	1.191936	-1.904662	2.650296
H	2.754032	-0.017204	-1.786311
H	1.197602	-2.065490	-2.568863
H	-1.251569	-1.082019	-3.121888
H	-1.204098	1.569472	-2.667803
H	1.271940	2.230545	-1.852031

E = -467.853084003
G = -467.664300

Cp_2SmSiH_3

Sm	0.012178	0.013956	-0.055232
C	2.717161	0.446808	0.083382
C	2.575666	-0.905991	-0.310994
C	2.025039	-0.921480	-1.619741
C	1.838723	0.421996	-2.036394
C	2.262398	1.268920	-0.981395
C	-2.671303	0.522888	0.242215
C	-2.216176	1.470050	-0.712783
C	-1.857685	0.766744	-1.890007
C	-2.084640	-0.615234	-1.659263
C	-2.596116	-0.763898	-0.343066
H	3.134369	0.790319	1.023565
H	2.858054	-1.771854	0.274441
H	1.829896	-1.805269	-2.216811
H	1.473499	0.744348	-3.004086
H	2.285375	2.353091	-1.007688
H	-3.042962	0.743361	1.236439
H	-2.197243	2.547282	-0.585750
H	-1.509858	1.209521	-2.815597
H	-1.947184	-1.411062	-2.382679
H	-2.895282	-1.692513	0.126324
Si	-0.002566	-2.047720	2.140529
H	-1.177208	-2.074483	3.096339
H	-0.001463	-3.463900	1.596108
H	1.187329	-2.068744	3.078551

E = -427.451102323
G = -427.307459

CH_4

C	0.039072	-0.035042	-0.040623
H	-0.024998	0.044660	1.046342
H	1.085768	0.014133	-0.347286
H	-0.388475	-0.986596	-0.362681
H	-0.512749	0.787595	-0.499680

E = -40.5081085049
G = -40.482694

$Cp_2SmH + MeSiH_3$: Si(β)-C(α) activation

$Cp_2SmH + MeSiH_3 \rightarrow Cp_2SmCH_3 + SiH_4$

Transition state

Sm	-0.085043	-0.528591	-0.236680
C	2.644659	-0.909906	-0.381744
C	2.112242	-1.577115	-1.514872
C	1.588281	-0.596755	-2.395368
C	1.792835	0.676031	-1.801960
C	2.449366	0.481617	-0.559809
C	-2.127596	-0.430974	-2.034394
C	-2.656071	-1.175143	-0.948402
C	-2.801337	-0.298126	0.156064
C	-2.365377	0.989858	-0.246883
C	-1.948397	0.908450	-1.598691
H	3.149404	-1.376957	0.455735
H	2.146260	-2.645278	-1.700642
H	1.149295	-0.782772	-3.368474
H	1.535909	1.632100	-2.242869
H	2.767396	1.260616	0.121971
H	-1.943758	-0.805670	-3.034558
H	-2.942093	-2.221170	-0.974222
H	-3.211158	-0.554476	1.125975
H	-2.371016	1.880749	0.369283
H	-1.595256	1.732551	-2.207322
H	0.934949	0.020542	3.645474
Si	-0.356799	0.028282	2.890244
C	-0.091309	-1.898733	1.956035
H	0.157916	0.734782	1.441528
H	-0.946579	1.418858	3.112560
H	-1.411002	-0.713748	3.706954
H	0.816013	-2.214807	1.403687
H	-0.987180	-2.377415	1.525934
H	0.033258	-2.363978	2.935603

E = -467.922508193
G = -467.732888

Cp_2SmCH_3

Sm	-0.004844	-0.164908	-0.053501
C	2.671275	0.454573	0.256658
C	2.652999	-0.831945	-0.329390
C	2.154424	-0.701376	-1.652771
C	1.883549	0.671484	-1.887207
C	2.194388	1.386002	-0.705366
C	-2.705172	0.371265	0.192254
C	-2.238993	1.302171	-0.775484
C	-1.880950	0.579189	-1.938624
C	-2.112533	-0.797804	-1.686723
C	-2.633662	-0.923387	-0.371702
H	3.023237	0.691010	1.254730
H	2.970444	-1.751290	0.146459
H	2.059011	-1.500994	-2.379319
H	1.525521	1.100780	-2.815369
H	2.133182	2.461539	-0.578068
H	-3.085709	0.612287	1.178723
H	-2.214633	2.381000	-0.664983
H	-1.518239	1.004831	-2.866646
H	-1.976616	-1.605466	-2.397766
H	-2.931017	-1.844829	0.112895
C	0.006960	-1.849234	1.728586
H	0.883128	-1.781247	2.391285
H	-0.883306	-1.810348	2.374677
H	0.027555	-2.871399	1.314523

E = -461.642535917
G = -461.486467

SiH_4

Si	0.039477	-0.034937	-0.040692
H	-0.049434	0.074062	1.444033
H	1.471253	0.032766	-0.459854
H	-0.546669	-1.335733	-0.480347
H	-0.716009	1.088593	-0.667068

E = -6.28910490369
G = -6.279886

$Cp_2SmH + MeSiH_3$: C-H activation

$Cp_2SmH + MeSiH_3 \rightarrow Cp_2SmCH_2SiH_3 + H_2$

Transition state

C	-0.286290	-0.299139	-2.881720
C	-0.281415	1.042556	-2.423362
C	1.015971	1.331666	-1.926418
C	1.815922	0.174133	-2.087922
C	1.010845	-0.834684	-2.681272
Sm	1.349141	1.020568	-4.644056
C	2.440598	0.168763	-7.016504
C	2.891491	1.504417	-6.873168
C	3.797318	1.547183	-5.780298
C	3.899939	0.240122	-5.245266
C	3.056050	-0.612068	-6.005779
C	-0.417048	2.854064	-5.741875
H	-1.442401	2.948667	-5.371395
H	-0.435361	1.413543	-5.843102
H	-0.344035	0.401003	-5.846274
H	-1.134047	1.711263	-2.406723
H	-1.137023	-0.828133	-3.292781
H	1.321311	-1.849972	-2.899315
H	2.846774	0.062998	-1.772664
H	1.330168	2.262985	-1.469703
H	4.538697	-0.064277	-4.424508
H	2.939404	-1.680829	-5.868117
H	1.759645	-0.196292	-7.775197
H	2.631700	2.336033	-7.517776
H	4.346091	2.418493	-5.441904
H	-0.417683	3.041233	-6.820053
Si	0.667001	4.108101	-4.894012
H	1.798372	3.350393	-4.162234
H	1.416378	5.028758	-5.799946
H	0.015444	4.875706	-3.791324

E = -467.927272094
G = -467.741621

$Cp_2SmCH_2SiH_3$

C	-2.651873	-1.283477	-1.030480
C	-2.958137	-0.175722	-0.206242
C	-2.458728	0.994845	-0.838047
C	-1.844762	0.607743	-2.053391
C	-1.952616	-0.803208	-2.168840
Sm	-0.206169	-0.410900	-0.096436
C	2.050727	1.169308	0.044919
C	2.443664	-0.069784	0.617615
C	2.458561	-1.041610	-0.409666
C	2.066027	-0.409734	-1.618737
C	1.822962	0.960625	-1.336838
C	-0.374603	-2.231527	1.628568
H	2.716850	-0.234010	1.653240
H	2.739635	-2.081864	-0.296026
H	2.021444	-0.874728	-2.597185
H	1.543348	1.718782	-2.058795
H	1.982236	2.117520	0.566632
H	-3.509846	-0.209387	0.725938
H	-2.571479	2.010880	-0.476006
H	-1.396219	1.272715	-2.781868
H	-1.618843	-1.399080	-3.011103
H	-2.920489	-2.314589	-0.835677
H	0.538559	-2.809944	1.797532
Si	-0.645582	-0.982445	2.953183
H	-1.229723	-2.906188	1.526589
H	0.425723	-0.786903	3.979933
H	-0.608777	0.396568	2.202211
H	-1.987515	-0.921210	3.613298

E = -466.759831327
G = -466.588778

Reactions with Me_2SiH_2

Me_2SiH_2

C	0.075207	-0.074383	-0.071596
Si	-0.028990	0.078345	1.812233
C	1.684510	0.239997	2.599609
H	-0.724777	-1.126452	2.373155
H	-0.858924	1.275137	2.171599
H	0.657857	-0.954934	-0.359967
H	-0.922588	-0.170145	-0.510165
H	0.554270	0.807147	-0.509068
H	2.202396	1.130186	2.229022
H	1.606514	0.322311	3.687869
H	2.303541	-0.632824	2.369488

E = -84.9213705266
G = -84.858656

$Cp_2SmH + Me_2SiH_2$: Si(α)-H(β) activation

$Cp_2SmH + Me_2SiH_2 \rightarrow Cp_2SmSiHMe_2 + H_2$

Transition state

C	0.415778	1.399489	-2.017145
C	1.583818	0.610728	-1.856923
C	1.280571	-0.710344	-2.266436
C	-0.077106	-0.736555	-2.687918
C	-0.608938	0.568105	-2.537667
Sm	-0.205256	-0.372308	0.004625
C	-1.160724	-1.695139	2.229065
C	-1.935256	-2.168303	1.139016
C	-1.084975	-2.928192	0.297882
C	0.215862	-2.929944	0.871794
C	0.165003	-2.171993	2.066876
Si	0.231780	1.907908	1.839857
C	0.832998	3.636507	1.331896
H	1.394861	0.918371	1.518376
C	-0.023964	1.857247	3.721595
H	-1.257655	1.353144	0.890798
H	-1.974360	0.802612	0.226472
H	-1.383419	-3.456048	-0.600490
H	1.080460	-3.459174	0.488057
H	0.989066	-2.010078	2.752341
H	-1.533640	-1.112710	3.062741
H	-2.994324	-1.997632	0.991537
H	-0.598405	-1.594185	-3.097237
H	-1.611824	0.883359	-2.796791
H	0.330862	2.462817	-1.828648
H	2.548774	0.963532	-1.511042
H	1.973355	-1.543378	-2.299334
H	1.674192	3.960836	1.953137
H	1.148542	3.658801	0.285759
H	0.023999	4.364528	1.454632
H	0.851914	2.247238	4.250266
H	-0.885549	2.474605	3.997605
H	-0.214211	0.839980	4.073077

E = -507.247978623
G = -507.035658

$Cp_2SmSiHMe_2$

C	-2.408572	-0.933915	-0.810308
C	-2.677333	0.039806	0.183940
C	-2.347126	1.312797	-0.350984
C	-1.874777	1.128287	-1.673795
C	-1.906757	-0.262854	-1.954750
Sm	0.049371	0.006579	-0.080716
C	1.121983	-2.485390	-0.272376
C	2.248245	-1.621845	-0.290721
C	2.369393	-1.032525	0.990298
C	1.322626	-1.536032	1.805905
C	0.552349	-2.435935	1.027045
Si	1.709776	2.074213	-1.527754
H	1.055972	3.448321	-1.408244
C	3.507598	2.392318	-0.903136
C	1.876073	1.831572	-3.436641
H	-2.470794	2.267534	0.148581
H	-1.573496	1.912703	-2.355881
H	-1.639059	-0.727215	-2.897275
H	-2.587310	-1.998924	-0.722528
H	-3.108833	-0.151982	1.160332
H	3.143434	-0.338450	1.295394
H	1.169250	-1.313275	2.856733
H	-0.294239	-3.016633	1.373819
H	0.788972	-3.117021	-1.088032
H	2.913291	-1.456475	-1.129357
H	2.429117	2.659403	-3.894223
H	2.412562	0.904680	-3.670426
H	0.895748	1.776082	-3.922024
H	3.999930	3.179990	-1.484639
H	3.514586	2.702898	0.147683
H	4.119113	1.486335	-0.983186

E = -506.070197646
G = -505.872011

$Cp_2SmH + Me_2SiH_2$: Si(β)-H(α) activation

$Cp_2SmH + Me_2SiH_2 \rightarrow Cp_2SmH + Me_2SiH_2$

Transition state

C	-2.377033	-0.810980	-1.255386
C	-2.718818	-0.477990	0.079881
C	-2.572665	0.924972	0.233887
C	-2.137158	1.458634	-1.005317
C	-2.013103	0.385468	-1.924940
Sm	-0.016471	-0.035134	-0.096498
C	1.022618	-2.420166	-0.926994
C	1.877196	-1.433356	-1.482740
C	2.593302	-0.823394	-0.420921
C	2.177863	-1.429238	0.791706
C	1.204675	-2.413705	0.479812
C	-0.094122	3.831842	1.449844
Si	1.239036	2.482715	1.461926
H	2.502494	3.046803	0.831314
C	1.883064	2.268286	3.256936
H	-2.793789	1.494067	1.128618
H	-1.964418	2.505927	-1.220557
H	-1.736581	0.470469	-2.970095
H	-2.423768	-1.799279	-1.697358
H	-3.077238	-1.168017	0.835975
H	3.346202	-0.051034	-0.520562
H	2.562759	-1.204639	1.779013
H	0.722728	-3.080420	1.186482
H	0.375978	-3.089069	-1.482508
H	1.997276	-1.217612	-2.538690
H	0.379195	1.038468	1.738655
H	1.000349	1.855829	-0.129250
H	0.279651	4.705321	1.994131
H	-0.343520	4.144918	0.432885
H	-1.009636	3.495248	1.945086
H	2.391389	3.183923	3.582647
H	1.066886	2.041659	3.951742
H	2.609177	1.449548	3.312890

E = -507.258214425
G = -507.042490

$Cp_2SmH + Me_2SiH_2$: Si(β)-C(α) activation

$Cp_2SmH + Me_2SiH_2 \rightarrow Cp_2SmCH_3 + MeSiH_3$

Transition state

C	-1.954161	0.776828	-1.796985
C	-2.149501	-0.606051	-2.051257
C	-2.687737	-1.192928	-0.877221
C	-2.818439	-0.177545	0.102063
C	-2.366780	1.040617	-0.467709
Sm	-0.102483	-0.495983	-0.249616
C	-0.127426	-1.913576	1.908223
Si	-0.293827	-0.002226	2.923457
C	2.626398	-0.892384	-0.364970
C	2.104379	-1.523749	-1.523775
C	1.601775	-0.515079	-2.384057
C	1.806387	0.738868	-1.751997
C	2.444823	0.504534	-0.507006
H	3.113290	-1.386822	0.467268
H	2.132489	-2.586540	-1.738872
H	1.172978	-0.670290	-3.367046
H	1.563825	1.709021	-2.169897
H	2.758357	1.261326	0.201202
H	-1.970433	-1.111937	-2.992948
H	-2.985793	-2.229609	-0.763962
H	-3.227042	-0.301198	1.098092
H	-2.364211	2.007159	0.021350
H	-1.590696	1.508516	-2.508850
H	1.065074	-0.072193	3.551607
H	0.120598	0.737630	1.446066
C	-1.039629	1.726683	3.336830
H	-1.267602	-0.800149	3.792630
H	0.732464	-2.251357	1.292929
H	-1.063391	-2.348151	1.521010
H	0.044472	-2.410844	2.863991
H	-1.214054	1.796043	4.417268
H	-0.379279	2.540334	3.018722
H	-2.006914	1.859990	2.838151

E = -507.236728630
G = -507.019817

Reactions with Me_3SiH

Me_3SiH

Si	0.080402	-0.071848	-0.062515
C	-0.044099	0.055025	1.824096
H	1.531181	0.009010	-0.448728
C	-0.607334	-1.732263	-0.663685
C	-0.839495	1.366158	-0.885396
H	-1.087076	0.002577	2.154115
H	0.503228	-0.759206	2.309656
H	0.374294	1.001077	2.182213
H	-1.666365	-1.836869	-0.404903
H	-0.516375	-1.824324	-1.750688
H	-0.066327	-2.568695	-0.209802
H	-0.433987	2.329242	-0.559244
H	-0.751582	1.316803	-1.975404
H	-1.904975	1.347206	-0.632711

E = -124.237241384
G = -124.148080

$Cp_2SmH + Me_3SiH$: Si(α)-H(β) activation

$Cp_2SmH + Me_3SiH \rightarrow Cp_2SmSiMe_3 + H_2$

Transition state

C	1.196512	1.138406	-1.929115
C	1.842855	-0.126526	-1.951343
C	0.927258	-1.078983	-2.463237
C	-0.290642	-0.407878	-2.743688
C	-0.120736	0.963919	-2.417251
Sm	-0.049724	-0.354755	-0.004730
C	1.788057	0.288035	1.887797
C	0.837291	1.342900	1.947347
C	-0.364299	0.815065	2.480836
C	-0.161776	-0.563597	2.743771
C	1.172047	-0.887774	2.383996
Si	-2.792139	-1.640791	0.019347
H	-1.031509	-2.300582	0.040173
H	0.019070	-2.486183	0.043659
C	-3.631222	-2.191728	1.637894
C	-3.116982	0.259746	-0.203988
C	-3.639616	-2.535172	-1.431552
H	2.817723	0.379225	1.561870
H	1.016622	2.377763	1.679244
H	-1.267850	1.377009	2.689421
H	-0.878892	-1.241928	3.189432
H	1.641555	-1.857053	2.495082
H	2.870692	-0.320792	-1.667372
H	1.128614	-2.129570	-2.629875
H	-1.171877	-0.852646	-3.189607
H	-0.854667	1.749319	-2.559157
H	1.644979	2.077113	-1.625170
H	-4.721626	-2.361868	-1.428280
H	-3.244693	-2.200026	-2.395221
H	-3.472913	-3.615059	-1.362733
H	-4.720986	-2.096047	1.568505
H	-3.400393	-3.239098	1.857896
H	-3.292794	-1.590741	2.487140
H	-3.998204	0.548126	0.379417
H	-2.330193	0.957905	0.142838
H	-3.305974	0.497760	-1.254467

E = -546.557640229
G = -546.317170

$Cp_2SmSiMe_3$

C	-2.496369	-0.902142	-0.598320
C	-2.703649	0.220654	0.238282
C	-2.330062	1.382415	-0.485738
C	-1.888790	0.977296	-1.770822
C	-1.988012	-0.437229	-1.839113
Sm	0.030323	0.030444	-0.079403
C	2.358931	1.170425	-0.994972
C	2.771887	0.262917	0.015678
C	2.520338	-1.052817	-0.443101
C	1.942109	-0.959167	-1.736552
C	1.849152	0.414625	-2.079726
Si	-0.002679	-2.003327	2.169012
H	3.232257	0.524900	0.961676
H	2.753809	-1.966242	0.088721
H	1.670635	-1.792802	-2.374335
H	1.485460	0.813569	-3.019137
H	2.462418	2.249972	-0.966107
H	-3.099597	0.192353	1.246177
H	-2.416988	2.406265	-0.136926
H	-1.575478	1.633496	-2.574148
H	-1.767265	-1.047701	-2.707224
H	-2.708033	-1.932283	-0.339778
C	-1.535173	-1.920445	3.340348
C	0.018696	-3.834417	1.556832
C	1.505166	-1.885725	3.369836
H	0.010994	-4.529526	2.405927
H	-0.855261	-4.063032	0.936012
H	0.911333	-4.053238	0.959836
H	-1.474856	-2.683981	4.126336
H	-1.613843	-0.945137	3.835485
H	-2.468948	-2.085329	2.790570
H	1.460409	-2.665625	4.140661
H	2.455871	-2.001111	2.837019
H	1.534365	-0.917867	3.884632

E = -545.380872545
G = -545.154305

$Cp_2SmH + Me_3SiH$: Si(β)-H(α) activation

$Cp_2SmH + Me_3SiH \rightarrow Cp_2SmH + Me_3SiH$

Transition state

C	-2.362138	-0.799330	-1.253069
C	-2.710696	-0.388961	0.059369
C	-2.537910	1.015875	0.139676
C	-2.084778	1.474521	-1.124124
C	-1.981866	0.354071	-1.987047
Sm	0.003032	-0.002067	-0.141736
C	2.295592	0.766681	-1.443006
C	2.749261	0.149185	-0.249093
C	2.453042	-1.234674	-0.332231
C	1.814959	-1.472302	-1.577184
C	1.722691	-0.235691	-2.266056
Si	0.076124	-0.016150	3.090633
H	3.262888	0.641195	0.567539
H	2.702265	-1.983503	0.409672
H	1.499219	-2.437311	-1.958111
H	1.319718	-0.089998	-3.261341
H	2.410409	1.813678	-1.701815
H	-3.075058	-1.031248	0.851770
H	-2.748905	1.634958	1.002973
H	-1.896238	2.507067	-1.397127
H	-1.699307	0.379143	-3.032879
H	-2.425306	-1.809036	-1.643444
C	1.897192	-0.299240	3.543351
H	0.244519	1.033662	1.727604
H	-0.096805	-1.058708	1.722804
C	-0.537923	1.574234	3.980309
C	-0.997198	-1.345254	3.973820
H	1.982973	-0.369909	4.633448
H	2.286978	-1.226978	3.115440
H	2.528807	0.529321	3.210793
H	-0.976850	-1.204698	5.061068
H	-2.043103	-1.276485	3.652866
H	-0.644449	-2.354715	3.738603
H	-0.564090	1.429427	5.066936
H	0.109713	2.426505	3.750125
H	-1.553299	1.833372	3.658888

E = -546.571766212
G = -546.329368

$Cp_2SmH + Me_3SiH$: Si(β)-C(α) activation

$Cp_2SmH + Me_3SiH \rightarrow Cp_2SmCH_3 + Me_2SiH_2$

Transition state

C	-1.952000	0.814527	-1.811721
C	-2.147593	-0.565480	-2.079663
C	-2.703580	-1.160315	-0.917841
C	-2.844512	-0.152669	0.067693
C	-2.381470	1.068719	-0.485828
Sm	-0.124834	-0.478881	-0.242334
C	-0.194843	-1.939864	1.870647
Si	-0.274581	-0.002568	2.944291
C	2.613152	-0.838543	-0.277902
C	2.128504	-1.535096	-1.414569
C	1.629902	-0.579370	-2.335768
C	1.802622	0.708087	-1.764442
C	2.414530	0.546612	-0.495060
H	3.083668	-1.283361	0.590665
H	2.175992	-2.606923	-1.574098
H	1.228163	-0.790866	-3.319699
H	1.556188	1.651777	-2.236992
H	2.702820	1.343952	0.178557
H	-1.956582	-1.064427	-3.022759
H	-3.004096	-2.197530	-0.816534
H	-3.263493	-0.283539	1.058396
H	-2.383369	2.031312	0.011025
H	-1.576511	1.550682	-2.512687
C	1.439719	-0.007683	3.762221
H	0.090174	0.738280	1.462052
C	-1.112076	1.685574	3.346504
H	-1.222686	-0.844934	3.798682
H	0.571788	-2.355586	1.178579
H	-1.186524	-2.323786	1.587724
H	0.047513	-2.426480	2.816479
H	1.328883	0.202868	4.831093
H	1.955523	-0.966293	3.658176
H	2.076202	0.771946	3.332565
H	-1.301128	1.752579	4.425111
H	-0.491296	2.532336	3.032688
H	-2.080105	1.772559	2.839481

E = -546.550520610
G = -546.308220

$Cp_2SmCH_2CH_2CH_3$ and alkylsilanes

$Cp_2SmCH_2CH_2CH_3$

C	2.280756	3.420334	-1.116375
C	3.199026	3.738073	-0.082524
C	2.524034	4.536137	0.876929
C	1.186082	4.698738	0.442401
C	1.034349	4.008083	-0.789481
Sm	1.402965	2.020697	1.093000
C	0.908540	-0.613524	1.768246
C	2.085613	-0.647353	0.982422
C	1.739164	-0.298224	-0.348705
C	0.344250	-0.046637	-0.384721
C	-0.168546	-0.239881	0.923807
H	-0.365473	2.721623	2.561235
C	0.119826	2.599202	3.591580
C	1.617189	2.352129	3.507504
C	-0.321354	3.847509	4.358101
H	2.961492	4.967240	1.768372
H	0.423190	5.287203	0.939706
H	0.137943	3.979034	-1.399047
H	2.500734	2.851962	-2.012483
H	4.248976	3.466679	-0.059161
H	2.412257	-0.271996	-1.197848
H	-0.233184	0.207245	-1.266446
H	-1.210180	-0.166158	1.216543
H	0.840264	-0.855222	2.821414
H	3.073902	-0.926352	1.331167
H	0.167237	4.741385	3.955814
H	-0.030793	3.759360	5.409660
H	-1.405682	4.003938	4.313502
H	-0.402745	1.716884	3.980892
H	2.183924	3.243654	3.798295
H	1.928973	1.515677	4.138318

E = -540.244424824
G = -540.032604

Reactions of $Cp_2SmCH_2CH_2CH_3$ with propene : cf. [15]

Reactions with $MeSiH_3$

$Cp_2SmCH_2CH_2CH_3 + MeSiH_3$: Si(α)-H(β) activation

$Cp_2SmCH_2CH_2CH_3 + MeSiH_3 \rightarrow Cp_2SmSiH_2Me + propane$

Transition state

C	0.838115	1.476469	-1.953328
C	1.737409	0.395755	-2.156753
C	0.998220	-0.695903	-2.678795
C	-0.355003	-0.294147	-2.792617
C	-0.452941	1.049658	-2.349521
Sm	0.159316	-0.401643	-0.069445
C	-0.165995	-2.969767	-0.273500
C	-0.667650	-4.040117	0.692432
C	-0.135904	-5.447115	0.414248
C	0.288385	0.921399	2.341814
C	1.582272	1.033308	1.779239
C	2.170185	-0.260315	1.772822
C	1.239606	-1.166485	2.340747
C	0.073363	-0.439350	2.685158
Si	-2.781393	-0.873429	0.325888
H	-3.351599	-1.101588	1.694543
C	-4.149582	-1.090072	-0.974961
H	-2.384195	0.610741	0.336656
H	-1.377169	-1.951151	0.016335
H	3.175151	-0.499486	1.443419
H	2.055374	1.948827	1.444215
H	-0.406031	1.736753	2.509452
H	-0.808974	-0.841453	3.168377
H	1.401395	-2.224552	2.505640
H	1.400800	-1.660909	-2.963208
H	-1.164877	-0.896391	-3.186733
H	-1.351941	1.655199	-2.345345
H	1.101897	2.466119	-1.598986
H	2.808471	0.420477	-1.991151
H	0.944892	-2.954194	-0.233878
H	-0.416931	-3.244681	-1.307511
H	-0.415811	-3.756252	1.723511
H	-1.768259	-4.063896	0.661721
H	-0.537281	-6.181375	1.122737
H	-0.404916	-5.775549	-0.596218
H	0.957428	-5.476645	0.487443
H	-5.026779	-0.482963	-0.734007
H	-3.792074	-0.801647	-1.967381
H	-4.462222	-2.137930	-1.020267

E = -585.834479928
G = -585.569680

Propane

C	0.000007	0.088835	0.000106
H	0.019158	0.133981	1.095157
H	1.038564	0.135147	-0.347477
C	-0.688300	-1.183920	-0.487090
H	-0.722302	-1.183920	-1.584375
C	0.000007	-2.456675	0.000106
H	-1.734365	-1.183920	-0.153958
H	-0.510552	0.988095	-0.360075
H	-0.510552	-3.355935	-0.360075
H	1.038564	-2.502987	-0.347477
H	0.019158	-2.501821	1.095157

E = -119.110587845
G = -119.032363

$Cp_2SmCH_2CH_2CH_3$ + $MeSiH_3$: Si(β)-H(α) activation

$Cp_2SmCH_2CH_2CH_3$ + $MeSiH_3$ → Cp_2SmH + $MeSiH_2$-CH_2-CH_2-CH_3

Transition state

C	0.938977	1.275399	-1.899755
C	1.767078	0.143806	-2.124716
C	0.966294	-0.882253	-2.687571
C	-0.356575	-0.393190	-2.793180
C	-0.372298	0.943611	-2.311167
Sm	0.150456	-0.633925	-0.067142
C	0.335631	-3.095666	-0.278423
C	-0.142844	-4.041220	0.828496
C	0.031038	-5.532082	0.515194
C	-0.007721	0.539026	2.452165
C	1.131320	1.104490	1.831070
C	2.106147	0.081723	1.693548
C	1.569441	-1.112982	2.239750
C	0.261990	-0.832987	2.700538
Si	-3.252475	-0.604571	0.234824
H	-3.857028	-0.698675	1.593279
C	-4.525364	-0.484483	-1.143303
H	-2.322731	0.585489	0.228751
H	-2.334971	-1.785175	0.041970
H	3.106002	0.206372	1.293798
H	1.252034	2.141988	1.542574
H	-0.908757	1.072817	2.733256
H	-0.401039	-1.536245	3.190911
H	2.074513	-2.068593	2.301922
H	1.306486	-1.865542	-2.986173
H	-1.197180	-0.930782	-3.217509
H	-1.227056	1.610827	-2.303103
H	1.261260	2.233157	-1.508903
H	2.835829	0.093440	-1.950572
H	1.403112	-3.303597	-0.482587
H	-0.176153	-3.369177	-1.219742
H	0.384543	-3.820798	1.767441
H	-1.207308	-3.860546	1.049080
H	-0.322961	-6.174440	1.332070
H	-0.521685	-5.807730	-0.390882
H	1.086398	-5.769408	0.336119
H	-5.163915	0.391544	-0.998776
H	-4.035383	-0.400969	-2.116770
H	-5.159738	-1.375428	-1.150354

E = -585.851249380
G = -585.587235

$MeSiH_2$-CH_2-CH_2-CH_3 ('linear' hydrosilylation product)

C	-0.937593	1.396204	-0.518616
Si	-0.042956	-0.042445	0.328566
C	1.795233	-0.175746	-0.180542
C	2.560666	1.117072	0.175196
C	2.429602	-1.427369	0.439558
H	-0.116758	0.126077	1.818847
H	-0.745209	-1.325541	-0.012448
H	-0.492058	2.359019	-0.251070
H	-0.900140	1.292814	-1.607672
H	-1.989737	1.418939	-0.218584
H	1.795651	-0.295699	-1.274488
H	3.466211	-1.566130	0.109308
H	2.447308	-1.360953	1.533848
H	1.875728	-2.333869	0.173180
Si	4.352174	1.258670	-0.466626
H	2.033152	1.996684	-0.219288
H	2.584132	1.252583	1.265629
H	4.849603	2.635615	-0.136053
H	5.263347	0.291408	0.227825
C	4.454395	0.985061	-2.337522
H	5.479730	1.131032	-2.690570
H	4.147524	-0.029881	-2.608148
H	3.809267	1.689613	-2.871823

E = -207.928792304
G = -207.776118

$Cp_2SmCH_2CH_2CH_3$ + $MeSiH_3$: Si(β)-C(α) activation

$Cp_2SmCH_2CH_2CH_3$ + $MeSiH_3$ → Cp_2SmCH_3 + SiH_3-CH_2-CH_2-CH_3

Transition state

C	-1.983790	1.405265	-0.946922
C	-1.941084	0.376950	-1.920534
C	-2.410619	-0.817284	-1.316954
C	-2.767799	-0.518114	0.024675
C	-2.502363	0.851786	0.255136
Sm	-0.026832	-0.293641	-0.108435
C	2.418091	0.437908	-1.179792
C	2.650683	-0.837029	-0.606111
C	1.929089	-1.794206	-1.363301
C	1.248632	-1.111318	-2.401487
C	1.550349	0.270463	-2.287218
C	-0.032854	-1.990376	1.867115
Si	-0.714895	-0.261126	2.968659
H	3.298595	-1.047770	0.236783
H	1.926404	-2.865581	-1.197760
H	0.637352	-1.567888	-3.170855
H	1.213721	1.053608	-2.955985
H	2.854710	1.373760	-0.849882
H	-1.625332	0.487110	-2.950557
H	-2.532339	-1.774376	-1.811872
H	-3.184963	-1.207568	0.748176
H	-2.683497	1.384448	1.180665
H	-1.722586	2.445345	-1.108316
H	0.147204	-0.550947	4.159318
C	0.635994	1.085785	1.978877
H	-1.425020	1.057141	3.328220
H	-1.999579	-1.092105	3.124220
H	0.995467	-1.986090	1.452373
H	-0.727184	-2.352938	1.072550
C	-0.050725	-3.087562	2.936464
H	1.627579	0.812665	1.572976
H	0.216056	1.925027	1.394727
H	0.859285	1.530195	2.950860
H	-0.998123	-3.022589	3.488053
C	0.122214	-4.502819	2.383223
H	0.739490	-2.879385	3.667183
H	0.108941	-5.245853	3.188362
H	-0.684113	-4.757306	1.685186
H	1.072124	-4.612476	1.847205

E = -585.811889389
G = -585.539166

$SiH_3-CH_2-CH_2-CH_3$

H	-0.128379	0.058547	1.839349
Si	-0.025272	-0.075569	0.351520
H	-0.770503	1.066549	-0.266882
C	1.790321	-0.069821	-0.199026
C	2.555235	1.206072	0.177771
C	4.015159	1.181302	-0.273020
H	-0.702056	-1.348616	-0.051353
H	2.281762	-0.948694	0.239284
H	1.816930	-0.220033	-1.286566
H	2.054028	2.078481	-0.261542
H	2.513309	1.352169	1.265067
H	4.537167	2.102158	0.007983
H	4.553952	0.341228	0.179604
H	4.090919	1.073837	-1.360997

E = -124.206080166
G = -124.117276

$Cp_2SmCH_2CH_2CH_3$ + $MeSiH_3$: C-H activation

$Cp_2SmCH_2CH_2CH_3$ + $MeSiH_3$ → $Cp_2SmCH_2SiH_3$ + propane

Transition state

C	0.715031	1.394202	-1.971110
C	1.588571	0.286278	-2.119267
C	0.872837	-0.755657	-2.756847
C	-0.449153	-0.294772	-2.996694
C	-0.545742	1.030581	-2.504965
Sm	1.112342	1.159726	-4.704266
C	-0.521130	3.165904	-5.190785
C	-1.044788	4.297201	-4.305713
C	-2.443893	4.792413	-4.677189
C	2.274570	-0.553662	-6.506070
C	0.908062	-0.923250	-6.469987
C	0.154484	0.123623	-7.061509
C	1.058943	1.132576	-7.476666
C	2.367249	0.718704	-7.131262
C	2.253790	3.680324	-4.600509
H	2.420964	4.284645	-5.498926
H	2.069371	4.364925	-3.765851
Si	3.830763	2.742529	-4.234929
H	0.962573	3.326885	-4.858291
H	-1.255179	-0.873078	-3.433598
H	1.254083	-1.744367	-2.983745
H	2.614556	0.233324	-1.774681
H	0.954595	2.334656	-1.489049
H	-1.435477	1.647943	-2.512252
H	-0.919162	0.130456	-7.210366
H	0.795240	2.051597	-7.985281
H	3.283824	1.254269	-7.350607
H	3.106724	-1.154538	-6.157613
H	0.510167	-1.853779	-6.082972
H	-1.252021	2.333750	-5.163680
H	-0.494641	3.490226	-6.240319
H	-1.044367	3.976430	-3.254684
H	-0.347147	5.146006	-4.350826
H	-2.773110	5.610338	-4.025340
H	-2.468557	5.157652	-5.710210
H	-3.181505	3.985343	-4.598120
H	3.515934	1.238230	-4.222465
H	4.894189	2.869204	-5.276182
H	4.407323	2.986893	-2.878414

E = -585.829293111
G = -585.562299

Reactions with Me_2SiH_2

$Cp_2SmCH_2CH_2CH_3 + Me_2SiH_2$: Si(α)-H(β) activation

$Cp_2SmCH_2CH_2CH_3 + Me_2SiH_2 \rightarrow Cp_2SmSiHMe_2 + propane$

Transition state

C	0.766831	1.438456	-1.972319
C	1.705367	0.388603	-2.120424
C	1.014940	-0.747683	-2.621333
C	-0.349225	-0.396217	-2.778461
C	-0.501850	0.955554	-2.384153
Sm	1.025053	1.028422	-4.696978
C	-1.146485	0.540481	-6.072012
C	-2.621343	0.720450	-5.720787
C	-3.574422	-0.187470	-6.500118
C	3.065849	-0.386928	-5.843883
C	2.181198	-0.117434	-6.918573
C	2.224194	1.273431	-7.182885
C	3.140166	1.864486	-6.276707
C	3.657875	0.840790	-5.445126
Si	-0.198509	3.693724	-5.168623
C	0.116421	4.765568	-6.708132
C	-1.412127	4.590487	-4.010749
H	1.153933	3.636194	-4.406568
H	-0.697479	1.986346	-5.622355
H	1.446810	-1.725445	-2.801309
H	2.756488	0.430990	-1.859670
H	0.976384	2.428794	-1.584941
H	-1.433477	1.507587	-2.359042
H	-1.141961	-1.053676	-3.114668
H	1.593737	-0.849272	-7.460274
H	1.677493	1.787539	-7.964201
H	3.416685	2.911820	-6.242188
H	4.407535	0.964892	-4.672275
H	3.288498	-1.363764	-5.430571
H	-0.863637	-0.512138	-5.864149
H	-0.993532	0.672289	-7.152177
H	-2.766494	0.556146	-4.644178
H	-2.908997	1.769446	-5.894781
H	-4.621554	-0.009355	-6.227680
H	-3.477016	-0.022781	-7.579317
H	-3.355670	-1.244580	-6.309803
H	0.377708	5.792402	-6.432523
H	0.927551	4.356291	-7.316483
H	-0.782936	4.803295	-7.332016
H	-1.084716	5.616180	-3.811663
H	-2.405361	4.636999	-4.469317
H	-1.509544	4.069560	-3.054656

E = -625.148265379
G = -624.854574

$Cp_2SmCH_2CH_2CH_3$ + Me_2SiH_2 : Si(β)-H(α) activation

$Cp_2SmCH_2CH_2CH_3$ + Me_2SiH_2 → Cp_2SmH + Me_2SiH-CH_2-CH_2-CH_3

Transition state

C	2.032762	-3.530694	-1.803019
C	2.230411	-4.716512	-1.051490
C	1.098712	-5.549702	-1.244244
C	0.206529	-4.881997	-2.121786
C	0.782460	-3.634418	-2.465448
Sm	0.172370	-3.428581	0.218781
C	0.935833	-2.495145	2.689537
C	-0.444737	-2.782530	2.828023
C	-0.610778	-4.188342	2.743710
C	0.667180	-4.769567	2.548532
C	1.624778	-3.722308	2.513155
C	-0.902986	-1.111045	-0.331156
C	-1.122512	-0.239159	-1.570587
C	-0.502047	1.155520	-1.455362
Si	-2.853679	-2.465890	-0.354626
C	-3.251060	-2.880470	-2.164481
H	0.360701	-2.905600	-3.146778
H	2.737371	-2.711476	-1.895825
H	3.107413	-4.960105	-0.463446
H	0.962217	-6.542884	-0.831839
H	-0.734538	-5.271071	-2.490345
H	2.697516	-3.843848	2.418022
H	1.390504	-1.512370	2.745904
H	-1.231461	-2.058493	3.002629
H	-1.546785	-4.724700	2.841849
H	0.881865	-5.829727	2.479433
H	-1.885723	-3.775973	-0.063153
C	-4.134837	-3.293165	0.809324
H	-3.308772	-1.030426	-0.142311
H	-4.214630	-2.436519	-2.435738
H	-2.498737	-2.497425	-2.858870
H	-3.321525	-3.964176	-2.299637
H	0.219678	-1.165208	-0.244944
H	-1.193992	-0.549353	0.565458
H	-0.714729	-0.744671	-2.455369
H	-2.199217	-0.128841	-1.749375
H	0.582251	1.101011	-1.301478
H	-0.928867	1.704244	-0.608451
H	-0.679160	1.747266	-2.360615
H	-5.123703	-2.849828	0.643272
H	-4.191845	-4.375568	0.651221
H	-3.874294	-3.121166	1.860162

E = -625.147750465
G = -624.850405

$Me_2SiH-CH_2-CH_2-CH_3$ ('linear' hydrosilylation product)

C	-0.175930	0.014104	1.854724
Si	-0.014490	-0.084125	-0.031920
C	-0.976143	1.322818	-0.880158
C	-2.493428	1.326977	-0.652300
C	-3.203426	2.475835	-1.368254
C	-0.593816	-1.779542	-0.653173
H	1.437135	0.079576	-0.389822
H	0.429352	-0.760325	2.336726
H	0.162860	0.985509	2.228799
H	-1.213706	-0.127034	2.173928
H	-1.641828	-1.961896	-0.393759
H	-0.497682	-1.854091	-1.741079
H	0.004326	-2.581176	-0.208132
H	-0.547303	2.276347	-0.540801
H	-0.763650	1.271149	-1.957472
H	-2.921705	0.373910	-0.989946
H	-2.707174	1.386760	0.423141
H	-4.284354	2.456100	-1.191334
H	-2.826845	3.446319	-1.025505
H	-3.041576	2.424729	-2.450996

E = -202.837182523
G = -202.695094

Reactions with Me_3SiH

$Cp_2SmCH_2CH_2CH_3 + Me_3SiH$: Si(α)-H(β) activation

$Cp_2SmCH_2CH_2CH_3 + Me_3SiH \rightarrow Cp_2SmSiMe_3 + propane$

Transition state

C	1.454387	0.973051	-1.965276
C	1.664439	-0.381905	-2.330547
C	0.420477	-0.926174	-2.732181
C	-0.561544	0.089295	-2.613182
C	0.077750	1.264163	-2.138754
Sm	0.174014	-0.465907	-0.006920
C	0.366142	-3.017516	0.114794
C	1.259390	1.348840	1.740126
C	1.759558	0.092098	2.167834
C	0.678492	-0.651438	2.703811
C	-0.491520	0.141082	2.601692
C	-0.132870	1.377721	2.004008
Si	-2.745723	-1.662152	0.099209
H	-1.024906	-2.246664	0.143705
C	-3.511190	-2.467683	1.650747
C	-3.438504	0.130564	0.023643
C	-3.423180	-2.596489	-1.420746
H	2.796232	-0.224177	2.132585
H	1.844014	2.157320	1.317509
H	-0.795893	2.216913	1.825566
H	-1.475530	-0.128511	2.964782
H	0.741144	-1.639424	3.142847
H	2.618257	-0.897817	-2.337169
H	0.252566	-1.932713	-3.094983
H	-1.604619	0.000452	-2.891768
H	-0.392870	2.227744	-1.978671
H	2.218359	1.673445	-1.648898
H	1.410879	-2.682759	0.327124
C	0.018348	-4.142321	1.084192
H	0.382041	-3.398450	-0.914890
C	0.990218	-5.323402	1.050789
H	-0.038975	-3.748683	2.107673
H	-0.992417	-4.507021	0.853896
H	0.690328	-6.114709	1.747666
H	1.040819	-5.762105	0.047799
H	2.004145	-5.007248	1.321934
H	-4.534964	0.096318	-0.007136
H	-3.153135	0.715023	0.904685
H	-3.104398	0.671534	-0.867942
H	-4.519260	-2.591266	-1.428965
H	-3.078758	-2.147099	-2.357575
H	-3.094946	-3.641208	-1.415574
H	-4.605266	-2.408121	1.610362
H	-3.236530	-3.524237	1.726988
H	-3.184130	-1.973635	2.571022

E = -664.457954175
G = -664.137832

$Cp_2SmCH_2CH_2CH_3$ + Me_3SiH : Si(β)-H(α) activation

$Cp_2SmCH_2CH_2CH_3$ + Me_3SiH → Cp_2SmH + Me_3Si-CH_2-CH_2-CH_3

Transition state

C	1.694031	-3.297646	-2.079199
C	2.338195	-4.224920	-1.219225
C	1.517773	-5.378300	-1.128924
C	0.365122	-5.160298	-1.924554
C	0.476285	-3.875041	-2.513483
Sm	0.129029	-3.417375	0.197265
C	0.865648	-2.653669	2.734724
C	-0.528084	-2.897044	2.824889
C	-0.742444	-4.287682	2.653692
C	0.518191	-4.903299	2.450924
C	1.514029	-3.892860	2.502629
C	-0.889185	-1.034166	-0.228900
C	-0.832116	-0.328002	-1.589323
C	-0.087203	1.008692	-1.553100
Si	-2.913540	-2.325388	-0.271804
C	-3.335679	-2.670926	-2.095822
H	-0.233240	-3.429814	-3.200103
H	2.087174	-2.334008	-2.383584
H	3.310435	-4.097886	-0.756995
H	1.749692	-6.281122	-0.576101
H	-0.440728	-5.865990	-2.088493
H	2.583527	-4.048876	2.423168
H	1.353938	-1.693702	2.860340
H	-1.291755	-2.154501	3.022381
H	-1.698994	-4.793780	2.695022
H	0.695916	-5.964864	2.324088
H	-1.909899	-3.673075	-0.154547
C	-4.068542	-3.357391	0.875515
C	-3.688354	-0.597530	0.139670
H	-4.322226	-2.258517	-2.333685
H	-2.615954	-2.225635	-2.788208
H	-3.358731	-3.749262	-2.280168
H	0.183527	-1.110463	0.102504
H	-1.283312	-0.347004	0.526178
H	-0.360373	-0.985197	-2.330811
H	-1.849720	-0.154533	-1.956522
H	0.951875	0.876534	-1.228131
H	-0.563351	1.704676	-0.853276
H	-0.068634	1.486027	-2.539444
H	-5.100636	-2.991018	0.837029
H	-4.052162	-4.413966	0.588184
H	-3.739955	-3.293583	1.919392
H	-4.762437	-0.687534	-0.064107
H	-3.582762	-0.365915	1.205930
H	-3.308731	0.253536	-0.430609

E = -664.452876384
G = -664.127508

Me_3Si-CH_2-CH_2-CH_3 ('linear' hydrosilylation product)

C	-0.187787	0.019961	1.841585
Si	0.017419	-0.076906	-0.043880
C	-0.971561	1.328795	-0.850731
C	-0.644900	-1.745129	-0.662165
C	1.859763	0.059849	-0.513069
H	-1.241125	-0.080466	2.124440
H	0.369250	-0.778251	2.343668
H	0.171026	0.976716	2.235057
H	-1.703092	-1.867891	-0.407851
H	-0.551452	-1.829284	-1.750104
H	-0.095728	-2.580365	-0.214689
H	-0.632994	2.309272	-0.500213
H	-0.872104	1.310423	-1.941221
H	-2.037014	1.241947	-0.612043
H	2.385581	-0.799179	-0.071444
H	1.942227	-0.074581	-1.601503
C	2.564225	1.359165	-0.102420
C	4.036071	1.402350	-0.513287
H	2.042860	2.218414	-0.544630
H	2.490702	1.492171	0.985039
H	4.514356	2.339714	-0.208551
H	4.596853	0.578285	-0.057469
H	4.144173	1.310779	-1.600160

E = -242.152691682
G = -241.984008

Hydrosilylation of propene by $MeSiH_3$ catalyzed by Cp_2SmSiH_2Me

Cp_2SmSiH_2Me

C	-2.405491	-0.982129	-0.839758
C	-2.703376	0.013717	0.127023
C	-2.371361	1.277142	-0.427954
C	-1.860549	1.063232	-1.730492
C	-1.882452	-0.333085	-1.986505
Sm	0.013207	-0.018494	-0.024789
C	0.648062	-0.921484	2.462017
C	0.165141	-2.064697	1.775440
C	1.106161	-2.399223	0.768687
C	2.172701	-1.464878	0.840841
C	1.892679	-0.552237	1.888072
Si	1.296593	2.690173	0.280661
H	1.140240	3.171169	1.716056
C	0.796073	4.212459	-0.792270
H	2.812322	2.628207	0.163871
H	3.067926	-1.469180	0.228302
H	2.526486	0.264591	2.208713
H	0.171270	-0.436650	3.306627
H	-0.744038	-2.608694	2.002402
H	1.045389	-3.251394	0.100622
H	-1.537496	1.836067	-2.417588
H	-1.599187	-0.815539	-2.916171
H	-2.584673	-2.045612	-0.734264
H	-3.159370	-0.157469	1.095512
H	-2.501537	2.240088	0.050908
H	1.355218	5.107784	-0.504119
H	0.988574	4.023078	-1.853909
H	-0.271495	4.431570	-0.683767

E = -466.760391005
G = -466.589548

Propene

C	0.095565	0.170828	0.183346
C	-0.104737	-0.168928	1.456348
C	1.392867	0.035693	-0.552125
H	0.694544	-0.582907	2.067684
H	-1.072368	-0.046697	1.934624
H	-0.738118	0.581751	-0.387801
H	1.284825	-0.615258	-1.428733
H	1.739273	1.007406	-0.925764
H	2.176441	-0.381887	0.087088

E = -117.868522821
G = -117.813606

Cp_2SmSiH_2Me + propene : 1,2 insertion

Cp_2SmSiH_2Me + propene → $Cp_2SmCH_2CH(CH_3)SiH_2Me$

Transition state

C	-3.694537	2.164475	1.037346
C	-3.282345	2.127351	-0.320456
C	-3.354289	3.446373	-0.833427
C	-3.797528	4.299180	0.206530
C	-4.012657	3.506927	1.362354
Sm	-1.269021	3.443071	1.003249
C	1.354471	2.864919	1.673006
C	0.973867	1.853814	0.751873
C	-0.003911	1.040568	1.371243
C	-0.228551	1.545239	2.680310
C	0.618590	2.665466	2.868335
C	-1.354466	5.529433	2.550802
C	-0.701619	6.305109	1.581250
C	0.677273	6.862893	1.861638
Si	0.013848	5.347718	-0.736921
H	1.510856	5.409907	-0.891086
H	-0.325222	3.908244	-1.250962
H	2.116356	3.617557	1.509111
H	1.379712	1.716138	-0.243329
H	-0.475816	0.167288	0.936490
H	-0.890624	1.114226	3.422812
H	0.714877	3.242439	3.779921
H	-3.791228	1.309322	1.696188
H	-3.008174	1.240139	-0.879214
H	-3.133382	3.743744	-1.851625
H	-3.979648	5.364193	0.121137
H	-4.392480	3.857208	2.315028
H	1.335121	6.099052	2.284951
H	0.585687	7.669063	2.602000
H	1.169605	7.278624	0.977551
H	-1.335719	6.942303	0.965708
H	-0.805220	5.234714	3.441967
H	-2.433754	5.608794	2.650638
C	-0.728519	6.568217	-1.999063
H	-0.317955	6.404345	-2.999653
H	-1.816850	6.470441	-2.048955
H	-0.496228	7.598694	-1.708598

E = -584.637238968
G = -584.385770

$Cp_2SmCH_2CH(CH_3)SiH_2Me$

C	-3.725379	1.926675	0.872450
C	-3.485025	2.493438	-0.401763
C	-3.525263	3.907247	-0.266343
C	-3.787552	4.212595	1.090377
C	-3.900998	2.988146	1.797760
Sm	-1.251490	3.115982	1.107841
C	1.298689	2.244163	1.759675
C	0.826931	1.310163	0.800265
C	-0.229715	0.572991	1.388525
C	-0.417377	1.056581	2.709357
C	0.534356	2.085164	2.938361
C	-0.671516	5.376641	2.009055
C	-0.755912	6.465049	0.918453
C	-0.342267	7.875951	1.366471
Si	0.274124	5.809934	-0.526271
H	1.713223	5.650301	-0.139872
H	-0.196826	4.365466	-0.778541
H	2.115543	2.942282	1.621467
H	1.235956	1.155673	-0.192401
H	-0.779084	-0.237594	0.924075
H	-1.123419	0.667227	3.434146
H	0.664179	2.641677	3.858930
H	-3.786987	0.868699	1.098082
H	-3.343658	1.944218	-1.326187
H	-3.422170	4.625605	-1.071768
H	-3.900486	5.203527	1.511593
H	-4.135885	2.881162	2.851041
H	0.700283	7.890390	1.705754
H	-0.959699	8.198429	2.214046
H	-0.449158	8.627562	0.572772
H	-1.789930	6.517817	0.540361
H	0.346396	5.374548	2.431404
H	-1.336285	5.650773	2.846812
C	0.145106	6.679960	-2.201082
H	0.730415	6.157569	-2.963518
H	-0.894206	6.731952	-2.539112
H	0.527323	7.703015	-2.123504

E = -584.660028395
G = -584.409701

Cp_2SmSiH_2Me + propene : 2,1 insertion

Cp_2SmSiH_2Me + propene → $Cp_2SmCH(CH_3)CH_2SiH_2Me$

Transition state

C	0.457330	2.873943	-1.151743
C	0.519297	1.740059	-0.300562
C	1.224406	2.111741	0.870433
C	1.589226	3.475382	0.750238
C	1.120107	3.945659	-0.502653
Sm	-1.184680	3.490691	0.951804
C	-3.843089	3.112182	1.603362
C	-3.450205	1.949924	0.888036
C	-3.217277	2.320560	-0.457716
C	-3.466224	3.714001	-0.578303
C	-3.862543	4.197588	0.692365
C	-1.098287	6.095478	1.579469
C	0.146681	6.837123	1.148702
C	-1.265829	5.667743	2.898772
Si	-0.934370	3.254928	3.801120
H	-2.265990	5.593264	3.316422
H	-1.048155	1.941664	2.958764
H	-4.132985	3.147919	2.646628
H	-3.369572	0.949295	1.296136
H	-2.929681	1.654048	-1.262169
H	-3.413957	4.291932	-1.494357
H	-4.165604	5.212630	0.920131
H	0.019356	2.902376	-2.142857
H	0.131048	0.753210	-0.523943
H	1.462901	1.458687	1.701420
H	2.167572	4.043495	1.469084
H	1.281937	4.934866	-0.912173
H	-0.489617	5.890573	3.629629
H	-2.009862	6.316432	1.023392
H	-2.106710	3.173533	4.743338
C	0.641281	3.105508	4.864553
H	0.120646	7.883576	1.487413
H	1.054770	6.388937	1.566588
H	0.262804	6.860528	0.061324
H	0.583970	2.246174	5.539291
H	1.531184	2.998042	4.238222
H	0.767329	4.003649	5.478798

E = -584.633345415
G = -584.382848

$Cp_2SmCH(CH_3)CH_2SiH_2Me$

C	0.334976	2.777699	-1.467825
C	0.376993	1.584487	-0.701872
C	1.137617	1.841374	0.465017
C	1.572348	3.191422	0.417487
C	1.080044	3.768428	-0.775861
Sm	-1.184762	3.334954	0.741102
C	-3.838132	2.973698	1.461132
C	-3.515301	1.843724	0.662534
C	-3.314341	2.290502	-0.664624
C	-3.500070	3.697205	-0.685974
C	-3.835849	4.116935	0.626432
C	-0.955938	5.616524	1.785264
C	0.412756	6.292531	1.868757
C	-1.567590	5.423973	3.196571
Si	-0.919790	3.921119	4.152938
H	-2.654312	5.276478	3.131639
H	-0.807180	2.763799	3.144517
H	-4.093590	2.953926	2.514639
H	-3.474227	0.814229	1.000960
H	-3.077351	1.666654	-1.518170
H	-3.450325	4.332038	-1.563795
H	-4.068259	5.130167	0.929428
H	-0.136206	2.894268	-2.437040
H	-0.070065	0.636095	-0.976428
H	1.384787	1.119386	1.235692
H	2.198030	3.687398	1.149217
H	1.262029	4.781840	-1.113230
H	-1.431549	6.310753	3.845966
H	-1.624851	6.308940	1.247604
H	-1.912005	3.403585	5.151606
C	0.773999	4.063474	4.974971
H	0.394410	7.228971	2.456012
H	1.176751	5.656688	2.336474
H	0.795907	6.550322	0.874562
H	1.036152	3.131250	5.483834
H	1.556364	4.295754	4.248115
H	0.757854	4.864987	5.720797

E = -584.653918688
G = -584.403801

Cp_2SmSiH_2Me + propene : allylic activation

Cp_2SmSiH_2Me + propene → Cp_2SmCH_2-CH=CH_2 + $MeSiH_3$

Transition state

C	-0.847708	-0.087639	-6.468026
C	0.368128	0.493149	-6.905989
C	0.481972	1.775672	-6.310550
C	-0.664096	1.985970	-5.504021
C	-1.483914	0.833524	-5.597478
Sm	0.723895	0.015181	-4.195436
C	0.533301	1.608761	-1.981971
C	1.638531	0.774183	-1.686772
C	1.158007	-0.545558	-1.507106
C	-0.251231	-0.525418	-1.677130
C	-0.637200	0.804148	-1.972859
Si	-0.563284	-2.844648	-4.334654
C	2.565717	-1.951192	-4.903980
C	3.316343	-0.866345	-4.329823
C	3.391794	0.414557	-4.824348
H	1.062256	0.054665	-7.613816
H	1.279917	2.489885	-6.476700
H	-0.888672	2.883078	-4.939046
H	-2.444820	0.692752	-5.116993
H	-1.246649	-1.044855	-6.781309
H	1.751986	-1.410015	-1.234142
H	2.668706	1.096430	-1.594048
H	0.569235	2.680161	-2.141311
H	-1.651288	1.152913	-2.126912
H	-0.922775	-1.365285	-1.549224
H	2.830646	-2.942780	-4.540543
H	2.451425	-1.927190	-5.990228
H	1.119951	-2.141710	-4.538356
H	3.721394	-1.037142	-3.331490
H	3.944702	1.181900	-4.293654
H	3.118821	0.631153	-5.855008
H	-1.941086	-2.297572	-4.059770
C	-0.210678	-4.222623	-3.064880
H	-0.662347	-3.493430	-5.690401
H	-0.983088	-4.996457	-3.107683
H	0.754038	-4.698434	-3.268196
H	-0.182067	-3.827365	-2.045083

E = -584.626584456
G = -584.378564

Cp_2SmCH_2-CH=CH_2 + $MeSiH_3$

C	0.524990	-0.334951	2.617508
C	0.002141	0.974978	2.742967
C	0.808881	1.845644	1.965591
C	1.835874	1.073366	1.366256
C	1.655676	-0.276023	1.762510
Sm	-0.456746	0.276938	0.110233
C	-0.017478	-0.541503	-2.500228
C	-1.203288	0.230043	-2.574118
C	-0.867698	1.578926	-2.300813
C	0.528345	1.642937	-2.058980
C	1.054270	0.331426	-2.182304
C	-2.130667	-1.783420	0.454996
H	0.691892	2.920731	1.884368
H	2.633583	1.451835	0.738542
H	2.299001	-1.108036	1.498080
H	0.147070	-1.222083	3.110834
H	-0.846356	1.267281	3.349528
H	-1.551600	2.420115	-2.314559
H	1.100459	2.541434	-1.858947
H	2.098070	0.053495	-2.093331
H	0.062711	-1.605398	-2.693145
H	-2.189072	-0.141355	-2.828210
H	-2.319045	-1.864096	-0.616834
H	-1.874869	-2.712224	0.955300
C	-2.729543	-0.747556	1.178806
C	-3.063687	0.512467	0.672546
H	-2.713558	-0.844158	2.266675
H	-3.490097	1.262032	1.331861
H	-3.326096	0.611542	-0.382002

E = -539.043369530
G = -538.851894

$Cp_2SmSiH_2Me + MeSiH_3$: Si(α)-H(β) activation

$Cp_2SmSiH_2Me + MeSiH_3 \rightarrow Cp_2SmSiH_2Me + MeSiH_3$

Transition state

C	0.550600	1.506109	-2.105822
C	1.768719	0.779847	-2.015816
C	1.521140	-0.546860	-2.448658
C	0.148399	-0.643480	-2.799867
C	-0.446822	0.626881	-2.593383
Sm	0.188257	-0.279933	-0.067171
C	0.387992	1.688043	1.814388
C	1.521009	0.854920	2.017857
C	1.065865	-0.389687	2.521955
C	-0.349839	-0.329821	2.622105
C	-0.765121	0.956263	2.190754
Si	1.629416	-3.015276	0.216925
H	1.543516	-3.713145	1.547113
C	1.687091	-4.356076	-1.137362
Si	-2.059276	-2.141233	-0.055862
H	-2.740685	-2.525891	1.226189
C	-2.926389	-3.047127	-1.484944
H	2.555424	1.138686	1.861171
H	1.690482	-1.220153	2.827310
H	-0.993154	-1.108999	3.012275
H	-1.784500	1.324479	2.177884
H	0.407103	2.716222	1.471765
H	2.729065	1.183110	-1.715608
H	2.262708	-1.329925	-2.547131
H	-0.340258	-1.516804	-3.214523
H	-1.478713	0.887196	-2.798933
H	0.418244	2.558362	-1.882543
H	2.976529	-2.321811	0.228929
H	1.818363	-3.914684	-2.129961
H	2.512862	-5.051982	-0.963038
H	0.755859	-4.931661	-1.146670
H	-0.118498	-2.481573	0.061823
H	-2.363768	-0.621837	-0.200394
H	-2.569722	-2.692222	-2.455290
H	-2.723327	-4.120993	-1.421413
H	-4.010175	-2.905209	-1.439600

E = -512.355745013
G = -512.128427

Cp_2SmSiH_3 + $MeSiH_3$: Si(β)-H(α) activation

Cp_2SmSiH_2Me + $MeSiH_3$ → Cp_2SmH + MeH_2Si-SiH_2Me

Transition state

C	-1.715347	1.049805	-1.541797
C	-1.816378	-0.216603	-2.172378
C	-2.486570	-1.095484	-1.286354
C	-2.813648	-0.369586	-0.109319
C	-2.340273	0.955510	-0.269994
Sm	-0.100560	-0.634068	-0.082017
C	-0.459585	-2.542692	1.841822
C	-0.046805	-3.248337	0.679985
C	1.310122	-2.926396	0.430213
C	1.735333	-2.012262	1.427173
C	0.641367	-1.780780	2.302564
C	0.963515	1.749694	1.290217
Si	1.910373	1.580207	-0.410292
H	1.631738	2.867385	-1.123959
Si	2.166286	-0.143024	-2.429224
H	1.533535	-0.444824	-3.772594
C	3.265975	1.331067	-3.057008
H	3.344385	1.612894	0.021729
H	3.176351	-1.186067	-2.047814
H	2.734903	-1.606900	1.530946
H	0.656499	-1.165199	3.195057
H	-1.431973	-2.608599	2.315556
H	-0.650946	-3.945106	0.110785
H	1.921190	-3.320193	-0.372164
H	-3.369882	-0.749692	0.739406
H	-2.480645	1.769427	0.432423
H	-1.289241	1.945316	-1.978354
H	-1.456440	-0.463126	-3.163499
H	-2.744499	-2.128494	-1.488146
H	0.915914	-1.097728	-1.846804
H	1.057328	2.804233	1.567695
H	-0.125915	1.571944	1.309103
H	1.433424	1.156019	2.078502
H	3.839659	0.891328	-3.883116
H	2.659864	2.144762	-3.466027
H	3.973839	1.744573	-2.333504

E = -512.351081107
G = -512.118362

$MeH_2Si-SiH_2Me$

C	-0.144390	0.052984	1.864145
Si	0.071801	-0.069228	-0.018968
H	-0.741235	0.999666	-0.689420
Si	-0.565965	-2.180412	-0.877062
H	0.247067	-3.249305	-0.206606
C	-0.349763	-2.302622	-2.760175
H	1.504477	0.195486	-0.379835
H	-1.998642	-2.445124	-0.516204
H	0.156765	1.041963	2.222125
H	-1.188743	-0.110365	2.145139
H	0.467195	-0.697213	2.373539
H	-0.961345	-1.552425	-3.269571
H	0.694592	-2.139273	-3.041162
H	-0.650916	-3.291601	-3.118156

E = -90.0262926167
G = -89.951084

$Cp_2SmCH_2CH(CH_3)SiH_2Me$

$Cp_2SmCH_2CH(CH_3)SiH_2Me$ + propene : allylic activation

$Cp_2SmCH_2CH(CH_3)SiH_2Me$ + propene → Cp_2SmCH_2-CH=CH_2 + $MeSiH_2$-CH(CH_3)CH_3

Transition state

C	-0.424936	0.614049	-1.696331
C	0.758114	1.384547	-1.795125
C	1.864986	0.504580	-1.669829
C	1.364767	-0.807993	-1.503760
C	-0.052643	-0.742362	-1.526337
Sm	0.710437	-0.173919	-4.095775
C	2.075756	-2.492134	-4.667311
C	2.016676	-1.833711	-5.919916
C	0.667422	-1.816300	-6.345819
C	-0.109635	-2.479500	-5.362566
C	0.759204	-2.900300	-4.327897
C	-1.736020	0.480343	-5.008964
C	-2.703738	1.649137	-5.257299
Si	-2.948297	2.762020	-3.729848
C	-4.063716	1.162870	-5.788798
C	0.562984	2.191291	-5.585085
C	1.905164	1.657844	-5.790826
C	2.882106	1.554854	-4.845234
H	-2.271870	2.311448	-6.026671
H	0.804370	2.462637	-1.896143
H	2.910931	0.788223	-1.663076
H	1.958897	-1.701648	-1.355793
H	-0.731015	-1.576335	-1.387798
H	-1.436661	0.997373	-1.718699
H	0.296770	-1.402790	-7.276444
H	2.863804	-1.435903	-6.465975
H	2.973565	-2.694394	-4.095113
H	0.474542	-3.462733	-3.446918
H	-1.177839	-2.654892	-5.407029
H	-1.742322	-0.167191	-5.898584
H	-2.125269	-0.136277	-4.181359
H	0.101872	2.549781	-6.507751
H	0.507356	2.957569	-4.806378
H	-0.424797	1.349911	-5.249036
H	-4.733710	1.990495	-6.052483
H	-3.928848	0.549573	-6.688736
H	-4.578764	0.539514	-5.048104
H	2.090730	1.178605	-6.753277
H	3.832614	1.082971	-5.071346
H	2.806797	2.082552	-3.897401
C	-4.098414	4.228953	-4.072960
H	-3.523985	1.942812	-2.608957
H	-1.628238	3.294455	-3.252652
H	-4.172311	4.871767	-3.190398
H	-3.722144	4.836805	-4.902064
H	-5.107295	3.891835	-4.328328

E = -702.511931878
G = -702.185364

$MeSiH_2$-$CH(CH_3)CH_3$ ('branched' hydrosilylation product)

H	-0.083097	0.071015	1.812620
Si	-0.010616	-0.046354	0.317033
C	-0.976244	1.377057	-0.476254
C	1.823937	-0.087072	-0.209376
C	2.533730	-1.309517	0.386111
C	2.553169	1.213148	0.151962
H	-0.655060	-1.349311	-0.058679
H	-0.574159	2.348258	-0.172716
H	-0.935118	1.317089	-1.568405
H	-2.027865	1.339929	-0.175926
H	1.823502	-0.189307	-1.304957
H	3.580005	-1.356434	0.057741
H	2.539500	-1.271566	1.482042
H	2.052020	-2.247930	0.091490
H	3.601347	1.178931	-0.171682
H	2.094263	2.089828	-0.317498
H	2.554087	1.381002	1.235696

E = -163.519148949
G = -163.403730

$Cp_2SmCH_2CH(CH_3)SiH_2Me + MeSiH_3$: Si(α)-H(β) activation

$Cp_2SmCH_2CH(CH_3)SiH_2Me$ + propene → Cp_2SmSiH_2Me + $MeSiH_2$-$CH(CH_3)CH_3$

Transition state

C	0.455537	-1.631436	-2.375667
C	-0.211389	-0.382416	-2.432996
C	0.761048	0.642171	-2.291305
C	2.028253	0.025569	-2.147404
C	1.838613	-1.380565	-2.192615
Sm	0.688712	-0.579489	0.166247
C	-0.397029	-2.811116	0.840088
C	-1.496118	-3.740776	0.304489
C	-2.705434	-3.782788	1.247921
C	2.430691	-0.753879	2.297810
C	1.191467	-0.397507	2.882305
C	0.872301	0.920451	2.466800
C	1.918624	1.379825	1.625940
C	2.882187	0.344573	1.520157
Si	-0.812313	-5.494914	-0.022505
Si	-2.252993	0.077741	0.688897
H	-2.685029	0.288734	2.111536
C	-3.798040	-0.210624	-0.383364
H	-1.646074	1.409461	0.272713
H	-1.247174	-1.401975	0.735273
H	1.989323	2.363059	1.174822
H	0.004221	1.491444	2.774249
H	0.602252	-1.010923	3.552765
H	2.962138	-1.687084	2.448020
H	3.820029	0.399422	0.979762
H	2.978264	0.537887	-2.051671
H	2.621664	-2.129417	-2.148206
H	-0.003871	-2.606176	-2.484815
H	-1.269023	-0.232406	-2.612114
H	0.572395	1.709083	-2.328739
H	-0.290821	-2.939493	1.924711
H	0.590537	-3.107434	0.409377
H	-1.841839	-3.372127	-0.674136
H	-1.879267	-6.374508	-0.613644
H	0.289043	-5.386649	-1.039193
C	-0.129745	-6.310815	1.544347
H	-3.528597	-4.371446	0.828989
H	-2.439968	-4.223319	2.216386
H	-3.091756	-2.777001	1.455658
H	-4.511188	0.609378	-0.258399
H	-3.538937	-0.280025	-1.443451
H	-4.296331	-1.141281	-0.096758
H	0.297799	-7.290375	1.310153
H	0.655929	-5.695369	1.992801
H	-0.916947	-6.457066	2.290121

E = -630.241384902
G = -629.937532

$Cp_2SmCH_2CH(CH_3)SiH_2Me + MeSiH_3$: Si(β)-H(α) activation

$Cp_2SmCH_2CH(CH_3)SiH_2Me$ + propene → Cp_2SmH + $MeSiH_2$-$CH(CH_3)$-CH_2-SiH_2Me

Transition state

C	2.113274	-4.160007	-1.860332
C	2.340497	-5.082443	-0.806860
C	1.215624	-5.943592	-0.731259
C	0.296587	-5.555446	-1.738747
C	0.850950	-4.453505	-2.435798
Sm	0.297401	-3.515373	0.107771
C	0.887790	-2.302888	2.499656
C	-0.512798	-2.516321	2.540527
C	-0.740331	-3.914709	2.611838
C	0.518272	-4.564662	2.613686
C	1.527585	-3.568793	2.540549
C	-0.686745	-1.380380	-0.946063
C	-1.177281	-0.136572	-1.712115
Si	-0.515364	1.477816	-0.933773
Si	-2.654682	-2.458254	-0.439885
C	-3.420547	-2.713114	-2.156941
H	0.404039	-3.948800	-3.283937
H	2.806879	-3.397876	-2.198636
H	3.234454	-5.148195	-0.197949
H	1.098982	-6.779802	-0.052176
H	-0.649215	-6.035798	-1.957206
H	2.597004	-3.742733	2.568774
H	1.385425	-1.339396	2.486442
H	-1.276656	-1.747797	2.553474
H	-1.709714	-4.394286	2.673637
H	0.684029	-5.632408	2.694366
H	-1.756672	-3.848493	-0.246406
H	-3.614757	-3.176007	0.509642
H	-2.964862	-1.058500	0.066158
H	-4.487461	-2.477199	-2.097623
H	-2.976316	-2.088312	-2.933756
H	-3.324489	-3.760543	-2.457774
H	0.087261	-1.832104	-1.602442
H	-0.201605	-1.062733	0.000957
C	-0.854790	-0.198775	-3.211998
H	-2.270750	-0.056276	-1.591165
C	1.365603	1.650623	-1.086806
H	-0.890032	1.489807	0.518394
H	-1.170963	2.657124	-1.592143
H	-1.318591	0.632360	-3.753982
H	0.225098	-0.150714	-3.397246
H	-1.216710	-1.128937	-3.666267
H	1.702265	2.564504	-0.587821
H	1.882917	0.805447	-0.621707
H	1.676540	1.706859	-2.134252

E = -630.239284652
G = -629.930800

$MeSiH_2$-$CH(CH_3)$-CH_2-SiH_2Me

C	-0.937593	1.396204	-0.518616
Si	-0.042956	-0.042445	0.328566
C	1.795233	-0.175746	-0.180542
C	2.560666	1.117072	0.175196
C	2.429602	-1.427369	0.439558
H	-0.116758	0.126077	1.818847
H	-0.745209	-1.325541	-0.012448
H	-0.492058	2.359019	-0.251070
H	-0.900140	1.292814	-1.607672
H	-1.989737	1.418939	-0.218584
H	1.795651	-0.295699	-1.274488
H	3.466211	-1.566130	0.109308
H	2.447308	-1.360953	1.533848
H	1.875728	-2.333869	0.173180
Si	4.352174	1.258670	-0.466626
H	2.033152	1.996684	-0.219288
H	2.584132	1.252583	1.265629
H	4.849603	2.635615	-0.136053
H	5.263347	0.291408	0.227825
C	4.454395	0.985061	-2.337522
H	5.479730	1.131032	-2.690570
H	4.147524	-0.029881	-2.608148
H	3.809267	1.689613	-2.871823

E = -207.928792304
G = -207.776118

$Cp_2SmCH(CH_3)CH_2SiH_2Me$

$Cp_2SmCH(CH_3)CH_2SiH_2Me + MeSiH_3$: Si(α)-H(β) activation

$Cp_2SmCH_2CH(CH_3)SiH_2Me$ + propene → Cp_2SmSiH_2Me + Me_2SiH-CH_2-CH_2-CH_3

Transition state

C	3.330975	3.997507	3.970886
C	4.636322	3.557620	4.309558
C	4.579752	2.962583	5.595181
C	3.239725	3.035194	6.051513
C	2.466852	3.671550	5.046684
Sm	3.154018	1.259194	3.943512
C	4.985053	-0.510816	4.646354
C	5.645362	0.000268	3.367276
C	2.222155	-0.637154	2.172538
C	1.084308	-0.222477	2.910962
C	0.800135	1.121715	2.558834
C	1.758790	1.535580	1.598375
C	2.636638	0.448478	1.360650
C	4.937531	-2.040805	4.712472
Si	6.630808	-2.899634	4.882346
Si	2.058236	-0.414540	6.338032
H	4.328732	-2.370008	5.567671
C	2.747386	-0.452887	8.113813
H	1.469605	-1.763766	6.033452
H	0.881933	0.532726	6.315235
H	3.519416	-0.329282	5.331133
H	1.410290	3.905137	5.108617
H	2.876741	2.712031	7.019468
H	5.420296	2.563195	6.149890
H	5.529269	3.699747	3.711224
H	3.051352	4.524704	3.066349
H	1.791437	2.500011	1.105297
H	3.455609	0.438812	0.650292
H	2.665535	-1.625166	2.193037
H	0.505974	-0.838962	3.588536
H	-0.028300	1.715332	2.927868
H	5.530021	-0.115858	5.512770
H	4.428731	-2.444014	3.825920
C	6.468674	-4.780303	5.045232
H	7.494680	-2.580752	3.696748
H	7.327953	-2.343804	6.090685
H	6.728376	0.141581	3.466943
H	5.469170	-0.675102	2.524431
H	5.322674	1.014013	3.004728
H	1.967919	-0.730511	8.829385
H	3.559276	-1.182185	8.195773
H	3.145498	0.523491	8.405581
H	7.451874	-5.247122	5.158116
H	5.864617	-5.047214	5.917985
H	5.990723	-5.209051	4.158812

E = -630.243933365
G = -629.939017

Hydrosilylation of 1-hexene by SiH_4

1-hexene

C	0.129750	-0.337390	0.012558
C	0.240134	-0.370397	1.507948
C	1.013184	0.429322	2.242323
H	-0.381379	-1.112055	2.013620
H	1.044356	0.357811	3.325947
H	1.648110	1.184898	1.783910
C	-1.296122	-0.050272	-0.478686
H	0.820248	0.413471	-0.392482
H	0.451024	-1.307789	-0.395620
C	-1.423941	-0.066458	-2.002054
H	-1.985082	-0.790869	-0.048138
H	-1.619205	0.925133	-0.090892
C	-2.842817	0.218087	-2.488874
H	-0.733346	0.672517	-2.430750
H	-1.094314	-1.043286	-2.382036
H	-2.903305	0.199836	-3.581909
H	-3.550487	-0.525562	-2.105081
H	-3.187399	1.203006	-2.153950

E = -235.774619963
G = -235.640683

SiH_4

Si	0.039477	-0.034937	-0.040692
H	-0.049434	0.074062	1.444033
H	1.471253	0.032766	-0.459854
H	-0.546669	-1.335733	-0.480347
H	-0.716009	1.088593	-0.667068

E = -6.28910490369
G = -6.279886

Cp_2SmH

Sm	-0.012028	-0.360917	-0.032744
C	2.651518	0.166910	0.400364
C	2.628053	-1.035725	-0.347190
C	2.153089	-0.727706	-1.648215
C	1.896905	0.667000	-1.707315
C	2.201572	1.220440	-0.439044
C	-2.676905	0.192820	0.357255
C	-2.204661	1.238468	-0.479754
C	-1.885825	0.676625	-1.740853
C	-2.155637	-0.715416	-1.679663
C	-2.653000	-1.013341	-0.384672
H	2.995320	0.268995	1.424094
H	2.924893	-2.013303	0.009195
H	2.049911	-1.428719	-2.469134
H	1.563384	1.217923	-2.578639
H	2.150921	2.271424	-0.175649
H	-3.035485	0.302623	1.375108
H	-2.148484	2.290123	-0.220217
H	-1.534462	1.220687	-2.609468
H	-2.046267	-1.421049	-2.495806
H	-2.964166	-1.986614	-0.028729
H	-0.026518	-2.217018	0.902785

E = -422.333039019
G = -422.201852

Reactions of Cp_2SmH with SiH_4 : cf. [15]

Cp_2SmH + 1-hexene : 1,2 insertion

Cp_2SmH + 1-hexene → $Cp_2SmCH_2(CH_2)_4CH_3$

Transition state

C	0.067280	-0.460144	0.714922
C	1.197090	-0.806169	1.499427
C	2.353822	-0.668263	0.691119
C	1.941479	-0.224095	-0.589714
C	0.527735	-0.098345	-0.575217
Sm	1.454533	1.893950	1.111880
C	3.118094	2.242253	3.248279
C	2.239558	3.353114	3.316070
C	2.526860	4.202626	2.219501
C	3.587431	3.622583	1.478127
C	3.954327	2.410152	2.113165
C	0.128696	3.580794	-0.537554
C	-0.869318	3.634189	0.397642
C	-2.223578	3.001462	0.212267
H	-2.756253	3.636494	-0.514087
H	-0.377378	2.363814	1.980854
H	-0.094603	0.175856	-1.419210
H	-0.965020	-0.492288	1.039145
H	1.175264	-1.155002	2.525634
H	3.370889	-0.890847	0.991343
H	2.588340	-0.061896	-1.445247
H	4.759524	1.750314	1.811937
H	3.172918	1.428911	3.962880
H	1.493583	3.531614	4.079972
H	2.047715	5.152027	2.009990
H	4.067025	4.053584	0.605672
H	-2.112544	2.024224	-0.273508
C	-3.077076	2.881967	1.472826
H	-0.803349	4.392459	1.176022
H	0.020033	2.969874	-1.432289
H	0.937433	4.310218	-0.525280
C	-4.474919	2.326044	1.199941
H	-2.550309	2.248337	2.195690
H	-3.166342	3.872433	1.941934
C	-5.327546	2.216367	2.461787
H	-4.988015	2.962322	0.465245
H	-4.386604	1.335904	0.731711
H	-6.320959	1.812533	2.241285
H	-4.857124	1.558606	3.201074
H	-5.464335	3.196003	2.933698

E = -658.120428715
G = -657.834204

$Cp_2SmCH_2(CH_2)_4CH_3$ (hexyl complex)

C	0.288256	-0.528921	0.588507
C	1.363293	-0.874581	1.450132
C	2.568591	-0.742353	0.718425
C	2.239912	-0.305155	-0.590878
C	0.829213	-0.182028	-0.673688
Sm	1.645411	1.838436	1.025647
C	3.277609	2.326635	3.185945
C	2.323812	3.376034	3.214422
C	2.563125	4.218380	2.097693
C	3.660804	3.688075	1.379448
C	4.103977	2.517919	2.049436
C	0.175179	3.267117	-0.307770
C	-0.843885	3.243278	0.820161
C	-2.295906	2.944598	0.429935
H	-2.629298	3.740534	-0.248900
H	-0.607218	2.450332	1.613287
H	0.264794	0.101744	-1.552790
H	-0.765976	-0.571187	0.838082
H	1.274851	-1.226839	2.471875
H	3.563893	-0.962483	1.086155
H	2.941051	-0.146738	-1.403211
H	4.953672	1.905453	1.770673
H	3.384150	1.539355	3.923556
H	1.577039	3.537295	3.984256
H	2.019152	5.121427	1.850508
H	4.104718	4.119805	0.489257
H	-2.319708	2.016383	-0.157714
C	-3.260799	2.832104	1.609722
H	-0.803304	4.169887	1.407549
H	-0.224430	2.795204	-1.212485
H	0.487795	4.285786	-0.551644
C	-4.705197	2.552907	1.191742
H	-2.920577	2.033494	2.286357
H	-3.227479	3.760178	2.198857
C	-5.664657	2.435102	2.373641
H	-5.046386	3.352270	0.520091
H	-4.737383	1.628117	0.599612
H	-6.688528	2.235260	2.041331
H	-5.369156	1.620733	3.045032
H	-5.682135	3.358017	2.964526

E = -658.151183176
G = -657.860257

Cp_2SmH + 1-hexene : 2,1 insertion

Cp_2SmH + 1-hexene → $Cp_2SmCH(CH_3)(CH_2)_3CH_3$

Transition state

C	-0.621837	0.195924	1.387552
C	-1.274332	1.382363	0.964110
C	-1.235767	2.312432	2.033418
C	-0.552318	1.705381	3.116348
C	-0.176401	0.396507	2.717348
Sm	1.346017	2.105949	1.145546
C	0.860293	3.754911	-0.979309
C	2.156836	3.243501	-1.233274
C	3.038689	3.794718	-0.270521
C	2.289133	4.655035	0.571420
C	0.941636	4.629656	0.136749
C	3.291434	0.816686	2.479755
C	3.680502	2.170397	2.997677
C	3.551082	0.318841	1.225972
H	3.407697	-0.733859	1.014594
H	2.131872	0.558529	0.000250
H	0.317287	-0.341231	3.338275
H	-0.509505	-0.710633	0.806692
H	-1.752965	1.536350	0.004068
H	-1.680493	3.300560	2.033937
H	-0.396320	2.143571	4.096144
H	0.126387	5.208774	0.553930
H	-0.030644	3.546377	-1.559999
H	2.429217	2.568789	-2.034387
H	4.109561	3.632902	-0.225750
H	2.683755	5.261916	1.378833
H	4.206386	0.847884	0.537505
H	2.779893	0.169011	3.190501
C	4.298700	2.128655	4.402540
H	4.365160	2.667867	2.299186
H	2.802170	2.872271	3.085537
C	4.634459	3.508742	4.966321
H	3.606836	1.611690	5.081467
H	5.204719	1.510773	4.360272
C	5.253552	3.446892	6.360642
H	5.321879	4.023550	4.281605
H	3.722001	4.120386	4.997767
H	5.482650	4.447544	6.740134
H	4.574872	2.968051	7.075309
H	6.186296	2.872043	6.355374

E = -658.119204957
G = -657.831039

$Cp_2SmCH(CH_3)(CH_2)_3CH_3$

C	-0.593207	0.216828	1.568268
C	-1.275176	1.352832	1.057908
C	-1.281231	2.347905	2.065167
C	-0.602807	1.827610	3.198959
C	-0.184847	0.507413	2.893847
Sm	1.330531	2.157963	1.280425
C	0.794416	3.702986	-0.966729
C	2.073630	3.144249	-1.209100
C	2.992364	3.737803	-0.305364
C	2.277299	4.658088	0.499125
C	0.918883	4.637204	0.094115
C	3.178070	0.947806	2.296671
C	3.713458	2.215151	2.892531
C	3.613321	0.448528	0.952213
H	3.811323	-0.628243	0.937690
H	2.828451	0.563759	0.126797
H	0.327903	-0.169476	3.564601
H	-0.453212	-0.726608	1.052222
H	-1.741924	1.431795	0.083001
H	-1.752346	3.321215	1.994556
H	-0.475725	2.331183	4.150993
H	0.124918	5.258011	0.492642
H	-0.112462	3.481893	-1.517336
H	2.317778	2.431026	-1.988371
H	4.059568	3.555993	-0.271784
H	2.702205	5.301722	1.260958
H	4.487210	0.967010	0.537147
H	2.970081	0.166120	3.025253
C	4.217967	2.103520	4.336106
H	4.490503	2.669040	2.259215
H	2.922974	3.050131	2.936763
C	4.618863	3.437855	4.964247
H	3.438544	1.629184	4.948613
H	5.072753	1.414521	4.345236
C	5.121544	3.299833	6.399503
H	5.395841	3.910033	4.347473
H	3.758595	4.121693	4.942696
H	5.398414	4.270734	6.822924
H	4.354233	2.861670	7.047768
H	6.003943	2.652053	6.450327

E = -658.139828856
G = -657.849204

Cp_2SmH + 1-hexene : allylic activation

Cp_2SmH + 1-hexene → $Cp_2SmCH(C_3H_7)$-$CH=CH_2$ + H_2

Transition state

C	-0.245458	-2.075765	-6.662003
C	-0.149019	-2.972989	-5.567026
C	-1.272258	-2.762968	-4.730242
C	-2.062694	-1.735999	-5.308103
C	-1.430534	-1.316023	-6.504469
Sm	0.206268	-0.469878	-4.447829
C	0.767502	1.244126	-2.341550
C	1.045977	-0.052524	-1.841058
C	-0.176295	-0.761706	-1.757082
C	-1.214443	0.102498	-2.198896
C	-0.630899	1.342304	-2.554190
C	2.847440	0.145250	-5.015208
C	2.901001	-1.210911	-4.845171
C	2.127374	0.865143	-6.052556
H	-0.254117	1.318446	-5.559301
H	1.486983	2.041346	-2.487177
H	2.018871	-0.428075	-1.546456
H	-0.304660	-1.768516	-1.376935
H	-2.271857	-0.132799	-2.219859
H	-1.160291	2.217399	-2.909420
H	0.439461	-2.016985	-7.500311
H	0.621767	-3.720459	-5.418600
H	-1.506810	-3.315871	-3.828243
H	-3.003985	-1.363057	-4.921877
H	-1.799790	-0.560482	-7.186489
H	0.814049	1.180788	-5.775320
H	2.596776	-1.892512	-5.636799
H	3.424193	-1.644742	-3.999568
H	3.270490	0.762649	-4.219065
C	2.594376	2.285452	-6.359595
H	1.991010	0.265939	-6.962104
C	3.921912	2.351024	-7.120731
H	1.818082	2.802135	-6.940271
H	2.683815	2.844596	-5.417114
C	4.351723	3.779267	-7.447134
H	4.702257	1.852821	-6.530357
H	3.830444	1.771409	-8.049252
H	5.300115	3.796378	-7.993568
H	3.603071	4.287211	-8.065545
H	4.483295	4.373447	-6.535664

E = -658.113126661
G = -657.827695

$Cp_2SmCH(C_3H_7)-CH=CH_2$ (π-allylic complex)

C	1.037052	0.272545	-2.188660
C	-0.063005	-0.580933	-2.459430
C	-1.228889	0.220113	-2.540917
C	-0.852958	1.567282	-2.318886
C	0.548328	1.601237	-2.101385
Sm	-0.433899	0.341004	0.130996
C	1.690523	-0.156829	1.789130
C	0.566113	-0.162986	2.654596
C	0.058386	1.157286	2.722903
C	0.866595	1.980660	1.897841
C	1.880333	1.169604	1.326887
C	-2.693812	-0.642763	1.262712
C	-2.976911	0.630290	0.730593
C	-2.162173	-1.721593	0.560616
H	0.758840	3.051507	1.764571
H	2.675877	1.509400	0.674738
H	2.324178	-1.006687	1.560383
H	0.185606	-1.020794	3.195453
H	-0.782634	1.486952	3.320427
H	-1.514575	2.425615	-2.348525
H	1.147243	2.489962	-1.939834
H	2.074482	-0.030526	-2.107115
H	-0.014068	-1.652017	-2.621157
H	-2.228617	-0.132046	-2.766326
H	-2.333751	-1.744693	-0.521685
C	-1.859991	-3.054718	1.197803
H	-2.665340	-0.721633	2.353382
H	-3.369456	1.399048	1.389320
H	-3.306601	0.702514	-0.307258
C	-2.991582	-4.083256	1.041486
H	-0.941844	-3.489185	0.774165
H	-1.656501	-2.908935	2.268085
C	-2.666934	-5.433898	1.674859
H	-3.906355	-3.669570	1.484903
H	-3.207681	-4.217362	-0.027006
H	-3.488356	-6.146118	1.545742
H	-1.770009	-5.877940	1.227506
H	-2.481717	-5.333723	2.750613

E = -656.950399006
G = -656.680282

H_2
E = -1.17751649843
G = -1.178858

$Cp_2SmCH_2(CH_2)_4CH_3$ (hexyl complex)

$Cp_2SmCH_2(CH_2)_4CH_3$ + 1-hexene : 1,2 insertion

$Cp_2SmCH_2(CH_2)_4CH_3$ + 1-hexene → $Cp_2SmCH_2CH(C_4H_9)C_6H_{13}$

Transition state

E = -893.917378142
G = -893.467331

$Cp_2SmCH_2(CH_2)_4CH_3$ + 1-hexene : allylic activation

$Cp_2SmCH_2(CH_2)_4CH_3$ + 1-hexene → $Cp_2SmCH(C_3H_7)$-CH=CH_2 + hexane

Transition state

E = -893.916813336
G = -893.470404

Hexane

C	-0.148651	0.000000	0.175585
C	1.277210	0.000000	-0.369901
C	1.338941	0.000000	-1.896946
C	2.762280	0.000000	-2.453053
C	2.824010	0.000000	-3.980098
C	4.249871	0.000000	-4.525584
H	-0.162312	0.000000	1.270442
H	-0.702892	-0.883185	-0.162489
H	1.817264	0.876733	0.013525
H	1.817264	-0.876733	0.013525
H	0.797909	-0.877238	-2.280989
H	0.797909	0.877238	-2.280989
H	3.303311	0.877238	-2.069010
H	3.303311	-0.877238	-2.069011
H	2.283956	-0.876733	-4.363524
H	2.283956	0.876733	-4.363524
H	4.263533	0.000000	-5.620441
H	4.804112	0.883185	-4.187510
H	4.804112	-0.883185	-4.187510
H	-0.702892	0.883185	-0.162489

E = -237.016889259
G = -236.859778

$Cp_2SmCH_2(CH_2)_4CH_3 + SiH_4$: Si(α)-H(β) activation

$Cp_2SmCH_2(CH_2)_4CH_3 + SiH_4 \rightarrow Cp_2SmSiH_3 + hexane$

Transition state

C	-0.189983	-0.149206	2.633380
C	0.147121	1.147430	2.162960
C	1.506648	1.129174	1.765073
C	2.008484	-0.181075	1.981050
C	0.960754	-0.968068	2.523643
Sm	0.218473	-0.435378	-0.077822
C	0.042533	-2.977956	-0.231309
C	-0.417121	-4.098038	0.695323
C	0.261285	-5.450843	0.453156
C	1.338773	1.170614	-1.996839
C	1.444255	-0.143431	-2.523959
C	0.139457	-0.597849	-2.834935
C	-0.775690	0.430948	-2.495379
C	-0.033543	1.524943	-1.978747
Si	-2.804750	-1.156361	0.204865
H	-3.432147	-1.671926	1.461767
H	-3.675526	-1.542892	-0.949673
H	-2.867324	0.350811	0.293050
H	-1.304277	-2.003215	-0.006016
H	3.029277	-0.506450	1.812799
H	2.072326	1.974879	1.392393
H	-0.507836	2.011299	2.151819
H	-1.145127	-0.446244	3.050218
H	1.036152	-2.003972	2.830288
H	-0.113636	-1.551710	-3.280880
H	-1.847520	0.407227	-2.653822
H	-0.440126	2.479132	-1.663328
H	2.164903	1.807011	-1.701907
H	2.366839	-0.685461	-2.700484
H	1.146607	-2.850882	-0.114342
H	-0.109949	-3.269278	-1.279292
H	-0.264835	-3.804491	1.743669
H	-1.505272	-4.228076	0.585901
C	-0.235623	-6.563429	1.377198
H	0.104689	-5.747008	-0.594010
H	1.348354	-5.334829	0.573246
C	0.443898	-7.911436	1.133202
H	-0.080668	-6.264337	2.424159
H	-1.322556	-6.678809	1.256030
C	-0.057463	-9.017021	2.059521
H	0.287993	-8.210108	0.087495
H	1.529765	-7.795569	1.254080
H	0.447735	-9.968069	1.861484
H	0.115730	-8.762103	3.111309
H	-1.133903	-9.180936	1.934654

E = -664.426963956
G = -664.109705

Cp_2SmSiH_3

Sm	0.012178	0.013956	-0.055232
C	2.717161	0.446808	0.083382
C	2.575666	-0.905991	-0.310994
C	2.025039	-0.921480	-1.619741
C	1.838723	0.421996	-2.036394
C	2.262398	1.268920	-0.981395
C	-2.671303	0.522888	0.242215
C	-2.216176	1.470050	-0.712783
C	-1.857685	0.766744	-1.890007
C	-2.084640	-0.615234	-1.659263
C	-2.596116	-0.763898	-0.343066
H	3.134369	0.790319	1.023565
H	2.858054	-1.771854	0.274441
H	1.829896	-1.805269	-2.216811
H	1.473499	0.744348	-3.004086
H	2.285375	2.353091	-1.007688
H	-3.042962	0.743361	1.236439
H	-2.197243	2.547282	-0.585750
H	-1.509858	1.209521	-2.815597
H	-1.947184	-1.411062	-2.382679
H	-2.895282	-1.692513	0.126324
Si	-0.002566	-2.047720	2.140529
H	-1.177208	-2.074483	3.096339
H	-0.001463	-3.463900	1.596108
H	1.187329	-2.068744	3.078551

E = -427.451102323
G = -427.307459

$Cp_2SmCH_2(CH_2)_4CH_3 + SiH_4$: Si(β)-H(α) activation

$Cp_2SmCH_2(CH_2)_4CH_3 + SiH_4 \rightarrow Cp_2SmH + SiH_3CH_2(CH_2)_4CH_3$

Transition state

C	-1.893081	-4.677795	-0.928879
C	-1.547752	-3.632266	-1.823787
C	-0.268228	-3.917862	-2.361326
C	0.177811	-5.143285	-1.802956
C	-0.825382	-5.613669	-0.920119
Sm	0.170071	-3.399678	0.307354
C	0.835118	-2.762632	2.911361
C	-0.574051	-2.925104	2.913047
C	-0.857738	-4.294121	2.675449
C	0.377623	-4.975312	2.522171
C	1.423030	-4.028828	2.671826
Si	2.661411	-2.140803	-1.232093
C	0.967122	-1.033298	-0.444266
C	1.324502	0.414755	-0.783832
C	0.261286	1.434670	-0.360923
H	3.660732	-1.431069	-0.370720
H	1.371641	-1.840593	3.102044
H	-1.305466	-2.149236	3.111725
H	-1.841748	-4.747591	2.656705
H	0.501751	-6.040289	2.364620
H	2.484518	-4.240153	2.634198
H	-2.829195	-4.774631	-0.391280
H	-2.173612	-2.785521	-2.083664
H	0.261911	-3.325451	-3.097776
H	1.113498	-5.638820	-2.032299
H	-0.800758	-6.543719	-0.364869
H	2.214065	-3.432062	-0.228793
H	3.474819	-3.244054	-1.908923
H	2.416154	-1.343946	-2.509742
H	0.853820	-1.055929	0.659616
H	-0.020883	-1.223890	-0.917111
H	2.280716	0.668659	-0.307860
H	1.496263	0.495847	-1.864398
H	0.086786	1.358354	0.722194
H	-0.695378	1.182486	-0.841634
C	0.638261	2.875077	-0.710777
C	-0.420881	3.899592	-0.301852
H	1.593198	3.127319	-0.228170
H	0.818270	2.950684	-1.792573
C	-0.034260	5.335412	-0.649114
H	-1.373626	3.648559	-0.788022
H	-0.603394	3.819771	0.778653
H	-0.810784	6.045044	-0.345662
H	0.896040	5.627225	-0.148901
H	0.121117	5.454319	-1.727368

E = -664.428613113
G = -664.106052

$SiH_3CH_2(CH_2)_4CH_3$ ('linear' hydrosilylation product)

C	-0.046354	-0.218367	-0.282949
C	0.656796	-0.521505	1.048220
C	1.762269	0.468120	1.420562
C	2.491085	0.097390	2.712223
C	3.602998	1.076828	3.090532
C	4.328913	0.694945	4.378416
H	2.487669	0.526821	0.596199
H	1.340223	1.477983	1.521152
H	1.765025	0.038157	3.535875
H	2.915933	-0.912008	2.612499
H	4.326125	1.138136	2.265799
H	3.177562	2.084360	3.193787
H	5.116344	1.414791	4.624197
H	3.636996	0.657356	5.227511
H	4.796887	-0.292307	4.292059
H	-0.745808	-1.028941	-0.525224
H	0.684039	-0.198284	-1.102791
H	1.090142	-1.530573	0.999824
H	-0.085803	-0.553084	1.857160
Si	-1.053722	1.392835	-0.350353
H	-1.865682	1.429689	-1.607958
H	-1.991044	1.470799	0.814982
H	-0.192509	2.616561	-0.331406

E = -242.110923505
G = -241.943411

Cp_2SmSiH_3

Sm	0.012178	0.013956	-0.055232
C	2.717161	0.446808	0.083382
C	2.575666	-0.905991	-0.310994
C	2.025039	-0.921480	-1.619741
C	1.838723	0.421996	-2.036394
C	2.262398	1.268920	-0.981395
C	-2.671303	0.522888	0.242215
C	-2.216176	1.470050	-0.712783
C	-1.857685	0.766744	-1.890007
C	-2.084640	-0.615234	-1.659263
C	-2.596116	-0.763898	-0.343066
H	3.134369	0.790319	1.023565
H	2.858054	-1.771854	0.274441
H	1.829896	-1.805269	-2.216811
H	1.473499	0.744348	-3.004086
H	2.285375	2.353091	-1.007688
H	-3.042962	0.743361	1.236439
H	-2.197243	2.547282	-0.585750
H	-1.509858	1.209521	-2.815597
H	-1.947184	-1.411062	-2.382679
H	-2.895282	-1.692513	0.126324
Si	-0.002566	-2.047720	2.140529
H	-1.177208	-2.074483	3.096339
H	-0.001463	-3.463900	1.596108
H	1.187329	-2.068744	3.078551

E = -427.451102323
G = -427.307459

Reactions of Cp_2SmSiH_3 with SiH_4 : cf. [15]

Cp_2SmSiH_3 + 1-hexene : 1,2 insertion

Cp_2SmSiH_3 + 1-hexene → $Cp_2SmCH_2CH(C_4H_9)SiH_3$

Transition state

C	-3.525221	1.945738	0.760045
C	-3.177076	2.227740	-0.581351
C	-3.386000	3.615361	-0.806166
C	-3.873675	4.184566	0.395759
C	-3.948972	3.156978	1.369410
Sm	-1.246074	3.482320	0.903608
C	0.755172	1.868316	-0.039178
C	1.374848	2.582838	1.019110
C	1.492721	3.936931	0.622295
C	0.945941	4.064611	-0.677769
C	0.494476	2.783686	-1.089815
C	-1.157655	5.910836	1.736529
C	-1.077614	5.491451	3.085363
C	-2.157017	5.920334	4.068565
Si	-1.181051	3.093462	3.765718
H	-1.098707	1.847184	2.838978
H	-4.326067	3.259915	2.379841
H	-3.500311	0.971154	1.233383
H	-2.840439	1.507567	-1.317770
H	-3.248892	4.133912	-1.748497
H	-4.172219	5.216250	0.534007
H	0.061712	2.540969	-2.053241
H	0.556506	0.802926	-0.058154
H	1.732984	2.157508	1.949219
H	1.951228	4.730136	1.200937
H	0.918020	4.970839	-1.272182
H	-3.145774	5.727546	3.633746
C	-2.030464	7.411172	4.417390
H	-2.110819	5.339590	4.999144
H	-0.074625	5.479584	3.515271
H	-2.077429	6.388890	1.405367
H	-0.247390	6.242555	1.242867
H	-2.383734	2.820134	4.620563
H	0.013824	2.960682	4.665654
C	-3.082316	7.877695	5.424765
H	-1.026618	7.604231	4.821432
H	-2.106706	8.003468	3.497069
C	-2.960255	9.360068	5.770359
H	-4.084109	7.675782	5.021768
H	-2.999167	7.278740	6.341846
H	-3.724311	9.666867	6.491816
H	-1.981080	9.586246	6.207235
H	-3.075193	9.986073	4.878384

E = -663.229908691
G = -662.926578

$Cp_2SmCH_2CH(C_4H_9)SiH_3$

C	-3.354681	1.372176	-0.043150
C	-2.731586	1.791403	-1.243829
C	-3.124681	3.131648	-1.495508
C	-4.001900	3.533602	-0.454040
C	-4.139922	2.450210	0.443962
Sm	-1.513089	3.299484	0.709101
C	1.114994	2.533471	0.313730
C	1.175068	3.497261	1.356189
C	0.829462	4.756677	0.811910
C	0.545996	4.572447	-0.566463
C	0.735177	3.200150	-0.875219
C	-2.266740	5.065137	2.318844
C	-1.624240	4.897721	3.712515
C	-2.083033	5.869513	4.821420
Si	-1.949246	3.093063	4.167634
H	-1.510846	2.218973	2.986977
H	-4.758648	2.437419	1.333306
H	-3.284114	0.384766	0.400333
H	-2.092803	1.186419	-1.876620
H	-2.850838	3.721722	-2.362819
H	-4.493501	4.495352	-0.368280
H	0.628858	2.747437	-1.853842
H	1.365420	1.481879	0.401897
H	1.479468	3.307475	2.379254
H	0.804663	5.697579	1.347004
H	0.289066	5.353663	-1.273254
H	-3.174240	5.791323	4.933811
C	-1.712743	7.328835	4.550522
H	-1.651057	5.572011	5.790090
H	-0.528606	4.983056	3.622415
H	-3.363352	5.055573	2.426464
H	-2.016767	6.055627	1.903964
H	-3.403900	2.791710	4.337125
H	-1.199940	2.513562	5.329713
C	-2.181959	8.288029	5.645241
H	-0.621069	7.409555	4.440483
H	-2.140922	7.637519	3.588329
C	-1.802653	9.742224	5.374117
H	-3.272330	8.207347	5.752555
H	-1.760352	7.973566	6.609988
H	-2.150815	10.404633	6.173482
H	-0.715828	9.860189	5.295464
H	-2.240239	10.097644	4.434289

E = -663.248971318
G = -662.946459

Cp_2SmSiH_3 + 1-hexene : 2,1 insertion

Cp_2SmSiH_3 + 1-hexene → $Cp_2Sm\ CH(C_4H_9)CH_2SiH_3$

Transition state

C	0.483405	2.836477	-1.123496
C	0.529910	1.696593	-0.278796
C	1.209364	2.061350	0.909396
C	1.576176	3.426210	0.804967
C	1.133018	3.904205	-0.453868
Sm	-1.198427	3.434206	0.946548
C	-3.828460	2.853289	1.564985
C	-3.391605	1.817257	0.697453
C	-3.197288	2.375855	-0.588945
C	-3.510070	3.759460	-0.518054
C	-3.907508	4.049428	0.809728
C	-1.145947	5.977821	1.672562
C	0.078592	6.764315	1.246665
C	-1.277958	5.518586	2.995784
Si	-0.956644	3.182161	3.809338
H	-2.266083	5.474360	3.446630
H	-1.064067	1.842946	3.033464
H	-4.108639	2.734586	2.604962
H	-3.263788	0.774766	0.965072
H	-2.895047	1.836432	-1.478604
H	-3.495415	4.457776	-1.347546
H	-4.249565	5.010262	1.175578
H	0.067850	2.870585	-2.124052
H	0.147749	0.710904	-0.517511
H	1.432845	1.404737	1.741741
H	2.138248	3.988844	1.540757
H	1.299697	4.897349	-0.852121
H	-0.483457	5.750297	3.705881
H	-2.078563	6.217370	1.159883
H	-2.040214	3.113311	4.844607
H	0.345574	3.087881	4.551488
C	0.077128	8.232588	1.717168
H	0.982960	6.278268	1.635366
H	0.177922	6.756900	0.153347
H	1.047898	8.683420	1.465345
C	-1.038481	9.084745	1.113199
H	0.001509	8.258016	2.813378
C	-0.992815	10.541215	1.569872
H	-0.971070	9.041782	0.016793
H	-2.011610	8.650696	1.375990
H	-1.801307	11.128460	1.122266
H	-1.090953	10.618090	2.658755
H	-0.044736	11.015392	1.291550

E = -663.225581410
G = -662.924069

$Cp_2Sm\ CH(C_4H_9)CH_2SiH_3$

C	0.341868	2.751027	-1.437306
C	0.525695	1.668614	-0.539451
C	1.256846	2.146174	0.576314
C	1.530508	3.522867	0.367019
C	0.967365	3.895195	-0.875931
Sm	-1.211770	3.386770	0.727094
C	-3.815126	2.828986	1.511564
C	-3.393210	1.683077	0.784713
C	-3.247186	2.056764	-0.571877
C	-3.562267	3.435780	-0.683080
C	-3.925582	3.909282	0.604482
C	-1.161049	5.718489	1.711308
C	0.142951	6.530169	1.699729
C	-1.744842	5.560515	3.138583
Si	-0.852575	4.197071	4.093566
H	-2.799231	5.254691	3.097615
H	-0.793376	2.966924	3.182567
H	-4.059363	2.855546	2.567591
H	-3.255464	0.686252	1.189022
H	-2.960310	1.401771	-1.385864
H	-3.581756	4.011648	-1.601848
H	-4.252378	4.913589	0.843728
H	-0.143598	2.699496	-2.405020
H	0.193428	0.648916	-0.696422
H	1.590259	1.552846	1.420705
H	2.093299	4.170791	1.027316
H	1.027988	4.876427	-1.332381
H	-1.734611	6.480966	3.747514
H	-1.910434	6.273695	1.120148
H	-1.540879	3.700663	5.326521
H	0.577337	4.472362	4.422573
C	0.060852	8.000810	2.157058
H	0.898424	6.029870	2.325142
H	0.566403	6.524820	0.684691
H	1.080721	8.407434	2.225012
C	-0.765087	8.901204	1.238172
H	-0.346737	8.059034	3.176470
C	-0.793621	10.359589	1.690845
H	-0.358765	8.841708	0.218276
H	-1.792385	8.520158	1.176163
H	-1.389905	10.981311	1.014390
H	-1.224960	10.454568	2.694154
H	0.216352	10.784095	1.727829

E = -663.241659304
G = -662.939481

Cp_2SmSiH_3 + 1-hexene : allylic activation

Cp_2SmSiH_3 + 1-hexene → $Cp_2SmCH(C_3H_7)$-$CH=CH_2$ + SiH_4

Transition state

C	-0.893950	-0.014909	-6.465193
C	0.328958	0.545924	-6.908628
C	0.472210	1.821084	-6.304442
C	-0.664208	2.047481	-5.488174
C	-1.506327	0.911642	-5.583034
Sm	0.698868	0.044708	-4.199818
C	0.442546	1.614812	-1.982317
C	1.625397	0.877727	-1.729845
C	1.263988	-0.477444	-1.531726
C	-0.146563	-0.577357	-1.650000
C	-0.654563	0.714331	-1.932125
Si	-0.675028	-2.767596	-4.294092
C	2.487382	-1.998202	-4.945665
C	3.254060	-0.927434	-4.372970
C	3.346635	0.362307	-4.848539
H	1.009464	0.099400	-7.624562
H	1.282924	2.520566	-6.471417
H	-0.868468	2.945369	-4.916858
H	-2.466903	0.786948	-5.097531
H	-1.314877	-0.960673	-6.785370
H	1.937130	-1.288520	-1.280208
H	2.627019	1.286474	-1.672655
H	0.381676	2.684895	-2.142621
H	-1.699519	0.976605	-2.047045
H	-0.736433	-1.472473	-1.493945
C	2.843056	-3.421576	-4.542211
H	2.312747	-1.886476	-6.022710
H	0.998134	-2.122866	-4.534409
H	3.673287	-1.123070	-3.383329
H	3.918611	1.110074	-4.310069
H	3.082528	0.596216	-5.877628
H	-2.018986	-2.142102	-4.044454
H	-0.466745	-3.768186	-3.195647
H	-0.811656	-3.545821	-5.571250
C	4.141719	-3.931547	-5.177661
H	2.924581	-3.476921	-3.447444
H	2.024607	-4.101482	-4.816206
C	4.467202	-5.372116	-4.789924
H	4.060531	-3.851537	-6.270007
H	4.968712	-3.270660	-4.887132
H	5.398026	-5.710410	-5.256088
H	4.582476	-5.475277	-3.704988
H	3.671188	-6.057276	-5.102667

E = -663.219721919
G = -662.920168

$Cp_2SmCH_2CH(C_4H_9)SiH_3$

C	-3.354681	1.372176	-0.043150
C	-2.731586	1.791403	-1.243829
C	-3.124681	3.131648	-1.495508
C	-4.001900	3.533602	-0.454040
C	-4.139922	2.450210	0.443962
Sm	-1.513089	3.299484	0.709101
C	1.114994	2.533471	0.313730
C	1.175068	3.497261	1.356189
C	0.829462	4.756677	0.811910
C	0.545996	4.572447	-0.566463
C	0.735177	3.200150	-0.875219
C	-2.266740	5.065137	2.318844
C	-1.624240	4.897721	3.712515
C	-2.083033	5.869513	4.821420
Si	-1.949246	3.093063	4.167634
H	-1.510846	2.218973	2.986977
H	-4.758648	2.437419	1.333306
H	-3.284114	0.384766	0.400333
H	-2.092803	1.186419	-1.876620
H	-2.850838	3.721722	-2.362819
H	-4.493501	4.495352	-0.368280
H	0.628858	2.747437	-1.853842
H	1.365420	1.481879	0.401897
H	1.479468	3.307475	2.379254
H	0.804663	5.697579	1.347004
H	0.289066	5.353663	-1.273254
H	-3.174240	5.791323	4.933811
C	-1.712743	7.328835	4.550522
H	-1.651057	5.572011	5.790090
H	-0.528606	4.983056	3.622415
H	-3.363352	5.055573	2.426464
H	-2.016767	6.055627	1.903964
H	-3.403900	2.791710	4.337125
H	-1.199940	2.513562	5.329713
C	-2.181959	8.288029	5.645241
H	-0.621069	7.409555	4.440483
H	-2.140922	7.637519	3.588329
C	-1.802653	9.742224	5.374117
H	-3.272330	8.207347	5.752555
H	-1.760352	7.973566	6.609988
H	-2.150815	10.404633	6.173482
H	-0.715828	9.860189	5.295464
H	-2.240239	10.097644	4.434289

E = -663.248971318
G = -662.946459

$Cp_2SmCH_2CH(C_4H_9)SiH_3$ + 1-hexene : allylic activation

$Cp_2SmCH_2CH(C_4H_9)SiH_3$ + 1-hexene → $Cp_2SmCH(C_3H_7)$-$CH{=}CH_2$ + $SiH_3CH(C_4H_9)CH_3$

Transition state

E = -899.003129673
G = -898.544374

$SiH_3CH(C_4H_9)CH_3$ ('branched' hydrosilylation product)

C	-0.072249	-0.217674	-0.266848
Si	0.852328	-0.503972	1.380261
C	0.397146	1.035677	-1.030025
C	0.206570	2.372262	-0.309588
C	0.659735	3.568858	-1.147919
C	0.480920	4.907060	-0.434862
H	0.812660	5.742313	-1.060139
H	-0.848686	2.506313	-0.036662
H	0.764504	2.367189	0.637890
H	1.715022	3.437731	-1.423812
H	0.100096	3.578740	-2.093323
H	-0.569819	5.082347	-0.177414
H	1.057459	4.940434	0.496455
H	0.203887	-1.086800	-0.882612
C	-1.592612	-0.264009	-0.057329
H	-0.138369	1.074777	-1.991270
H	1.460004	0.922259	-1.283246
H	0.588897	-1.895725	1.867338
H	2.330905	-0.343885	1.200716
H	0.405841	0.440364	2.452853
H	-1.909872	-1.216913	0.379986
H	-1.940684	0.530599	0.610898
H	-2.122566	-0.147210	-1.011287

E = -242.107367399
G = -241.939204

$Cp_2SmCH_2CH(C_4H_9)SiH_3 + SiH_4$: Si(α)-H(β) activation

$Cp_2SmCH_2CH(C_4H_9)SiH_3 + SiH_4 \rightarrow Cp_2SmSiH_3 + SiH_3CH(C_4H_9)CH_3$

Transition state

C	0.457608	-1.632628	-2.384291
C	-0.262243	-0.412248	-2.388593
C	0.672171	0.649031	-2.259755
C	1.968786	0.083571	-2.178763
C	1.836027	-1.327911	-2.248628
Sm	0.748152	-0.629750	0.166547
C	-0.311002	-2.864570	0.835802
C	-1.381829	-3.797854	0.249930
C	-2.633530	-3.832360	1.144871
C	2.624935	-0.667080	2.173109
C	1.389054	-0.523952	2.849930
C	0.866164	0.757936	2.541889
C	1.783362	1.409235	1.676513
C	2.871239	0.529258	1.449221
Si	-0.607458	-5.527794	0.004703
Si	-2.240773	-0.016890	0.699964
H	-2.815764	0.120916	2.074568
H	-3.351811	-0.355940	-0.243233
H	-1.753798	1.357626	0.302792
H	-1.207096	-1.415258	0.760058
H	1.689305	2.417619	1.289710
H	-0.045662	1.185878	2.941733
H	0.938089	-1.250938	3.513930
H	3.289632	-1.521833	2.233113
H	3.755226	0.747647	0.861546
H	2.899795	0.633449	-2.108544
H	2.650650	-2.043703	-2.253185
H	0.034601	-2.622764	-2.500448
H	-1.332317	-0.304278	-2.521081
H	0.438558	1.707624	-2.267556
H	-0.238772	-3.016237	1.920298
H	0.696447	-3.141721	0.435629
H	-1.682638	-3.439568	-0.747014
H	-1.500990	-6.531611	-0.662401
H	0.624537	-5.396209	-0.839384
H	-0.201702	-6.082056	1.336098
C	-3.854612	-4.516200	0.528836
H	-2.382315	-4.317276	2.099704
H	-2.909460	-2.799558	1.408380
C	-5.085600	-4.482387	1.435957
H	-4.095571	-4.031446	-0.428016
H	-3.617079	-5.560802	0.285566
C	-6.306700	-5.157441	0.815623
H	-4.843890	-4.967286	2.391530
H	-5.327356	-3.438785	1.679351
H	-7.171473	-5.116441	1.485751
H	-6.592138	-4.672594	-0.124774
H	-6.107580	-6.212226	0.594711

E = -669.517936073
G = -669.189626

$Cp_2SmCH_2CH(C_4H_9)SiH_3 + SiH_4$: Si(β)-H(α) activation

$Cp_2SmCH_2CH(C_4H_9)SiH_3 + SiH_4 \rightarrow Cp_2SmH + SiH_3CH(C_4H_9)CH_2SiH_3$

$SiH_3CH_2(CH_2)_4CH_2SiH_3$

C	0.012613	-0.139738	-0.362166
H	0.521523	-0.272913	0.602499
C	0.623586	1.048702	-1.136202
C	0.359402	2.369178	-0.384862
C	0.673943	3.648297	-1.162648
C	0.290323	4.918959	-0.401972
C	0.599235	6.198301	-1.176088
H	-0.703903	2.388709	-0.099798
H	0.917489	2.369617	0.562867
H	1.742602	3.689066	-1.410655
H	0.141978	3.627688	-2.124787
H	-0.780663	4.886008	-0.159279
H	0.817726	4.936339	0.561477
H	0.310968	7.089468	-0.609286
H	1.669090	6.278602	-1.399280
H	0.061401	6.223686	-2.130559
Si	-0.052845	-1.834075	-1.229208
H	-1.030558	0.102337	-0.108993
H	0.131790	1.111446	-2.118745
Si	2.480490	0.760998	-1.492566
H	-1.043655	-2.702542	-0.518215
H	-0.497359	-1.676950	-2.650072
H	1.262916	-2.542375	-1.222370
H	3.094306	1.883045	-2.266907
H	3.223784	0.618411	-0.199772
H	2.673762	-0.491001	-2.287165

E = -247.201315945
G = -247.022997

$Cp_2SmCH(C_4H_9)CH_2SiH_3$

$Cp_2Sm\ CH(C_4H_9)CH_2SiH_3$

C	0.341868	2.751027	-1.437306
C	0.525695	1.668614	-0.539451
C	1.256846	2.146174	0.576314
C	1.530508	3.522867	0.367019
C	0.967365	3.895195	-0.875931
Sm	-1.211770	3.386770	0.727094
C	-3.815126	2.828986	1.511564
C	-3.393210	1.683077	0.784713
C	-3.247186	2.056764	-0.571877
C	-3.562267	3.435780	-0.683080
C	-3.925582	3.909282	0.604482
C	-1.161049	5.718489	1.711308
C	0.142951	6.530169	1.699729
C	-1.744842	5.560515	3.138583
Si	-0.852575	4.197071	4.093566
H	-2.799231	5.254691	3.097615
H	-0.793376	2.966924	3.182567
H	-4.059363	2.855546	2.567591
H	-3.255464	0.686252	1.189022
H	-2.960310	1.401771	-1.385864
H	-3.581756	4.011648	-1.601848
H	-4.252378	4.913589	0.843728
H	-0.143598	2.699496	-2.405020
H	0.193428	0.648916	-0.696422
H	1.590259	1.552846	1.420705
H	2.093299	4.170791	1.027316
H	1.027988	4.876427	-1.332381
H	-1.734611	6.480966	3.747514
H	-1.910434	6.273695	1.120148
H	-1.540879	3.700663	5.326521
H	0.577337	4.472362	4.422573
C	0.060852	8.000810	2.157058
H	0.898424	6.029870	2.325142
H	0.566403	6.524820	0.684691
H	1.080721	8.407434	2.225012
C	-0.765087	8.901204	1.238172
H	-0.346737	8.059034	3.176470
C	-0.793621	10.359589	1.690845
H	-0.358765	8.841708	0.218276
H	-1.792385	8.520158	1.176163
H	-1.389905	10.981311	1.014390
H	-1.224960	10.454568	2.694154
H	0.216352	10.784095	1.727829

E = -663.241659304
G = -662.939481

$Cp_2SmCH(C_4H_9)CH_2SiH_3 + SiH_4$: Si(α)-H(β) activation

$Cp_2SmCH(C_4H_9)CH_2SiH_3 + SiH_4 \rightarrow Cp_2SmSiH_3 + SiH_3CH_2(CH_2)_4CH_3$

Transition state

C	3.434237	3.917478	3.994608
C	4.733126	3.475292	4.356275
C	4.653804	2.877952	5.639903
C	3.305692	2.953294	6.070146
C	2.551128	3.594531	5.054981
Sm	3.286170	1.171586	3.936827
C	5.021513	-0.518525	4.508798
C	5.836005	0.013708	3.341299
C	2.594130	-0.378147	1.741345
C	1.625758	-0.696894	2.717775
C	0.818179	0.454228	2.928976
C	1.286935	1.479132	2.070189
C	2.393126	0.971479	1.344046
C	4.729248	-2.024753	4.469854
Si	6.253737	-3.137454	4.744913
Si	1.422581	-0.269534	6.823723
H	4.000107	-2.303982	5.242957
H	1.915760	-0.069837	8.214533
H	0.770073	-1.599886	6.674968
H	0.474862	0.816688	6.449544
H	2.625107	-0.246571	5.915451
H	1.494759	3.833610	5.098545
H	2.930818	2.633153	7.035959
H	5.481540	2.474324	6.209450
H	5.636493	3.613499	3.773376
H	3.171324	4.446402	3.085892
H	0.861944	2.471021	1.972099
H	2.947033	1.498522	0.575324
H	3.345119	-1.051419	1.345927
H	1.501474	-1.660764	3.197390
H	-0.048509	0.516947	3.577295
H	5.520258	-0.255470	5.451384
H	4.265446	-2.315460	3.517845
H	5.913775	-4.601261	4.757710
H	7.284991	-2.933741	3.675094
H	6.899317	-2.809694	6.057707
C	7.238202	0.544702	3.659524
H	5.895109	-0.731012	2.535284
H	5.330016	0.886505	2.798213
H	7.837122	-0.285675	4.055376
C	7.958256	1.173274	2.466355
H	7.163898	1.279453	4.472886
C	9.347852	1.702871	2.813593
H	8.038998	0.431044	1.660507
H	7.345324	1.991732	2.061865
H	9.839274	2.144804	1.940802
H	9.295704	2.473554	3.591045
H	9.994273	0.901458	3.188265

E = -669.532984931
G = -669.204494

Hydrosilylation of isobutylene by SiH_4

Isobutylene

C	0.004884	-0.202356	-0.053781
C	0.000698	-0.027903	1.271244
H	0.930075	-0.211043	-0.624231
H	-0.916727	-0.342211	-0.612805
C	-1.272675	-0.014826	2.071568
C	1.269006	0.167237	2.055833
H	2.153559	0.144105	1.413935
H	1.257656	1.126994	2.588524
H	1.381252	-0.611278	2.821567
H	-1.264674	-0.803351	2.835221
H	-1.390189	0.935676	2.607906
H	-2.152866	-0.161043	1.440018

E = -157.176444980
G = -157.095501

SiH_4

Si	0.039477	-0.034937	-0.040692
H	-0.049434	0.074062	1.444033
H	1.471253	0.032766	-0.459854
H	-0.546669	-1.335733	-0.480347
H	-0.716009	1.088593	-0.667068

E = -6.28910490369
G = -6.279886

Cp_2SmH

Sm	-0.012028	-0.360917	-0.032744
C	2.651518	0.166910	0.400364
C	2.628053	-1.035725	-0.347190
C	2.153089	-0.727706	-1.648215
C	1.896905	0.667000	-1.707315
C	2.201572	1.220440	-0.439044
C	-2.676905	0.192820	0.357255
C	-2.204661	1.238468	-0.479754
C	-1.885825	0.676625	-1.740853
C	-2.155637	-0.715416	-1.679663
C	-2.653000	-1.013341	-0.384672
H	2.995320	0.268995	1.424094
H	2.924893	-2.013303	0.009195
H	2.049911	-1.428719	-2.469134
H	1.563384	1.217923	-2.578639
H	2.150921	2.271424	-0.175649
H	-3.035485	0.302623	1.375108
H	-2.148484	2.290123	-0.220217
H	-1.534462	1.220687	-2.609468
H	-2.046267	-1.421049	-2.495806
H	-2.964166	-1.986614	-0.028729
H	-0.026518	-2.217018	0.902785

E = -422.333039019
G = -422.201852

Reactions with SiH_4 : cf. [15]

Cp_2SmH + isobutylene : 1,2 insertion

Cp_2SmH + isobutylene → $Cp_2SmCH_2CH(CH_3)_2$

Transition state

C	-0.132446	-0.364040	1.001102
C	1.096669	-0.719224	1.609505
C	2.124544	-0.578206	0.640995
C	1.528774	-0.140935	-0.567865
C	0.135861	-0.000460	-0.343148
Sm	1.283280	2.005608	1.135268
C	1.149913	3.914842	-0.824628
C	2.465909	3.395151	-0.921574
C	3.182261	3.801930	0.231137
C	2.311088	4.581349	1.035427
C	1.055748	4.653343	0.382440
C	1.623506	2.219383	3.776253
C	0.288075	2.550276	3.894002
C	-0.115135	3.988025	4.111433
H	-0.485928	2.548364	2.100784
H	2.576895	5.077624	1.961529
H	0.185295	5.194950	0.730213
H	0.365640	3.803959	-1.564907
H	2.863373	2.816698	-1.746985
H	4.227913	3.597600	0.435128
H	2.042907	0.028246	-1.506395
H	-0.601828	0.293238	-1.081351
H	-1.108293	-0.388376	1.469142
H	1.224209	-1.085433	2.621638
H	3.173264	-0.816010	0.783375
H	0.568593	4.680933	3.616260
H	-0.086628	4.198505	5.189858
H	-1.128212	4.180614	3.752551
C	-0.704936	1.522171	4.377270
H	2.383119	2.999775	3.777522
H	1.956181	1.200877	3.971424
H	-1.712369	1.733626	4.012987
H	-0.427322	0.511254	4.070924
H	-0.724930	1.547617	5.475957

E = -579.519935606
G = -579.285152

$Cp_2SmCH_2CH(CH_3)_2$ (isobutyl complex)

C	-0.088893	-0.359467	0.988988
C	1.134932	-0.727232	1.601628
C	2.159388	-0.614921	0.628098
C	1.567198	-0.190011	-0.589175
C	0.177879	-0.027023	-0.365281
Sm	1.375610	1.980218	1.099413
C	1.167519	3.936074	-0.833029
C	2.483088	3.427757	-0.968057
C	3.219777	3.809753	0.182829
C	2.363767	4.562763	1.024819
C	1.093885	4.636984	0.399105
C	1.557368	2.200427	3.536087
C	0.082874	2.564528	3.620329
C	-0.168247	3.991551	4.116990
H	-0.407739	2.561260	2.576780
H	2.640422	5.021738	1.965421
H	0.231453	5.177629	0.772780
H	0.372426	3.845056	-1.564590
H	2.867719	2.874994	-1.816997
H	4.269078	3.603443	0.364296
H	2.081194	-0.045222	-1.532018
H	-0.557670	0.255575	-1.110128
H	-1.065938	-0.376991	1.458667
H	1.262348	-1.061255	2.623450
H	3.205650	-0.860525	0.774953
H	0.418672	4.717656	3.545796
H	0.133808	4.072550	5.167117
H	-1.225713	4.272754	4.043427
C	-0.757590	1.549667	4.401112
H	2.198982	3.005517	3.907538
H	1.784534	1.283673	4.089267
H	-1.830391	1.768464	4.337639
H	-0.593887	0.532723	4.031108
H	-0.467091	1.569625	5.457360

E = -579.546804799
G = -579.308336

Cp_2SmH + isobutylene : 2,1 insertion

Cp_2SmH + isobutylene → $Cp_2SmC(CH_3)_3$

Transition state

C	-0.841625	0.448282	1.121982
C	-1.354391	1.767858	1.044623
C	-1.154675	2.392505	2.301965
C	-0.521498	1.455571	3.157740
C	-0.327790	0.256780	2.428363
Sm	1.346031	2.109489	1.215119
C	0.924180	3.607841	-1.028059
C	2.240279	3.111695	-1.198731
C	3.070878	3.742969	-0.239916
C	2.269881	4.634758	0.518041
C	0.942559	4.552264	0.032172
C	3.319028	0.865475	2.606842
C	3.626142	2.274127	3.027999
C	3.549266	0.400152	1.321663
H	3.551431	-0.668144	1.132262
H	2.196616	0.503302	0.202724
H	0.107963	-0.658168	2.808965
H	-0.862586	-0.292918	0.332714
H	-1.843107	2.212038	0.185857
H	-1.473687	3.391912	2.574617
H	-0.275255	1.616073	4.201666
H	0.098370	5.135083	0.381407
H	0.062835	3.343127	-1.629734
H	2.558171	2.397525	-1.947395
H	4.143067	3.613562	-0.146863
H	2.618776	5.298622	1.301350
H	4.152491	0.985391	0.630367
C	2.879835	-0.066865	3.710255
H	4.118427	2.299462	4.007526
H	4.254925	2.809869	2.311443
H	2.719083	2.922130	3.197521
H	3.707511	-0.236515	4.414590
H	2.044417	0.328567	4.300508
H	2.578091	-1.041411	3.317260

E = -579.513186687
G = -579.277528

$Cp_2SmC(CH_3)_3$

C	-0.669146	0.239546	1.531873
C	-1.291465	1.349925	0.903546
C	-1.392016	2.391914	1.857064
C	-0.828920	1.927264	3.074447
C	-0.388692	0.593579	2.874274
Sm	1.284207	2.165019	1.348946
C	0.867667	3.783438	-0.875760
C	2.143963	3.204316	-1.082741
C	3.038350	3.756969	-0.129781
C	2.310039	4.669262	0.671428
C	0.968042	4.686297	0.213654
C	3.063181	0.870783	2.420523
C	3.633417	2.141991	3.003051
C	3.539882	0.444552	1.054976
H	3.776347	-0.624637	1.006511
H	2.766871	0.558072	0.222598
H	0.055587	-0.050085	3.621651
H	-0.481036	-0.726470	1.076559
H	-1.659789	1.382383	-0.115195
H	-1.848060	3.360968	1.693581
H	-0.794135	2.475699	4.009576
H	0.172044	5.314640	0.595841
H	-0.021868	3.593170	-1.464602
H	2.404611	2.507081	-1.871121
H	4.100514	3.556366	-0.062332
H	2.717545	5.285835	1.464758
H	4.403589	1.004401	0.673903
C	2.913772	-0.263858	3.417436
H	3.974019	2.016737	4.037978
H	4.456665	2.577731	2.422897
H	2.887417	2.996436	3.093519
H	3.886146	-0.685744	3.731089
H	2.403993	0.060866	4.332598
H	2.327191	-1.094735	3.007536

E = -579.531551654
G = -579.293554

Cp_2SmH + isobutylene : allylic activation

Cp_2SmH + isobutylene → Cp_2SmCH_2-C(CH_3)=CH_2 + H_2

Transition state

C	-0.197002	-1.997298	-6.702428
C	-0.171020	-2.904683	-5.612375
C	-1.312168	-2.657406	-4.810844
C	-2.043914	-1.597780	-5.406354
C	-1.356976	-1.193818	-6.577544
Sm	0.232961	-0.421106	-4.455446
C	0.461879	1.403906	-2.377676
C	0.972446	0.194075	-1.850142
C	-0.097109	-0.730518	-1.755027
C	-1.275382	-0.081169	-2.210452
C	-0.929255	1.234895	-2.598613
C	2.983288	0.095880	-4.926243
C	2.893507	-1.254226	-4.701913
C	2.250853	0.761760	-5.998826
H	-0.107097	1.388444	-5.578017
H	1.019292	2.317915	-2.543968
H	1.995680	0.012347	-1.544666
H	-0.037944	-1.735446	-1.353125
H	-2.270024	-0.509914	-2.229847
H	-1.608612	1.990008	-2.974345
H	0.517166	-1.959302	-7.517143
H	0.564509	-3.683139	-5.444892
H	-1.595907	-3.206311	-3.920635
H	-2.981905	-1.190585	-5.047852
H	-1.673929	-0.419764	-7.265124
H	0.948289	1.215951	-5.765312
H	2.487509	-1.920416	-5.461046
H	3.421475	-1.720310	-3.876121
C	3.777133	0.971984	-3.990244
H	2.636240	1.749710	-6.256786
H	2.109165	0.152620	-6.895395
H	4.677180	1.321981	-4.510315
H	3.215343	1.862382	-3.692159
H	4.092857	0.437321	-3.091501

E = -579.512240411
G = -579.279077

Cp_2SmCH_2-C(CH_3)=CH_2 (π-allylic complex)

C	-1.099647	0.008860	-2.417382
C	-0.823830	1.390784	-2.556804
C	0.546442	1.597344	-2.251321
C	1.114390	0.343120	-1.914695
C	0.099748	-0.640401	-2.026282
Sm	0.594232	0.177026	-4.597304
C	2.400007	-1.511498	-5.852937
C	2.283750	-0.413783	-6.740702
C	2.855356	0.720589	-6.114145
C	3.328366	0.324073	-4.837198
C	3.047121	-1.056578	-4.675979
C	-0.863278	1.550672	-6.346497
H	1.057539	2.553576	-2.229808
H	2.138180	0.169885	-1.606102
H	0.209169	-1.696085	-1.803454
H	-2.063865	-0.465450	-2.551610
H	-1.539650	2.161095	-2.815005
H	2.950815	1.708444	-6.550695
H	3.852206	0.953812	-4.127495
H	3.316823	-1.665333	-3.820871
H	2.085373	-2.529234	-6.054779
H	1.860711	-0.443814	-7.737934
C	-1.741532	0.503152	-6.023747
C	-3.073803	0.841611	-5.398106
C	-1.351632	-0.845520	-6.088209
H	-0.092022	1.377641	-7.099163
H	-1.200861	2.579871	-6.262366
H	-2.058476	-1.621650	-5.808056
H	-0.611336	-1.142887	-6.832996
H	-3.397618	0.081435	-4.682022
H	-3.829957	0.887112	-6.191083
H	-3.061757	1.815545	-4.901501

E = -578.348456384
G = -578.130677

H_2
E = -1.17751649843
G = -1.178858

$Cp_2SmCH_2CH(CH_3)_2$ (isobutyl complex)

C	-0.088893	-0.359467	0.988988
C	1.134932	-0.727232	1.601628
C	2.159388	-0.614921	0.628098
C	1.567198	-0.190011	-0.589175
C	0.177879	-0.027023	-0.365281
Sm	1.375610	1.980218	1.099413
C	1.167519	3.936074	-0.833029
C	2.483088	3.427757	-0.968057
C	3.219777	3.809753	0.182829
C	2.363767	4.562763	1.024819
C	1.093885	4.636984	0.399105
C	1.557368	2.200427	3.536087
C	0.082874	2.564528	3.620329
C	-0.168247	3.991551	4.116990
H	-0.407739	2.561260	2.576780
H	2.640422	5.021738	1.965421
H	0.231453	5.177629	0.772780
H	0.372426	3.845056	-1.564590
H	2.867719	2.874994	-1.816997
H	4.269078	3.603443	0.364296
H	2.081194	-0.045222	-1.532018
H	-0.557670	0.255575	-1.110128
H	-1.065938	-0.376991	1.458667
H	1.262348	-1.061255	2.623450
H	3.205650	-0.860525	0.774953
H	0.418672	4.717656	3.545796
H	0.133808	4.072550	5.167117
H	-1.225713	4.272754	4.043427
C	-0.757590	1.549667	4.401112
H	2.198982	3.005517	3.907538
H	1.784534	1.283673	4.089267
H	-1.830391	1.768464	4.337639
H	-0.593887	0.532723	4.031108
H	-0.467091	1.569625	5.457360

E = -579.546804799
G = -579.308336

$Cp_2SmCH_2CH(CH_3)_2$ + isobutylene : 1,2 insertion

$Cp_2SmCH_2CH(CH_3)_2$ + isobutylene → $Cp_2SmCH_2C(CH_3)_2CH_2CH(CH_3)_2$

Transition state

C	-0.431909	4.525037	3.646754
C	-1.785457	4.141279	3.799968
C	-2.585293	5.054316	3.069736
C	-1.724437	6.009666	2.473550
C	-0.393223	5.681237	2.825367
Sm	-1.130893	3.629958	1.127600
C	0.469715	1.952368	-0.444196
C	1.041682	1.933791	0.852288
C	1.590571	3.214803	1.105946
C	1.346919	4.029768	-0.027458
C	0.661278	3.243291	-0.988522
C	-2.467788	1.581556	1.610915
C	-3.426585	1.895653	0.590616
C	-4.769510	2.400288	1.084522
C	-2.939102	3.472512	-0.793886
C	-2.785141	5.003266	-0.870074
C	-2.473075	5.447909	-2.307875
C	-4.025696	5.728371	-0.343759
H	-3.668037	5.062445	3.034048
H	-2.033528	6.868765	1.889323
H	0.495047	6.236920	2.548906
H	0.421393	4.044017	4.109936
H	-2.146227	3.316345	4.401729
H	2.126702	3.512305	1.998600
H	1.675457	5.054524	-0.157984
H	0.371722	3.564771	-1.982237
H	-0.001888	1.113772	-0.942379
H	1.085086	1.079452	1.517618
H	-4.650298	3.168906	1.852102
H	-5.310613	1.561432	1.542269
H	-5.394935	2.804984	0.283265
C	-3.532750	0.874009	-0.527260
H	-2.796474	1.706729	2.641020
H	-1.842227	0.706153	1.441847
H	-3.910771	3.247850	-1.231011
H	-2.189077	2.987662	-1.433674
H	-1.920510	5.399635	-0.277488
H	-4.258021	5.443211	0.684650
H	-3.896552	6.815348	-0.374723
H	-4.893547	5.478094	-0.964930
H	-2.346428	6.535557	-2.369407
H	-3.294670	5.165625	-2.975748
H	-1.559657	4.977950	-2.683793
H	-3.990821	-0.032282	-0.112115
H	-4.153337	1.204037	-1.365825
H	-2.547968	0.595854	-0.912996

E = -736.705886888
G = -736.360152

$Cp_2SmCH_2C(CH_3)_2CH_2CH(CH_3)_2$

C	-0.593615	4.426738	3.746226
C	-1.984868	4.333824	3.477350
C	-2.360396	5.477328	2.735229
C	-1.204714	6.281888	2.547375
C	-0.117068	5.637550	3.182717
Sm	-0.695849	3.980608	1.052634
C	1.020780	2.784232	-0.789400
C	1.240859	2.116173	0.436270
C	1.850709	3.032629	1.332368
C	2.017259	4.265795	0.651290
C	1.498053	4.114778	-0.657080
C	-2.207298	2.051681	0.580048
C	-3.715929	2.061939	0.244471
C	-4.545108	2.464651	1.473800
C	-4.034254	3.021972	-0.930721
C	-3.539644	4.474788	-0.769258
C	-2.230259	4.718098	-1.532673
C	-4.589010	5.504567	-1.196907
H	-3.365595	5.726693	2.416878
H	-1.173769	7.249883	2.058614
H	0.898620	6.009444	3.241310
H	-0.010353	3.725374	4.331999
H	-2.645102	3.540217	3.802384
H	2.182343	2.814096	2.340672
H	2.483586	5.157178	1.053614
H	1.511081	4.868134	-1.437451
H	0.591549	2.345028	-1.682131
H	0.996222	1.082314	0.648297
H	-4.322878	3.481581	1.811550
H	-4.332168	1.791033	2.311973
H	-5.621224	2.406779	1.266972
C	-4.180994	0.655309	-0.183639
H	-2.056880	1.339607	1.414283
H	-1.686849	1.571222	-0.269706
H	-5.122876	3.027827	-1.080453
H	-3.612363	2.600283	-1.855052
H	-3.355859	4.639707	0.305200
H	-5.503558	5.402962	-0.604153
H	-4.223534	6.531590	-1.079480
H	-4.859071	5.366868	-2.250891
H	-1.738242	5.660846	-1.242788
H	-2.416586	4.797765	-2.610009
H	-1.527692	3.876625	-1.436594
H	-4.015389	-0.066002	0.624556
H	-5.249353	0.632094	-0.440244
H	-3.617753	0.307070	-1.057211

E = -736.745271214
G = -736.399063

$Cp_2SmCH_2CH(CH_3)_2$ + isobutylene : allylic activation

$Cp_2SmCH_2CH(CH_3)_2$ + isobutylene → Cp_2SmCH_2-$C(CH_3)$=CH_2 + isobutane

Transition state

C	2.023145	0.979898	1.866840
C	2.139155	-0.314766	1.308032
C	1.004383	-1.067154	1.705284
C	0.194641	-0.239213	2.522015
C	0.819842	1.025841	2.618298
Sm	0.026168	0.801877	-0.049114
C	-0.629604	0.543199	-2.740893
C	-0.364693	-0.771841	-2.281828
C	1.016430	-0.863247	-1.988636
C	1.607204	0.398716	-2.259519
C	0.589543	1.261939	-2.734812
C	-2.418975	-0.186013	0.310297
C	-3.412286	-0.220956	1.487960
C	-4.732942	0.470514	1.132627
C	-3.690439	-1.653022	1.961009
C	-1.890507	2.688340	0.625701
C	-0.971039	3.448228	-0.227727
C	0.352998	3.612875	0.075464
H	0.465753	1.866377	3.204351
H	2.749127	1.779242	1.772103
H	2.962792	-0.675083	0.703648
H	0.812932	-2.106112	1.462900
H	-0.730148	-0.530475	3.004053
H	-1.590067	0.912733	-3.079578
H	0.728449	2.286652	-3.057088
H	2.658814	0.643815	-2.166292
H	1.536358	-1.748823	-1.643799
H	-1.088660	-1.572997	-2.197019
H	-2.959780	-0.205384	-0.645885
H	-1.826060	-1.115984	0.327097
H	-2.935000	2.964521	0.470443
H	-1.646541	2.742753	1.690794
H	-2.068440	1.367804	0.401343
H	-2.978694	0.322912	2.343581
H	-4.382781	-1.672666	2.811852
H	-4.135516	-2.245962	1.152712
H	-2.767265	-2.156477	2.269547
H	-5.412896	0.498919	1.991658
H	-4.583124	1.500537	0.794842
H	-5.240337	-0.069252	0.323394
C	-1.524957	3.961307	-1.532741
H	1.021948	4.134477	-0.601722
H	0.730595	3.407266	1.074765
H	-0.740142	4.319159	-2.203205
H	-2.112030	3.197453	-2.052654
H	-2.203746	4.798386	-1.328114

E = -736.710766875
G = -736.370819

Isobutane

C	-0.017319	-0.029636	-0.082789
C	0.005003	0.008808	1.446592
C	1.439961	-0.029413	1.976629
C	-0.745690	1.231860	1.977245
H	1.463240	-0.033443	3.071973
H	1.972796	-0.920673	1.627233
H	2.004365	0.847978	1.636774
H	0.489811	0.848565	-0.501472
H	0.490889	-0.920168	-0.468742
H	-1.042585	-0.035139	-0.468870
H	-0.265705	2.159477	1.641328
H	-1.782873	1.249777	1.624642
H	-0.764475	1.247196	3.072572
H	-0.513274	-0.889511	1.813549

E = -158.413556573
G = -158.309154

$Cp_2SmCH_2CH(CH_3)_2 + SiH_4$: Si(α)-H(β) activation

$Cp_2SmCH_2CH(CH_3)_2 + SiH_4 \rightarrow Cp_2SmSiH_3 + isobutane$

Transition state

C	0.302977	1.547333	1.646053
C	1.659766	1.173900	1.805214
C	1.694643	-0.070017	2.487921
C	0.357671	-0.456049	2.764891
C	-0.501955	0.539955	2.241659
Sm	0.639417	-0.640334	0.026343
C	-0.207960	-3.028013	0.252715
C	-1.346611	-3.929201	0.734736
C	-0.971601	-5.415929	0.699248
C	2.437760	-1.385439	-1.929637
C	1.192521	-1.339456	-2.599410
C	0.771714	0.014892	-2.651008
C	1.762103	0.806122	-2.015681
C	2.791912	-0.059261	-1.565915
Si	-2.407234	-0.596411	-0.729561
H	-3.535572	-0.630854	0.252482
H	-2.913369	-1.084142	-2.050968
H	-2.060697	0.859800	-0.920210
H	-1.244162	-1.746906	-0.179193
H	0.048809	-1.341109	3.306043
H	2.588885	-0.600491	2.796584
H	2.520319	1.749451	1.485483
H	-0.056543	2.462550	1.189714
H	-1.582271	0.556668	2.325699
H	-0.123196	0.384608	-3.137747
H	1.752026	1.885795	-1.921277
H	3.711061	0.243996	-1.078039
H	3.035447	-2.273514	-1.755918
H	0.664670	-2.184479	-3.024385
H	0.630586	-3.104954	0.984726
H	0.179367	-3.410291	-0.704062
C	-1.833209	-3.531136	2.129383
H	-2.190965	-3.791353	0.037792
H	-1.813304	-6.051742	0.999974
H	-0.660403	-5.723022	-0.305032
H	-0.138208	-5.621362	1.382428
H	-2.683540	-4.144567	2.447043
H	-1.034515	-3.668713	2.869529
H	-2.144425	-2.481909	2.162092

E = -585.821593652
G = -585.557666

Cp_2SmSiH_3

Sm	0.012178	0.013956	-0.055232
C	2.717161	0.446808	0.083382
C	2.575666	-0.905991	-0.310994
C	2.025039	-0.921480	-1.619741
C	1.838723	0.421996	-2.036394
C	2.262398	1.268920	-0.981395
C	-2.671303	0.522888	0.242215
C	-2.216176	1.470050	-0.712783
C	-1.857685	0.766744	-1.890007
C	-2.084640	-0.615234	-1.659263
C	-2.596116	-0.763898	-0.343066
H	3.134369	0.790319	1.023565
H	2.858054	-1.771854	0.274441
H	1.829896	-1.805269	-2.216811
H	1.473499	0.744348	-3.004086
H	2.285375	2.353091	-1.007688
H	-3.042962	0.743361	1.236439
H	-2.197243	2.547282	-0.585750
H	-1.509858	1.209521	-2.815597
H	-1.947184	-1.411062	-2.382679
H	-2.895282	-1.692513	0.126324
Si	-0.002566	-2.047720	2.140529
H	-1.177208	-2.074483	3.096339
H	-0.001463	-3.463900	1.596108
H	1.187329	-2.068744	3.078551

E = -427.451102323
G = -427.307459

$Cp_2SmCH_2CH(CH_3)_2$ + SiH_4 : Si(β)-H(α) activation

$Cp_2SmCH_2CH(CH_3)_2 + SiH_4 \rightarrow Cp_2SmH + SiH_3CH_2CH(CH_3)_2$

Transition state

C	-1.949325	-4.655270	-0.752948
C	-1.757314	-3.558811	-1.632692
C	-0.540278	-3.763148	-2.330254
C	0.019829	-4.987837	-1.884538
C	-0.849771	-5.539002	-0.911100
Sm	0.188329	-3.328913	0.288954
C	1.011618	-2.677535	2.843184
C	-0.398774	-2.811268	2.923755
C	-0.722144	-4.176343	2.717603
C	0.489108	-4.883972	2.503033
C	1.559948	-3.957664	2.585821
Si	2.636635	-2.243912	-1.413044
C	1.065789	-1.003226	-0.524234
C	1.567387	0.434218	-0.770218
C	0.406359	1.401154	-1.031512
H	3.773029	-1.608375	-0.677327
H	1.575621	-1.764554	2.992444
H	-1.102548	-2.018926	3.154753
H	-1.714528	-4.609622	2.757923
H	0.582897	-5.952749	2.350370
H	2.613184	-4.191301	2.491568
H	-2.808267	-4.815114	-0.111812
H	-2.445026	-2.732877	-1.778853
H	-0.126426	-3.118998	-3.097244
H	0.941675	-5.429083	-2.243765
H	-0.719240	-6.487735	-0.404240
H	2.201420	-3.482522	-0.355431
H	3.289574	-3.402298	-2.167965
H	2.310781	-1.428341	-2.660814
H	0.847288	-1.027401	0.565487
H	0.117021	-1.124441	-1.083224
C	2.431429	0.932176	0.391267
H	2.189138	0.419932	-1.677941
H	-0.269779	1.448617	-0.168657
H	-0.180980	1.093475	-1.903649
H	0.775262	2.416092	-1.219447
H	2.861270	1.913483	0.164513
H	1.832838	1.038558	1.305259
H	3.256086	0.245878	0.602820

E = -585.822433160
G = -585.552015

$SiH_3CH_2CH(CH_3)_2$ *('linear' hydrosilylation product)*

H	-0.307096	-0.162134	1.769731
Si	-0.056502	-0.103070	0.295730
H	-0.737573	1.118839	-0.239517
C	1.794271	-0.075622	-0.134036
C	2.562636	1.214595	0.207494
C	3.988447	1.154216	-0.349077
H	-0.700072	-1.305428	-0.322091
H	2.272144	-0.935311	0.356907
H	1.865070	-0.270970	-1.212577
H	2.047785	2.054016	-0.282616
C	2.582716	1.492334	1.712832
H	4.534864	2.082100	-0.146415
H	4.550484	0.330643	0.108125
H	3.988549	0.995278	-1.432875
H	3.138655	2.409179	1.936020
H	1.574184	1.609388	2.123593
H	3.066534	0.670223	2.254416

E = -163.507662293
G = -163.392581

Cp_2SmSiH_3

Sm	0.012178	0.013956	-0.055232
C	2.717161	0.446808	0.083382
C	2.575666	-0.905991	-0.310994
C	2.025039	-0.921480	-1.619741
C	1.838723	0.421996	-2.036394
C	2.262398	1.268920	-0.981395
C	-2.671303	0.522888	0.242215
C	-2.216176	1.470050	-0.712783
C	-1.857685	0.766744	-1.890007
C	-2.084640	-0.615234	-1.659263
C	-2.596116	-0.763898	-0.343066
H	3.134369	0.790319	1.023565
H	2.858054	-1.771854	0.274441
H	1.829896	-1.805269	-2.216811
H	1.473499	0.744348	-3.004086
H	2.285375	2.353091	-1.007688
H	-3.042962	0.743361	1.236439
H	-2.197243	2.547282	-0.585750
H	-1.509858	1.209521	-2.815597
H	-1.947184	-1.411062	-2.382679
H	-2.895282	-1.692513	0.126324
Si	-0.002566	-2.047720	2.140529
H	-1.177208	-2.074483	3.096339
H	-0.001463	-3.463900	1.596108
H	1.187329	-2.068744	3.078551

E = -427.451102323
G = -427.307459

Reactions of Cp_2SmSiH_3 with SiH_4 : cf. [15]

Cp_2SmSiH_3 + isobutylene : 1,2 insertion

Cp_2SmSiH_3 + isobutylene → $Cp_2SmCH_2C(CH_3)_2SiH_3$

Transition state

C	-3.579929	2.128837	0.585295
C	-3.234747	2.582749	-0.708627
C	-3.395928	3.994456	-0.736027
C	-3.853989	4.406827	0.538903
C	-3.956432	3.257461	1.361456
Sm	-1.240171	3.547830	0.912188
C	0.846830	1.849700	0.319074
C	1.449822	2.909261	1.048310
C	1.403014	4.074870	0.243802
C	0.755092	3.743808	-0.971023
C	0.418796	2.363758	-0.926749
C	-1.037199	5.854458	1.929633
C	-0.989885	5.382581	3.286776
C	-2.196337	5.743425	4.146949
Si	-1.106985	3.002016	3.776405
H	-1.239540	1.863938	2.728806
H	-4.320175	3.231929	2.382150
H	-3.584716	1.097504	0.918532
H	-2.932284	1.960844	-1.542614
H	-3.248214	4.634447	-1.598724
H	-4.111673	5.419368	0.823347
H	-0.052991	1.798355	-1.721446
H	0.757367	0.821037	0.648597
H	1.920406	2.821953	2.020773
H	1.818410	5.042005	0.498078
H	0.594019	4.410664	-1.810678
H	-3.137409	5.506141	3.644101
H	-2.174780	6.828014	4.322067
H	-2.197340	5.251012	5.124714
C	0.339522	5.587790	4.005293
H	-1.938547	6.390438	1.635693
H	-0.115419	6.276691	1.531987
H	-2.274489	2.759542	4.685543
H	0.120788	2.611393	4.543473
H	0.388782	5.092506	4.980407
H	1.183243	5.240838	3.403173
H	0.469904	6.665716	4.174241

E = -584.623587715
G = -584.373123

$Cp_2SmCH_2C(CH_3)_2SiH_3$

C	-3.663437	2.426510	0.001622
C	-3.251075	3.195696	-1.112011
C	-3.274395	4.562786	-0.733149
C	-3.722838	4.639690	0.611092
C	-3.957650	3.320190	1.065940
Sm	-1.210343	3.491966	0.717988
C	0.949496	1.775280	0.509937
C	1.523564	3.071607	0.549891
C	1.169380	3.741654	-0.645131
C	0.379741	2.859201	-1.428561
C	0.246925	1.642154	-0.714447
C	-0.604733	5.317825	2.357792
C	-0.953787	5.137481	3.857656
C	-2.448635	5.375010	4.109260
Si	-0.560970	3.303811	4.148664
H	-1.263696	2.499032	3.047467
H	-4.341406	3.040642	2.040639
H	-3.782339	1.348851	0.022160
H	-2.983947	2.809567	-2.088273
H	-3.047751	5.405420	-1.377369
H	-3.878417	5.547711	1.179271
H	-0.272990	0.755940	-1.059928
H	1.069122	1.004229	1.262889
H	2.140544	3.471392	1.344573
H	1.477587	4.742093	-0.928030
H	-0.012088	3.062843	-2.418201
H	-3.078711	4.723223	3.494733
H	-2.704895	6.411389	3.847973
H	-2.723866	5.222058	5.159517
C	-0.132054	6.047859	4.784067
H	-1.051419	6.269809	2.014188
H	0.483883	5.464603	2.270952
H	-1.055691	2.661156	5.412666
H	0.891703	2.982794	3.996486
H	-0.366672	5.895685	5.846463
H	0.944343	5.893943	4.650081
H	-0.342237	7.099425	4.545268

E = -584.641272610
G = -584.391054

Cp_2SmSiH_3 + isobutylene : 2,1 insertion

Cp_2SmSiH_3 + isobutylene → $Cp_2Sm\ C(CH_3)_2CH_2SiH_3$

Transition state

C	0.510551	2.895687	-1.132169
C	0.416802	1.718599	-0.344058
C	1.045355	1.973638	0.898170
C	1.526949	3.307406	0.882732
C	1.203153	3.874619	-0.375079
Sm	-1.238711	3.539103	0.871140
C	-3.683874	2.455340	1.611933
C	-3.198598	1.664542	0.540413
C	-3.236045	2.452787	-0.638661
C	-3.747956	3.730598	-0.293307
C	-4.023130	3.730821	1.094376
C	-1.094220	6.117858	1.507313
C	0.276490	6.725561	1.267630
C	-1.374700	5.671047	2.824524
Si	-1.019452	3.519555	3.783150
H	-2.411528	5.700925	3.157595
H	-1.016249	2.055689	3.311047
H	-3.819422	2.126256	2.635216
H	-2.885548	0.628964	0.603901
H	-2.966706	2.121897	-1.634798
H	-3.929146	4.549391	-0.980123
H	-4.461301	4.544805	1.659026
H	0.164873	3.006319	-2.153836
H	-0.030649	0.780909	-0.651224
H	1.160618	1.265726	1.710340
H	2.089890	3.786379	1.674891
H	1.476556	4.865206	-0.715598
H	-0.670943	5.937715	3.616697
C	-2.198946	6.784244	0.702815
H	-2.104281	3.602283	4.812561
H	0.285500	3.693944	4.501546
H	0.318239	7.753969	1.663367
H	1.076904	6.159859	1.755030
H	0.520045	6.793854	0.202133
H	-2.184890	7.874952	0.865190
H	-2.084680	6.642642	-0.381036
H	-3.195155	6.430479	0.979764

E = -584.615669398
G = -584.366182

$Cp_2Sm\ C(CH_3)_2CH_2SiH_3$

C	0.276592	2.956486	-1.527223
C	0.391965	1.746732	-0.796295
C	1.174859	2.004594	0.355153
C	1.556443	3.371909	0.329342
C	1.004681	3.958930	-0.832182
Sm	-1.189271	3.399187	0.740324
C	-3.708142	2.685520	1.674707
C	-3.256294	1.569896	0.919973
C	-3.212313	1.953263	-0.441103
C	-3.620302	3.309054	-0.528335
C	-3.938667	3.756757	0.779720
C	-1.098566	5.766786	1.686521
C	0.333944	6.251712	1.931852
C	-1.806557	5.645947	3.056499
Si	-1.116520	4.248138	4.126366
H	-2.880842	5.451503	2.937938
H	-0.773160	3.066826	3.212737
H	-3.896597	2.694879	2.742343
H	-3.029743	0.584386	1.311678
H	-2.931080	1.318912	-1.273049
H	-3.728639	3.883482	-1.441660
H	-4.325453	4.733720	1.039774
H	-0.226066	3.077849	-2.480141
H	-0.027486	0.788984	-1.080525
H	1.475292	1.273581	1.097971
H	2.183967	3.872748	1.056155
H	1.138327	4.985803	-1.150807
H	-1.736580	6.583212	3.646696
C	-1.819768	6.826582	0.850184
H	-2.079018	3.678612	5.119477
H	0.169977	4.541175	4.824663
H	0.351430	7.213876	2.481078
H	0.937618	5.550129	2.525679
H	0.877140	6.415318	0.993901
H	-1.807247	7.820554	1.338616
H	-1.345089	6.960004	-0.131952
H	-2.872903	6.578458	0.669335

E = -584.637527876
G = -584.387283

Cp_2SmSiH_3 + isobutylene : allylic activation

Cp_2SmSiH_3 + isobutylene → Cp_2SmCH_2-C(CH_3)=CH_2 + SiH_4

Transition state

C	-0.810972	-0.111482	-6.488779
C	0.388429	0.519626	-6.900227
C	0.448514	1.794605	-6.281766
C	-0.716309	1.950892	-5.489693
C	-1.492602	0.772090	-5.613327
Sm	0.720333	0.017742	-4.181986
C	0.461209	1.623364	-1.984830
C	1.536554	0.768115	-1.637984
C	1.022597	-0.540063	-1.474553
C	-0.377121	-0.494199	-1.708318
C	-0.723826	0.842288	-2.021835
Si	-0.530435	-2.869267	-4.274830
C	2.556744	-1.883987	-4.987378
C	3.371211	-0.882486	-4.343938
C	3.369778	0.438538	-4.745436
H	1.107595	0.118980	-7.605379
H	1.222826	2.539312	-6.424981
H	-0.980743	2.829959	-4.913917
H	-2.454908	0.590171	-5.149876
H	-1.171430	-1.076461	-6.825157
H	1.583996	-1.415577	-1.171703
H	2.566697	1.071914	-1.499362
H	0.524950	2.693496	-2.144457
H	-1.722833	1.210139	-2.221982
H	-1.067718	-1.322038	-1.603357
H	2.818093	-2.917569	-4.763526
H	2.367514	-1.731484	-6.052294
H	1.089471	-2.146167	-4.530969
C	4.151431	-1.300124	-3.121674
H	3.965790	1.178617	-4.221391
H	3.019962	0.712376	-5.738803
H	-1.932108	-2.353210	-4.103614
H	-0.273556	-3.799931	-3.125007
H	-0.553365	-3.716669	-5.515202
H	5.064049	-1.814896	-3.446277
H	4.450614	-0.446144	-2.509454
H	3.592035	-2.003232	-2.498210

E = -584.618340519
G = -584.371286

$Cp_2SmCH_2C(CH_3)_2SiH_3$

C	-3.663437	2.426510	0.001622
C	-3.251075	3.195696	-1.112011
C	-3.274395	4.562786	-0.733149
C	-3.722838	4.639690	0.611092
C	-3.957650	3.320190	1.065940
Sm	-1.210343	3.491966	0.717988
C	0.949496	1.775280	0.509937
C	1.523564	3.071607	0.549891
C	1.169380	3.741654	-0.645131
C	0.379741	2.859201	-1.428561
C	0.246925	1.642154	-0.714447
C	-0.604733	5.317825	2.357792
C	-0.953787	5.137481	3.857656
C	-2.448635	5.375010	4.109260
Si	-0.560970	3.303811	4.148664
H	-1.263696	2.499032	3.047467
H	-4.341406	3.040642	2.040639
H	-3.782339	1.348851	0.022160
H	-2.983947	2.809567	-2.088273
H	-3.047751	5.405420	-1.377369
H	-3.878417	5.547711	1.179271
H	-0.272990	0.755940	-1.059928
H	1.069122	1.004229	1.262889
H	2.140544	3.471392	1.344573
H	1.477587	4.742093	-0.928030
H	-0.012088	3.062843	-2.418201
H	-3.078711	4.723223	3.494733
H	-2.704895	6.411389	3.847973
H	-2.723866	5.222058	5.159517
C	-0.132054	6.047859	4.784067
H	-1.051419	6.269809	2.014188
H	0.483883	5.464603	2.270952
H	-1.055691	2.661156	5.412666
H	0.891703	2.982794	3.996486
H	-0.366672	5.895685	5.846463
H	0.944343	5.893943	4.650081
H	-0.342237	7.099425	4.545268

E = -584.641272610
G = -584.391054

$Cp_2SmCH_2C(CH_3)_2SiH_3$ + isobutylene : allylic activation

$Cp_2SmCH_2C(CH_3)_2SiH_3$ + isobutylene → $Cp_2SmCH(C_3H_7)$-$CH{=}CH_2$ + $SiH_3C(CH_3)_3$

Transition state

C	-0.367466	0.732978	-1.719446
C	0.946835	1.253878	-1.714851
C	1.850308	0.167104	-1.581882
C	1.091314	-1.023945	-1.502324
C	-0.280506	-0.676899	-1.598809
Sm	0.734310	-0.193912	-4.095512
C	2.025854	-2.557964	-4.665327
C	1.987610	-1.893431	-5.916399
C	0.641362	-1.838974	-6.345153
C	-0.156301	-2.482288	-5.363984
C	0.699161	-2.933194	-4.331777
C	-1.648444	0.590419	-5.033277
C	-2.734010	1.649821	-5.333841
Si	-2.795417	3.034109	-4.012878
C	-4.123379	0.976775	-5.335683
C	0.784871	2.310777	-5.250376
C	2.076414	1.746266	-5.658735
C	3.024602	1.357694	-4.753212
C	-2.520737	2.284871	-6.718706
H	1.212975	2.303824	-1.754321
H	2.929509	0.236809	-1.508449
H	1.488671	-2.022256	-1.367048
H	-1.116760	-1.364154	-1.539551
H	-1.280799	1.310552	-1.779136
H	0.283880	-1.419565	-7.278115
H	2.845153	-1.514709	-6.458566
H	2.916511	-2.784742	-4.091009
H	0.395688	-3.489750	-3.453580
H	-1.228649	-2.629847	-5.411400
H	-1.638128	-0.099297	-5.892632
H	-2.006340	-0.007637	-4.176623
H	0.350802	2.962898	-6.009586
H	0.824610	2.840723	-4.294839
H	-0.292970	1.496567	-5.149333
H	-4.928169	1.687205	-5.565943
H	-4.153826	0.184909	-6.096789
H	-4.351122	0.511806	-4.369926
C	2.273301	1.497940	-7.131985
H	3.946258	0.882735	-5.074100
H	2.973741	1.678397	-3.715303
H	-3.858279	4.032357	-4.363412
H	-3.137572	2.475630	-2.665161
H	-1.502955	3.779971	-3.888041
H	2.363241	2.460556	-7.649818
H	3.175833	0.917563	-7.336188
H	1.414106	0.980947	-7.572201
H	-3.326311	2.985008	-6.968510
H	-1.576638	2.830123	-6.800736
H	-2.516421	1.502380	-7.490867

E = -741.797843065

G = -741.446588

$SiH_3C(CH_3)_3$ ('branched' hydrosilylation product)

C	2.528566	-1.299506	0.413016
C	1.808286	-0.100652	-0.222948
C	2.510861	1.203871	0.183910
Si	-0.004003	-0.056779	0.396503
H	-0.050334	0.080422	1.887590
H	-0.741182	1.100843	-0.203920
H	-0.722849	-1.316114	0.020209
C	1.815227	-0.240580	-1.752894
H	3.571956	-1.342196	0.070888
H	2.544715	-1.232582	1.506766
H	2.055731	-2.250368	0.142475
H	3.553637	1.199163	-0.162740
H	2.024027	2.083123	-0.252961
H	2.527540	1.336154	1.271673
H	2.847663	-0.268480	-2.128091
H	1.322408	-1.162869	-2.080871
H	1.311328	0.600597	-2.242287

E = -163.504475661
G = -163.389287

$Cp_2SmCH_2(CH_2)_4CH_3 + SiH_4$: Si(α)-H(β) activation

$Cp_2SmCH_2CH(C_4H_9)SiH_3 + SiH_4 \rightarrow Cp_2SmSiH_3 + SiH_3C(CH_3)_3$

Transition state

C	3.082409	-1.428285	-1.891277
C	2.030423	-2.241604	-2.389245
C	0.970264	-1.393309	-2.788068
C	1.362474	-0.052995	-2.535538
C	2.669303	-0.074988	-1.985101
Sm	1.091573	-1.165867	-0.027766
C	-0.959204	-2.645579	0.016867
C	-2.385367	-3.005831	0.445698
C	-2.660136	-2.561609	1.889429
C	1.163467	0.148847	2.388651
C	2.464311	0.282554	1.837184
C	3.075755	-0.996754	1.843138
C	2.149645	-1.921371	2.391999
C	0.970114	-1.212722	2.731868
Si	-2.552755	-4.916961	0.342575
Si	-1.316052	0.825601	-0.174688
H	-2.200762	1.150544	0.988868
H	-2.116763	0.996258	-1.428088
H	-0.248399	1.889345	-0.202774
H	-1.083091	-0.882850	-0.034778
H	2.332249	-2.976246	2.565633
H	4.085774	-1.221283	1.520874
H	2.926646	1.207181	1.511566
H	0.463068	0.956038	2.567819
H	0.088173	-1.629636	3.200940
H	0.788504	0.833824	-2.777311
H	3.263405	0.791431	-1.718779
H	4.049073	-1.777170	-1.547044
H	2.052887	-3.321731	-2.484395
H	0.036541	-1.707056	-3.238884
H	-0.241312	-3.203792	0.664470
H	-0.785233	-2.977369	-1.019947
C	-3.415200	-2.377307	-0.505403
H	-3.920384	-5.394301	0.739139
H	-2.286388	-5.381844	-1.056425
H	-1.553000	-5.565321	1.251683
H	-3.677952	-2.819314	2.204399
H	-1.966774	-3.030741	2.597013
H	-2.548343	-1.473960	1.986665
H	-4.437065	-2.674594	-0.243680
H	-3.376510	-1.281024	-0.459918
H	-3.237606	-2.668413	-1.546907

E = -590.911769307
G = -590.635600

$Cp_2SmCH_2(CH_2)_4CH_3 + SiH_4$: Si(β)-H(α) activation

$Cp_2SmCH_2CH(C_4H_9)SiH_3 + SiH_4 \rightarrow Cp_2H + SiH_3CH_2C(CH_3)_2SiH_3$

Transition state

C	-1.668409	-2.176863	1.760093
C	-0.890902	-1.099240	1.269342
C	-1.308317	-0.824029	-0.058982
C	-2.352682	-1.729269	-0.383847
C	-2.572418	-2.565946	0.737518
Sm	-0.108610	-3.262878	-0.229792
C	-0.557590	-3.718372	-2.872531
C	0.415548	-2.685887	-2.840328
C	1.627500	-3.243968	-2.359466
C	1.403826	-4.620238	-2.098844
C	0.055025	-4.913473	-2.417083
Si	-0.262658	-5.579048	1.944660
C	1.431751	-4.204779	1.655853
C	2.598677	-4.644375	2.572222
C	3.588272	-3.462248	2.684139
Si	2.152168	-5.094147	4.402109
H	-1.674575	-6.143616	2.139685
H	0.533245	-6.813968	1.671374
H	-0.123279	-5.098577	3.382526
H	-2.906717	-1.752168	-1.314540
H	-3.316392	-3.349706	0.815733
H	-1.611599	-2.606221	2.753480
H	-0.138317	-0.551114	1.825433
H	-0.937262	-0.026145	-0.691901
H	2.142625	-5.332501	-1.751412
H	-0.417104	-5.885851	-2.349308
H	-1.576581	-3.621585	-3.228062
H	0.270396	-1.663638	-3.169325
H	2.572017	-2.720610	-2.257884
H	-0.862741	-5.127268	0.471496
H	3.939294	-3.163463	1.686121
H	3.126545	-2.583595	3.150274
H	4.470472	-3.728845	3.277069
C	3.350518	-5.840612	1.963065
H	1.147056	-3.186050	1.991705
H	1.935799	-4.122624	0.662585
H	1.321275	-4.044306	5.069189
H	1.556956	-6.445940	4.613838
H	3.483574	-5.107523	5.102447
H	4.196029	-6.139392	2.593277
H	2.705966	-6.712608	1.829800
H	3.760869	-5.572064	0.978624

E = -590.907554219
G = -590.624990

$SiH_3CH_2C(CH_3)_2SiH_3$

C	1.778078	-0.026961	-0.171932
Si	-0.062315	-0.198556	0.315252
C	2.539423	1.266587	0.204192
C	2.560518	1.477832	1.725626
Si	4.347667	1.065581	-0.408002
H	-0.268262	-0.174830	1.796438
H	-0.923871	0.864480	-0.288708
H	-0.544349	-1.521521	-0.192315
H	2.279263	-0.901569	0.266850
H	1.812902	-0.181666	-1.259610
C	1.923684	2.493436	-0.485187
H	5.162158	2.281080	-0.084882
H	4.988625	-0.120319	0.244745
H	4.376811	0.858269	-1.891188
H	3.158533	2.354252	1.999876
H	1.546627	1.642854	2.113721
H	2.975533	0.611434	2.252942
H	2.500888	3.401282	-0.276505
H	1.877217	2.369302	-1.573015
H	0.899831	2.670325	-0.130791

E = -168.596960679
G = -168.471076

$Cp_2SmC(CH_3)_2CH_2SiH_3$

C	0.276592	2.956486	-1.527223
C	0.391965	1.746732	-0.796295
C	1.174859	2.004594	0.355153
C	1.556443	3.371909	0.329342
C	1.004681	3.958930	-0.832182
Sm	-1.189271	3.399187	0.740324
C	-3.708142	2.685520	1.674707
C	-3.256294	1.569896	0.919973
C	-3.212313	1.953263	-0.441103
C	-3.620302	3.309054	-0.528335
C	-3.938667	3.756757	0.779720
C	-1.098566	5.766786	1.686521
C	0.333944	6.251712	1.931852
C	-1.806557	5.645947	3.056499
Si	-1.116520	4.248138	4.126366
H	-2.880842	5.451503	2.937938
H	-0.773160	3.066826	3.212737
H	-3.896597	2.694879	2.742343
H	-3.029743	0.584386	1.311678
H	-2.931080	1.318912	-1.273049
H	-3.728639	3.883482	-1.441660
H	-4.325453	4.733720	1.039774
H	-0.226066	3.077849	-2.480141
H	-0.027486	0.788984	-1.080525
H	1.475292	1.273581	1.097971
H	2.183967	3.872748	1.056155
H	1.138327	4.985803	-1.150807
H	-1.736580	6.583212	3.646696
C	-1.819768	6.826582	0.850184
H	-2.079018	3.678612	5.119477
H	0.169977	4.541175	4.824663
H	0.351430	7.213876	2.481078
H	0.937618	5.550129	2.525679
H	0.877140	6.415318	0.993901
H	-1.807247	7.820554	1.338616
H	-1.345089	6.960004	-0.131952
H	-2.872903	6.578458	0.669335

E = -584.637527876
G = -584.387283

$Cp_2Sm\ C(CH_3)_2CH_2SiH_3 + SiH_4$: Si(α)-H(β) activation

$Cp_2Sm\ CH(C_4H_9)CH_2SiH_3 + SiH_4 \rightarrow Cp_2SmSiH_3 + SiH_3CH_2CH(CH_3)_2$

Transition state

C	3.239949	3.964625	3.535663
C	4.605445	3.677517	3.280156
C	5.195283	3.249428	4.499588
C	4.195696	3.256351	5.497994
C	2.982941	3.695456	4.902160
Sm	3.434376	1.242723	3.745640
C	4.834823	-0.596538	5.085617
C	5.703037	-0.434176	3.839704
C	2.284687	1.299396	1.260678
C	3.057929	0.111578	1.262786
C	2.450603	-0.804738	2.159452
C	1.305569	-0.182033	2.714169
C	1.205441	1.121613	2.162804
C	4.382168	-2.049958	5.261238
Si	5.710999	-3.390042	5.585857
Si	1.766272	0.363552	6.273467
H	3.672134	-2.127709	6.098240
H	2.129415	0.819089	7.653069
H	1.087241	-0.965477	6.393015
H	0.722744	1.322557	5.771304
H	3.274623	0.009472	5.514918
H	2.041262	3.848981	5.415536
H	4.334137	3.005431	6.542570
H	6.239876	2.999392	4.644949
H	5.122146	3.824980	2.338534
H	2.524025	4.343642	2.816266
H	0.600773	-0.638871	3.398750
H	0.417542	1.838389	2.363012
H	2.470045	2.178527	0.655064
H	3.929432	-0.079499	0.646603
H	2.772300	-1.822060	2.345562
C	5.561743	-0.077510	6.322269
H	3.823002	-2.390088	4.379860
H	5.059335	-4.738172	5.548088
H	6.785115	-3.374521	4.541706
H	6.371461	-3.245550	6.920539
H	5.375751	-1.070999	3.010741
H	5.774230	0.610007	3.440562
H	6.761506	-0.667452	4.027973
H	5.895015	0.958109	6.200457
H	4.919154	-0.108352	7.210590
H	6.457511	-0.676215	6.554434

E = -590.912772364
G = -590.635610