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 (hydride complex)

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

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

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 + propene : 1,2 insertion

Cp_2SmH + propene → $Cp_2SmCH_2CH_2CH_3$

Adduct of propene on Cp_2SmH

C	2.591307	3.340037	-0.838827
C	2.987296	3.928965	0.386317
C	1.912384	4.729113	0.854666
C	0.854010	4.638534	-0.081398
C	1.270112	3.772442	-1.124486
Sm	0.990098	2.124591	1.030419
C	0.659288	-0.536691	1.730788
C	1.875041	-0.495729	0.997890
C	1.562508	-0.179551	-0.346458
C	0.155985	-0.017992	-0.441743
C	-0.403202	-0.247746	0.840559
H	-0.928802	2.705015	1.601540
C	0.743322	2.482127	4.161658
C	2.035367	2.303814	3.835543
C	0.117401	3.779715	4.551920
H	1.913588	5.337776	1.751632
H	-0.100248	5.144274	-0.014855
H	0.696428	3.521337	-2.009388
H	3.202715	2.702555	-1.466365
H	3.959863	3.826111	0.855557
H	2.269165	-0.107824	-1.164553
H	-0.399319	0.201030	-1.346680
H	-1.455069	-0.213776	1.091523
H	0.555537	-0.798754	2.777997
H	2.863645	-0.720670	1.383626
H	0.830599	4.607310	4.512509
H	-0.279088	3.710714	5.572403
H	-0.726159	3.998463	3.888925
H	0.080999	1.614955	4.164058
H	2.742706	3.130247	3.846605
H	2.434596	1.309789	3.635917

E = -540.217940584
G = -540.013679

Transition state

C	2.335456	3.403161	-0.987212
C	3.098020	3.827942	0.128885
C	2.256225	4.610001	0.962026
C	0.973404	4.666173	0.363054
C	1.020914	3.914392	-0.838677
Sm	1.257175	2.033596	1.136292
C	0.809077	-0.640778	1.721732
C	2.019555	-0.621799	0.982803
C	1.716489	-0.229261	-0.344503
C	0.317423	-0.002581	-0.423819
C	-0.243637	-0.263338	0.852204
H	-0.497774	2.564230	2.130664
C	0.406400	2.565611	3.927497
C	1.736175	2.263122	3.787254
C	-0.093225	3.942956	4.255681
H	2.557278	5.118751	1.870481
H	0.114727	5.205097	0.742600
H	0.206154	3.789606	-1.542934
H	2.700495	2.817343	-1.822513
H	4.153231	3.634144	0.289221
H	2.421577	-0.154240	-1.163956
H	-0.231451	0.275436	-1.316412
H	-1.293043	-0.204539	1.111554
H	0.700059	-0.936404	2.758822
H	2.999147	-0.903564	1.354162
H	0.555239	4.716394	3.835485
H	-0.094278	4.066713	5.347194
H	-1.108880	4.102524	3.890238
H	-0.288846	1.751459	4.117004
H	2.487047	3.051734	3.800518
H	2.085589	1.236989	3.888197

E = -540.215011257
G = -540.007831

$Cp_2SmCH_2CH_2CH_3$ (propyl complex)

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

Cp_2SmH + propene : 2,1 insertion

Cp_2SmH + propene → $Cp_2SmCH(CH_3)_2$

Adduct of propene on Cp_2SmH

C	1.747280	3.110031	-1.746594
C	2.861873	3.525544	-0.980285
C	2.405975	4.442810	0.002279
C	1.006538	4.591056	-0.154027
C	0.598207	3.762767	-1.232645
Sm	1.283245	2.016751	0.738891
C	-1.345149	1.389710	1.108364
C	-1.113658	2.480356	1.987124
C	-0.270382	2.028202	3.029552
C	0.012602	0.655113	2.798142
C	-0.655999	0.259807	1.614571
C	3.533877	0.866946	2.719475
C	4.045119	1.498914	1.649354
H	4.031608	1.027498	0.665991
H	1.705001	0.309934	-0.376456
H	0.587338	0.004326	3.446712
H	-0.646932	-0.729177	1.176195
H	-1.972963	1.406687	0.224931
H	-1.533870	3.474529	1.893363
H	0.054898	2.615256	3.881718
H	0.367302	5.252098	0.419118
H	-0.408927	3.681304	-1.624858
H	1.771322	2.419111	-2.579050
H	3.889675	3.223892	-1.144945
H	3.025589	4.977282	0.714462
H	4.550280	2.458423	1.740587
H	3.083647	-0.115380	2.566937
C	3.592838	1.366449	4.128527
H	4.214800	0.695989	4.734271
H	4.019287	2.371656	4.187250
H	2.601329	1.376365	4.593496

E = -540.217437344
G = -540.011683

Transition state

C	2.193203	3.255490	-1.181829
C	3.066066	3.806452	-0.210747
C	2.307840	4.663161	0.627037
C	0.963826	4.635546	0.181727
C	0.893505	3.763199	-0.937010
Sm	1.366231	2.111112	1.187661
C	-1.254702	1.396112	0.993113
C	-1.214627	2.304601	2.080857
C	-0.531409	1.675222	3.151121
C	-0.157020	0.374227	2.725855
C	-0.603440	0.200668	1.392575
C	3.316210	0.843916	2.534910
C	3.582171	0.342534	1.283519
H	3.447684	-0.712564	1.078645
H	2.174004	0.569510	0.051522
H	0.337184	-0.376021	3.331229
H	-0.492421	-0.694479	0.794018
H	-1.734731	1.569433	0.037103
H	-1.659292	3.292573	2.101682
H	-0.374185	2.093801	4.139297
H	0.144021	5.212198	0.593359
H	0.007723	3.554323	-1.525375
H	2.473679	2.583700	-1.982609
H	4.137004	3.647534	-0.158415
H	2.694627	5.269936	1.438441
H	4.239644	0.871183	0.596927
H	2.807058	0.196870	3.246145
C	3.694739	2.205113	3.037267
H	4.108214	2.153193	4.050242
H	4.422880	2.703409	2.390790
H	2.836000	2.918600	3.150922

E = -540.212122322
G = -540.003145

$Cp_2SmCH(CH_3)_2$

C	2.153006	3.201317	-1.121562
C	3.040630	3.761565	-0.167516
C	2.298097	4.652586	0.645505
C	0.954155	4.647417	0.194224
C	0.865695	3.751363	-0.902295
Sm	1.329252	2.124877	1.307295
C	-1.283833	1.366409	1.017500
C	-1.293365	2.342266	2.043195
C	-0.644913	1.789875	3.179415
C	-0.242760	0.468755	2.857296
C	-0.629903	0.209977	1.519017
C	3.131612	0.857438	2.326843
C	3.624538	0.431463	0.975093
H	3.834522	-0.641553	0.917208
H	2.873239	0.580834	0.126818
H	0.248108	-0.228130	3.523873
H	-0.494600	-0.725713	0.987779
H	-1.730864	1.471137	0.035813
H	-1.747608	3.324092	1.982334
H	-0.527410	2.273449	4.143009
H	0.147113	5.254177	0.587829
H	-0.022124	3.550640	-1.490445
H	2.423330	2.516218	-1.917264
H	4.106347	3.578552	-0.104231
H	2.697206	5.269930	1.442394
H	4.510308	0.976069	0.622962
H	2.920546	0.035417	3.005789
C	3.641475	2.097934	2.997210
H	3.853940	1.950892	4.061066
H	4.529088	2.539200	2.525257
H	2.898385	2.968136	3.015199

E = -540.232819484
G = -540.021196

Cp_2SmH + propene : allylic activation

Cp_2SmH + propene → Cp_2SmCH_2-CH=CH_2 + H_2

Adduct of propene on Cp_2SmH

C	0.661625	-0.581834	-1.600776
C	-0.732105	-0.823859	-1.662565
C	-1.365355	0.373236	-2.085667
C	-0.364906	1.360286	-2.272269
C	0.887429	0.768365	-1.978849
Sm	0.003192	-0.490052	-4.285043
C	-0.054436	-3.019702	-5.402539
C	-1.254711	-2.899845	-4.661122
C	-2.072633	-1.936304	-5.306534
C	-1.382763	-1.469464	-6.454286
C	-0.134003	-2.134487	-6.509451
H	-0.305287	1.261827	-5.373717
C	2.640032	1.038846	-6.851920
C	2.712184	0.709502	-5.397959
C	2.936235	-0.511963	-4.882554
H	1.845985	1.275445	-1.986838
H	1.414491	-1.289017	-1.269433
H	-1.229799	-1.749543	-1.399414
H	-2.432639	0.520245	-2.206172
H	-0.531159	2.384480	-2.578819
H	0.611467	-2.017564	-7.287713
H	0.758977	-3.704348	-5.187463
H	-1.517416	-3.469786	-3.777925
H	-3.070208	-1.641795	-5.000947
H	-1.748296	-0.740196	-7.165184
H	1.681608	1.518759	-7.075643
H	3.099239	-1.376680	-5.522083
H	3.050600	-0.658453	-3.808861
H	2.586174	1.549793	-4.713434
H	3.431643	1.752102	-7.112681
H	2.752726	0.150913	-7.479529

E = -540.217923630
G = -540.014341

Transition state

C	1.034625	0.021193	-1.865953
C	-0.188974	-0.686763	-1.791306
C	-1.219200	0.169824	-2.265430
C	-0.629447	1.403872	-2.630657
C	0.765078	1.309417	-2.392572
Sm	0.240009	-0.437600	-4.478721
C	-0.087347	-2.949149	-5.586956
C	-1.220753	-2.741561	-4.763522
C	-2.010876	-1.722261	-5.355431
C	-1.368018	-1.304463	-6.546895
C	-0.176327	-2.057469	-6.687213
H	-0.209039	1.334051	-5.609956
C	2.191749	0.878160	-6.017482
C	2.901618	0.153314	-4.976326
C	2.951798	-1.203612	-4.826029
H	1.487121	2.104076	-2.540132
H	2.002171	-0.349107	-1.547841
H	-0.323888	-1.686975	-1.396301
H	-2.276195	-0.065648	-2.300099
H	-1.152237	2.272934	-3.009594
H	0.516916	-1.999509	-7.518681
H	0.685845	-3.691514	-5.426037
H	-1.462210	-3.291700	-3.861637
H	-2.958983	-1.353678	-4.981929
H	-1.734312	-0.554932	-7.237057
H	0.870043	1.224128	-5.805592
H	2.647294	-1.873384	-5.627736
H	3.467161	-1.651274	-3.982852
H	3.312045	0.756420	-4.165233
H	2.533983	1.904444	-6.155967
H	2.122611	0.351315	-6.973205

E = -540.206888511
G = -540.000399

Adduct of H_2 on Cp_2SmCH_2–CH=CH_2

C	1.137548	0.170318	-1.925403
C	0.015015	-0.685229	-1.796871
C	-1.128845	0.021956	-2.250570
C	-0.709238	1.307276	-2.670123
C	0.694169	1.398510	-2.471972
Sm	0.348811	-0.452435	-4.502358
C	-0.128096	-2.927513	-5.639315
C	-1.251882	-2.658418	-4.819136
C	-1.984115	-1.597833	-5.411610
C	-1.312625	-1.216105	-6.600374
C	-0.164156	-2.032703	-6.738971
H	-0.620546	1.580821	-5.626932
C	2.361368	0.714135	-5.944971
C	2.997409	0.021229	-4.909654
C	2.869321	-1.343528	-4.642364
H	1.308088	2.270763	-2.662952
H	2.153163	-0.069421	-1.636093
H	0.020734	-1.685242	-1.378654
H	-2.147496	-0.346512	-2.247483
H	-1.354694	2.100368	-3.030309
H	0.537958	-2.008887	-7.564161
H	0.605235	-3.708061	-5.475935
H	-1.525717	-3.194899	-3.918218
H	-2.916988	-1.185156	-5.045697
H	-1.642534	-0.458614	-7.302277
H	0.115127	1.618846	-5.823811
H	2.640034	-2.028521	-5.457981
H	3.386351	-1.778552	-3.793277
H	3.448076	0.632521	-4.124923
H	2.536054	1.779482	-6.061606
H	2.094762	0.180928	-6.858937

E = -540.222897155
G = -540.016555

Cp_2SmCH_2-CH=CH_2 (π-allylic complex)

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

H_2

E = -1.17751649843
G = -1.178858

Cp_2SmH + propene : vinylic activation

Cp_2SmH + propene → $Cp_2SmCH{=}CH{-}CH_3$ + H_2

Adduct of propene on Cp_2SmH

C	2.780107	-0.088350	-5.772654
C	2.721402	-1.013512	-4.697208
C	1.565159	-1.811590	-4.870668
C	0.913240	-1.383250	-6.056816
C	1.660687	-0.312663	-6.609369
Sm	3.198372	-2.575917	-6.933566
C	4.065284	-5.064400	-7.816892
C	3.779895	-5.240593	-6.436800
C	2.382335	-5.107189	-6.260388
C	1.805173	-4.843005	-7.530670
C	2.845356	-4.824364	-8.493122
C	5.848552	-1.265918	-6.931949
C	6.381123	-2.439945	-7.311295
C	7.268771	-3.300872	-6.469343
H	3.209514	-1.772763	-8.853815
H	3.409758	-1.066603	-3.860476
H	1.218782	-2.586194	-4.196973
H	-0.018893	-1.775361	-6.447072
H	1.416649	0.238507	-7.507809
H	3.523860	0.688567	-5.905647
H	4.495921	-5.487757	-5.660257
H	1.843700	-5.223315	-5.327665
H	0.747835	-4.721052	-7.735704
H	2.727915	-4.660227	-9.555995
H	5.038823	-5.154848	-8.284309
H	5.284068	-0.658457	-7.640180
H	6.026488	-0.850793	-5.941764
H	6.201998	-2.774563	-8.334531
H	8.272404	-3.339797	-6.910481
H	7.360841	-2.918675	-5.448874
H	6.906853	-4.333492	-6.428368

E = -540.217401484
G = -540.011948

Transition state

C	2.759952	-0.185230	-5.604109
C	2.387488	-1.126078	-4.612072
C	1.210213	-1.784884	-5.049978
C	0.857191	-1.250963	-6.316457
C	1.813923	-0.260985	-6.656972
Sm	3.155753	-2.658811	-6.763958
C	3.694608	-4.938828	-8.237583
C	3.757027	-5.355254	-6.887859
C	2.449108	-5.274865	-6.340851
C	1.576530	-4.821312	-7.363662
C	2.346565	-4.604836	-8.532985
C	5.597189	-1.931084	-6.771385
C	6.599021	-2.826192	-6.880573
C	7.961872	-2.725886	-6.259074
H	3.948145	-1.643949	-8.590450
H	2.891585	-1.286100	-3.665137
H	0.654055	-2.533120	-4.497219
H	-0.015201	-1.521761	-6.899941
H	1.807567	0.351241	-7.550766
H	3.603151	0.492727	-5.555381
H	4.643340	-5.700293	-6.368035
H	2.156721	-5.570252	-5.339456
H	0.504944	-4.688364	-7.272364
H	1.968492	-4.284106	-9.496819
H	4.522470	-4.903145	-8.935626
H	4.683528	-1.700547	-7.996198
H	5.838007	-1.026534	-6.196804
H	6.447791	-3.721875	-7.491422
H	8.742731	-2.722335	-7.031285
H	8.065096	-1.815828	-5.660972
H	8.170016	-3.589601	-5.614612

E = -540.186750970
G = -539.983866

Adduct of H_2 on $Cp_2SmCH{=}CH{-}CH_3$

C	2.677771	-0.109192	-5.779108
C	2.531219	-0.946015	-4.649525
C	1.372036	-1.744764	-4.839300
C	0.796174	-1.389119	-6.085438
C	1.606021	-0.384279	-6.670193
Sm	3.157121	-2.669194	-6.703486
C	3.773920	-4.892919	-8.228105
C	3.672047	-5.369548	-6.901964
C	2.311710	-5.272447	-6.502012
C	1.571974	-4.751199	-7.593367
C	2.474948	-4.504072	-8.655846
C	5.540676	-2.190094	-6.344784
C	6.589517	-3.011657	-6.577105
C	8.036990	-2.740344	-6.270535
H	3.836620	-1.413342	-8.970712
H	3.182050	-0.961139	-3.782960
H	0.964268	-2.457169	-4.130986
H	-0.118049	-1.794446	-6.502709
H	1.408805	0.127525	-7.605923
H	3.458910	0.626581	-5.927091
H	4.486881	-5.755171	-6.300835
H	1.900613	-5.601786	-5.554297
H	0.500816	-4.588916	-7.616180
H	2.211629	-4.144233	-9.644602
H	4.678601	-4.855938	-8.823169
H	4.470349	-1.485442	-8.562321
H	5.857374	-1.238349	-5.885200
H	6.417221	-3.992265	-7.035300
H	8.652849	-2.788075	-7.179130
H	8.170228	-1.753054	-5.817155
H	8.447256	-3.492542	-5.583094

E = -540.193543471
G = -539.992504

$Cp_2SmCH=CH-CH_3$ (vinylic complex)

C	2.115312	0.775220	1.590100
C	2.049102	-0.639969	1.560367
C	0.911468	-1.039857	2.311331
C	0.274786	0.125080	2.801370
C	1.014757	1.248329	2.349774
Sm	-0.108713	0.194546	0.070413
C	0.635228	1.708243	-2.107311
C	1.476338	0.569990	-2.166649
C	0.669358	-0.555990	-2.463657
C	-0.671877	-0.108510	-2.613089
C	-0.692552	1.287418	-2.392866
C	-2.469877	-0.136989	0.628704
C	-3.523953	-0.001874	-0.208091
C	-4.978533	-0.176640	0.133577
H	0.805308	2.285438	2.589249
H	2.887589	1.386008	1.137329
H	2.769726	-1.300417	1.091267
H	0.603320	-2.061034	2.507487
H	-0.611930	0.152754	3.421937
H	-1.564889	1.927458	-2.456071
H	0.958157	2.729905	-1.939501
H	2.550516	0.563922	-2.024174
H	1.023196	-1.569945	-2.616617
H	-1.525160	-0.724830	-2.869216
H	-2.790648	-0.405022	1.649426
H	-3.352723	0.263628	-1.257793
H	-5.440788	-0.962438	-0.479424
H	-5.110976	-0.441484	1.187340
H	-5.548789	0.741247	-0.064312

E = -539.013283696
G = -538.826746

$Cp_2SmH + SiH_4$: Si-H activation (Si at α position at the TS)

$Cp_2SmH + SiH_4 \rightarrow Cp_2SmSiH_3 + H_2$

Adduct of SiH_4 on Cp_2SmH

Sm	0.181588	-0.565831	-0.005027
Si	-3.008382	-1.568852	0.030746
H	-1.760280	-2.415482	0.045656
H	0.692799	-2.572838	0.062546
H	-3.792687	-1.769552	1.277240
H	-2.524470	-0.139484	-0.012833
H	-3.811906	-1.838727	-1.190153
C	1.850971	0.221109	1.993416
C	0.962974	1.317245	1.823816
C	-0.316766	0.914236	2.273492
C	-0.220227	-0.430681	2.721187
C	1.121322	-0.855463	2.557470
C	1.851211	0.028906	-2.069767
C	1.068546	-1.048023	-2.556458
C	-0.257035	-0.577633	-2.726902
C	-0.290610	0.794651	-2.360024
C	1.012253	1.169565	-1.954534
H	2.912735	0.223456	1.774349
H	1.227478	2.300510	1.453076
H	-1.202240	1.539095	2.313966
H	-1.018685	-1.014236	3.166053
H	1.517930	-1.827459	2.818508
H	2.915323	-0.001076	-1.864693
H	1.421228	-2.049472	-2.763486
H	-1.085998	-1.151826	-3.125974
H	-1.150155	1.452653	-2.425977
H	1.323612	2.161499	-1.649228

E = -428.626541161
G = -428.468914

Transition state

Sm	0.034745	-0.381276	-0.012811
Si	-2.687303	-1.678965	0.038226
H	-1.064542	-2.336147	0.054511
H	0.143360	-2.496470	0.056799
H	-3.458539	-2.025983	1.270464
H	-2.654819	-0.145989	-0.010212
H	-3.466840	-2.103297	-1.164259
C	1.802079	0.098877	1.999532
C	1.050432	1.300195	1.883486
C	-0.268967	1.032518	2.321295
C	-0.336229	-0.332873	2.705915
C	0.947462	-0.906505	2.515517
C	1.794980	-0.022884	-2.056499
C	0.943033	-1.062367	-2.505169
C	-0.343388	-0.506763	-2.728150
C	-0.280568	0.880559	-2.431385
C	1.038905	1.180474	-2.015163
H	2.857226	-0.014364	1.778132
H	1.432494	2.261430	1.559982
H	-1.076170	1.753488	2.388122
H	-1.199485	-0.833291	3.128960
H	1.227961	-1.927093	2.742160
H	2.851272	-0.117722	-1.831849
H	1.227012	-2.094237	-2.667236
H	-1.205888	-1.036577	-3.115477
H	-1.090533	1.592984	-2.542235
H	1.417832	2.161885	-1.754527

E = -428.618648141
G = -428.459709

Adduct of H_2 on Cp_2SmSiH_3

Sm	-0.098530	-0.404265	-0.008775
Si	-2.877277	-1.162073	0.020544
H	-0.438089	-2.862393	0.065247
H	0.326000	-2.905323	0.068269
H	-3.818876	-1.077512	1.198925
H	-2.387080	0.351772	-0.023577
H	-3.820078	-1.146035	-1.159785
C	1.783132	0.196803	1.868419
C	0.858053	1.273787	1.909265
C	-0.359986	0.783433	2.444922
C	-0.195097	-0.596283	2.726036
C	1.132615	-0.956958	2.373148
C	1.767736	0.048364	-1.942037
C	1.088432	-1.119680	-2.370141
C	-0.236897	-0.754273	-2.726505
C	-0.371965	0.642446	-2.523897
C	0.862251	1.138985	-2.033001
H	2.817262	0.258670	1.550049
H	1.064798	2.300309	1.629213
H	-1.256096	1.364381	2.627740
H	-0.937136	-1.246748	3.172181
H	1.584689	-1.932481	2.512590
H	2.807207	0.108313	-1.641278
H	1.520028	-2.110318	-2.458411
H	-0.997295	-1.414905	-3.124135
H	-1.259451	1.229122	-2.729162
H	1.092181	2.175801	-1.816045

E = -428.634732542
G = -428.474322

Cp_2SmSiH_3 (silyl complex)

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

$Cp_2SmH + SiH_4$: Si-H activation (Si at β position at the TS)

$Cp_2SmH + SiH_4 \rightarrow Cp_2SmH + SiH_4$

Adduct of SiH_4 on Cp_2SmH

Sm	-0.043384	0.058836	-0.161916
C	2.700898	0.133879	-0.105135
C	2.368251	-1.239648	-0.215097
C	1.791956	-1.448483	-1.494105
C	1.778051	-0.204812	-2.179374
C	2.336912	0.773339	-1.319382
C	-2.736381	-0.426100	-0.038722
C	-2.620451	0.985697	0.015956
C	-2.149539	1.437587	-1.245064
C	-1.974984	0.304938	-2.079082
C	-2.331451	-0.847802	-1.330835
H	3.187883	0.603362	0.741533
H	2.542606	-1.997448	0.538389
H	1.465794	-2.400403	-1.898009
H	1.437756	-0.040813	-3.195031
H	2.502730	1.816668	-1.565430
H	-3.089991	-1.065825	0.760068
H	-2.887513	1.612432	0.858811
H	-1.998856	2.471337	-1.536920
H	-1.662902	0.319925	-3.116725
H	-2.339754	-1.867482	-1.699347
H	1.208157	-0.773948	3.406303
H	0.179701	1.097243	1.842879
Si	0.051194	0.109599	3.069809
H	-0.168957	-1.076814	1.612880
H	0.258765	1.276104	4.033784
H	-1.308521	-0.371069	3.460419

E = -428.631607096
G = -428.470339

Transition state

Sm	-0.050149	0.023780	-0.158877
C	2.690609	0.110732	-0.104366
C	2.365338	-1.266357	-0.193515
C	1.795720	-1.500502	-1.472018
C	1.774572	-0.268200	-2.175596
C	2.324539	0.727478	-1.328565
C	-2.760797	-0.373554	-0.054916
C	-2.597163	1.032754	0.023644
C	-2.100796	1.486457	-1.225723
C	-1.959696	0.361486	-2.077546
C	-2.362104	-0.789879	-1.351191
H	3.163811	0.597985	0.739438
H	2.550389	-2.012570	0.569698
H	1.479941	-2.461307	-1.863285
H	1.435556	-0.122177	-3.194441
H	2.480956	1.768751	-1.588718
H	-3.151619	-1.012069	0.728155
H	-2.843581	1.655283	0.875314
H	-1.908237	2.518477	-1.497967
H	-1.641488	0.382293	-3.113199
H	-2.407370	-1.801733	-1.738311
H	1.475149	-0.196557	3.245487
H	0.112526	1.109821	1.712519
Si	0.016412	0.045497	3.026368
H	-0.252671	-1.008950	1.734026
H	-0.372033	1.284420	3.811604
H	-0.748166	-0.986061	3.835946

E = -428.628963675
G = -428.468002

$Cp_2SmCH_2CH_2CH_3$ (propyl complex)

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

$Cp_2SmCH_2CH_2CH_3$ + propene : 1,2 insertion

$Cp_2SmCH_2CH_2CH_3$ + propene → $Cp_2SmCH_2CH(CH_3)CH_2CH_2CH_3$

Adduct of propene on $Cp_2SmCH_2CH_2CH_3$

C	1.371471	2.561586	1.067047
C	1.526460	3.891530	0.594103
C	0.971871	3.966422	-0.702781
C	0.468718	2.680680	-1.037271
C	0.725240	1.812667	0.053811
Sm	-1.223402	3.553087	0.942457
C	-3.176308	2.765300	2.793394
C	-2.458605	1.583752	2.480141
C	-2.737670	1.250461	1.131094
C	-3.626161	2.226654	0.614065
C	-3.896615	3.165524	1.641503
C	-0.252464	4.622851	3.559157
C	-1.000100	5.705752	3.280103
C	-0.459335	7.059415	2.951155
C	-1.974154	5.750388	0.098834
C	-2.358606	5.109906	-1.228071
C	-3.785465	5.382036	-1.706674
H	-1.642909	5.378666	-2.014734
H	0.957129	4.842934	-1.338441
H	0.019393	2.398564	-1.982621
H	0.489545	0.756056	0.096029
H	1.730068	2.173008	2.013652
H	2.013904	4.703581	1.120858
H	-2.367856	0.381622	0.599771
H	-4.058286	2.229199	-0.379826
H	-4.568813	4.011607	1.571951
H	-3.213280	3.248634	3.763522
H	-1.840623	1.009556	3.161432
H	0.622915	7.036989	2.797090
H	-0.672635	7.751717	3.775701
H	-0.935991	7.467761	2.055996
H	-2.085082	5.626296	3.359227
H	0.833148	4.662837	3.533417
H	-0.704622	3.696699	3.909050
H	-1.219818	6.531379	-0.035407
H	-2.847528	6.189258	0.595750
H	-2.270777	3.977397	-1.211038
H	-4.027830	4.838814	-2.627863
H	-3.920521	6.452016	-1.895375
H	-4.512753	5.088931	-0.941705

E = -658.123070975
G = -657.835325

Transition state

C	1.219201	2.205316	0.889145
C	1.534007	3.585130	0.817134
C	1.012640	4.092529	-0.395873
C	0.383738	3.020636	-1.083407
C	0.517909	1.855225	-0.292757
Sm	-1.243607	3.443067	1.121422
C	-3.600481	2.714230	2.432241
C	-2.617222	1.798232	2.880435
C	-2.255579	0.974124	1.786001
C	-3.013081	1.382982	0.659272
C	-3.847092	2.456872	1.062589
C	-0.665279	4.752603	3.188666
C	-1.128321	5.931582	2.541682
C	-0.100152	6.941833	2.084396
C	-2.383283	5.800448	0.818857
C	-2.312199	5.462196	-0.675157
C	-3.579985	5.865201	-1.438148
H	-1.439797	5.950454	-1.124933
H	1.118882	5.107772	-0.759907
H	-0.073577	3.072873	-2.065088
H	0.164192	0.865144	-0.553781
H	1.508310	1.526323	1.683195
H	2.103539	4.144032	1.549270
H	-1.548522	0.153608	1.813644
H	-2.992493	0.925334	-0.323062
H	-4.573885	2.965156	0.438964
H	-4.096138	3.462080	3.040223
H	-2.234082	1.718701	3.890807
H	0.720865	6.457006	1.548732
H	0.331850	7.431011	2.966379
H	-0.516737	7.720045	1.438591
H	-2.027573	6.376792	2.964232
H	0.410038	4.628612	3.300892
H	-1.265367	4.353613	4.003213
H	-2.406795	6.886234	0.898394
H	-3.328190	5.429931	1.241714
H	-2.174778	4.379454	-0.903405
H	-3.506603	5.615210	-2.502735
H	-3.749770	6.943427	-1.354592
H	-4.460562	5.358294	-1.030163

E = -658.104820837
G = -657.812322

$Cp_2SmCH_2CH(CH_3)CH_2CH_2CH_3$

C	1.452436	2.279958	0.918943
C	1.508869	3.668066	0.628766
C	0.928695	3.867293	-0.646532
C	0.521818	2.602924	-1.150736
C	0.854160	1.622343	-0.186663
Sm	-1.168398	3.079330	1.001304
C	-3.686194	2.338871	1.930931
C	-2.762610	1.598751	2.702143
C	-2.130402	0.656301	1.847955
C	-2.675496	0.810602	0.547989
C	-3.630354	1.855431	0.596327
C	-1.223849	4.892861	2.709326
C	-1.304267	6.378036	2.310579
C	0.003825	6.889073	1.698313
C	-2.498322	6.666973	1.379446
C	-2.601358	5.757211	0.148234
C	-3.504492	6.308099	-0.955546
H	-1.595353	5.587606	-0.273208
H	0.858398	4.813146	-1.172014
H	0.082106	2.415145	-2.124211
H	0.695076	0.555031	-0.282582
H	1.851426	1.798658	1.805234
H	1.935307	4.434554	1.262383
H	-1.402413	-0.088919	2.147535
H	-2.423335	0.216537	-0.322515
H	-4.253606	2.186127	-0.227673
H	-4.338615	3.120561	2.300950
H	-2.583178	1.718487	3.764248
H	0.246889	6.379186	0.758913
H	0.841612	6.715509	2.382570
H	-0.040244	7.965670	1.493138
H	-1.478261	7.000789	3.205941
H	-0.366147	4.763310	3.393606
H	-2.108738	4.658745	3.327046
H	-2.447949	7.711208	1.039031
H	-3.434792	6.578733	1.946538
H	-3.031200	4.788236	0.463581
H	-3.592475	5.615746	-1.799448
H	-3.112239	7.255579	-1.339375
H	-4.512903	6.498434	-0.572873

E = -658.145767110
G = -657.852717

$Cp_2SmCH_2CH_2CH_3$ + propene : 2,1 insertion

$Cp_2SmCH_2CH_2CH_3$ + propene → $Cp_2SmCH(CH_3)CH_2CH_2CH_2CH_3$

Adduct of propene on $Cp_2SmCH_2CH_2CH_3$

C	-3.658120	2.166899	0.617784
C	-3.235324	2.823852	-0.564763
C	-3.317841	4.220563	-0.343272
C	-3.801673	4.424167	0.975078
C	-4.011336	3.158383	1.570268
Sm	-1.250355	3.318450	1.289858
C	0.758571	1.621828	0.458445
C	1.413034	2.525183	1.336136
C	1.437423	3.794180	0.712486
C	0.801096	3.680714	-0.550166
C	0.385100	2.335464	-0.708099
C	0.308822	7.242697	0.994339
C	-0.932831	6.600414	1.528064
C	-1.045936	5.997771	2.722738
C	-1.203737	2.871440	3.715974
C	-1.483723	1.397442	3.458924
C	-0.550921	0.405284	4.156255
H	-2.527343	1.154244	3.693854
H	-4.401995	2.978416	2.563958
H	-3.742909	1.094836	0.753399
H	-2.931670	2.342591	-1.486557
H	-3.101466	4.992566	-1.073323
H	-4.021351	5.382566	1.432311
H	-0.101822	1.917789	-1.581072
H	0.616677	0.560544	0.627074
H	1.845904	2.280995	2.297983
H	1.897575	4.688137	1.116177
H	0.695741	4.466989	-1.289305
H	-0.199618	5.903380	3.398449
H	-1.825132	6.695309	0.907638
H	-1.958977	3.319726	4.368389
H	-0.220088	3.012709	4.180272
H	-1.421176	1.125590	2.357379
H	-0.764620	-0.634348	3.880087
H	-0.649915	0.497933	5.242684
H	0.494548	0.612100	3.903228
H	0.145217	8.320858	0.873479
H	1.160196	7.101565	1.665245
H	0.575151	6.854635	0.005363
H	-2.000195	5.630005	3.090036

E = -658.121572658
G = -657.834534

Transition state

C	-3.517955	2.000459	0.586873
C	-3.152158	2.536246	-0.671323
C	-3.354282	3.938943	-0.627014
C	-3.865741	4.265248	0.654039
C	-3.962172	3.072325	1.405884
Sm	-1.216123	3.454217	1.059694
C	0.422308	1.690298	-0.287690
C	1.161264	2.009593	0.880008
C	1.560951	3.364158	0.789971
C	1.074138	3.884492	-0.434987
C	0.373626	2.849201	-1.102431
C	0.169601	6.710815	1.421286
C	-1.088235	5.917343	1.718531
C	-1.312441	5.440219	3.037133
C	-0.804336	3.494086	3.671248
C	-1.358808	2.066053	3.590618
C	-0.591509	1.083347	4.483258
H	-2.418695	2.068051	3.868133
H	-4.353706	2.986240	2.412726
H	-3.511636	0.950300	0.856251
H	-2.798150	1.970262	-1.524391
H	-3.193192	4.631909	-1.445047
H	-4.160154	5.252528	0.988961
H	-0.089972	2.921447	-2.079199
H	0.008816	0.719400	-0.535133
H	1.410945	1.322870	1.680806
H	2.164592	3.899742	1.512923
H	1.243476	4.885299	-0.812294
H	-0.604421	5.746191	3.804901
H	-1.982344	6.248933	1.189420
H	-1.049986	3.869840	4.663616
H	0.291102	3.481884	3.588964
H	-1.337657	1.601758	2.576678
H	-1.008206	0.071653	4.419966
H	-0.635258	1.403252	5.529158
H	0.463684	1.034972	4.195329
H	0.135061	7.719280	1.862364
H	1.066001	6.221150	1.818564
H	0.329177	6.841668	0.346182
H	-2.336240	5.389954	3.402482

E = -658.100107248
G = -657.807427

$Cp_2SmCH(CH_3)CH_2CH_2CH_2CH_3$

C	-3.671911	1.899661	0.367767
C	-3.385890	2.446214	-0.905463
C	-3.490866	3.857971	-0.809922
C	-3.864687	4.182505	0.520425
C	-3.970308	2.974612	1.248148
Sm	-1.262321	3.252265	0.666619
C	0.315411	1.555952	-0.825696
C	1.088697	1.819388	0.333064
C	1.489108	3.180320	0.295367
C	0.959809	3.757214	-0.882485
C	0.232593	2.755265	-1.576815
C	0.444399	5.969121	2.168412
C	-0.945520	5.349336	1.998250
C	-1.642571	5.194078	3.363538
C	-0.993830	4.185467	4.323788
C	-0.805089	2.787917	3.727312
C	-0.370325	1.726338	4.736809
H	-1.760280	2.462146	3.272087
H	-4.276271	2.882551	2.284133
H	-3.709707	0.843691	0.612651
H	-3.144078	1.884751	-1.799943
H	-3.367548	4.561546	-1.625942
H	-4.051291	5.177060	0.905693
H	-0.260365	2.872593	-2.534763
H	-0.108491	0.598761	-1.106997
H	1.374583	1.092252	1.085556
H	2.109443	3.686313	1.024230
H	1.109360	4.779507	-1.210463
H	-1.688833	6.161747	3.896966
H	-1.553534	6.081014	1.433569
H	-1.606318	4.100608	5.231793
H	-0.013386	4.552235	4.654654
H	-0.026652	2.842542	2.944847
H	-0.221392	0.748662	4.266995
H	-1.121536	1.608593	5.524733
H	0.570989	2.013769	5.216740
H	0.429014	6.894696	2.772338
H	1.150679	5.292604	2.669758
H	0.898024	6.229101	1.204751
H	-2.692265	4.893732	3.220321

E = -658.142828378
G = -657.849334

$Cp_2SmCH_2CH_2CH_3$ + propene : allylic activation

$Cp_2SmCH_2CH_2CH_3$ + propene → Cp_2SmCH_2-CH=CH_2 + propane

Adduct of propene on $Cp_2SmCH_2CH_2CH_3$

C	1.374362	0.853455	-1.655441
C	1.433118	-0.542093	-1.427024
C	0.102883	-1.034286	-1.392575
C	-0.776143	0.061072	-1.592772
C	0.008623	1.225039	-1.761373
Sm	0.475991	-0.355722	-4.012855
C	1.067426	-1.809308	-6.327061
C	-0.020459	-2.475129	-5.717520
C	0.440837	-3.042587	-4.502866
C	1.822115	-2.741293	-4.372526
C	2.208306	-1.976369	-5.496605
C	-1.768459	0.236648	-4.882053
C	-2.423165	1.576668	-4.528986
H	-1.744820	2.412437	-4.769813
C	-3.762524	1.839671	-5.227643
C	0.786726	2.219129	-7.011226
C	1.862675	1.669532	-6.131244
C	2.086878	2.034691	-4.857589
H	-0.372121	2.228622	-1.910772
H	2.222591	1.528215	-1.684804
H	2.332508	-1.125046	-1.267325
H	-0.190937	-2.058614	-1.195398
H	-1.857911	0.016231	-1.605561
H	1.044254	-1.308352	-7.288182
H	3.212589	-1.625354	-5.708745
H	2.471104	-3.063347	-3.567022
H	-0.145117	-3.647049	-3.820175
H	-1.026803	-2.542725	-6.110571
H	-1.698578	0.159603	-5.983825
H	-2.460127	-0.578327	-4.600880
H	1.235330	2.710593	-7.883163
H	0.160242	2.944629	-6.486969
H	0.142493	1.420834	-7.395117
H	-2.580058	1.641691	-3.443021
H	-4.198345	2.807210	-4.946315
H	-3.643141	1.830309	-6.317698
H	-4.489026	1.058578	-4.974887
H	2.532021	0.939804	-6.587036
H	2.935924	1.646873	-4.298208
H	1.480786	2.794149	-4.367236

E = -658.123292402
G = -657.837740

Transition state

C	1.587586	0.669355	-1.695690
C	1.063290	-0.630737	-1.504643
C	-0.343340	-0.565815	-1.679511
C	-0.686257	0.777692	-1.969698
C	0.505736	1.540526	-1.988133
Sm	0.689842	-0.153492	-4.186553
C	0.944928	-1.825133	-6.393598
C	-0.003878	-2.449152	-5.545641
C	0.668419	-2.879593	-4.377035
C	2.037752	-2.523043	-4.502433
C	2.206752	-1.880787	-5.752445
C	-1.720042	0.404452	-5.202183
C	-2.640047	1.620367	-5.097778
H	-2.321624	2.391372	-5.815083
C	-4.117763	1.306927	-5.344693
C	0.552106	2.118509	-5.800315
C	1.929684	1.647140	-5.883255
C	2.837362	1.630900	-4.865283
H	0.572665	2.611393	-2.142627
H	2.628620	0.953635	-1.596087
H	1.632184	-1.514252	-1.240877
H	-1.037741	-1.390175	-1.565495
H	-1.688132	1.157459	-2.124667
H	0.745469	-1.416754	-7.377556
H	3.144468	-1.515920	-6.154890
H	2.822506	-2.745502	-3.788989
H	0.225098	-3.419488	-3.548881
H	-1.055693	-2.588903	-5.762904
H	-1.815759	-0.055039	-6.196018
H	-2.060475	-0.357849	-4.481423
H	0.134027	2.398110	-6.769472
H	0.403287	2.922145	-5.072755
H	-0.417164	1.245691	-5.479556
H	-2.534183	2.084573	-4.107448
H	-4.742626	2.205021	-5.271383
H	-4.265257	0.877427	-6.342149
H	-4.492720	0.578777	-4.616344
H	2.209083	1.138642	-6.807176
H	3.824118	1.201397	-5.003295
H	2.668576	2.191990	-3.948825

E = -658.106202773
G = -657.819270

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

$Cp_2SmCH_2CH_2CH_3$ + propene : vinylic activation

$Cp_2SmCH_2CH_2CH_3$ + propene → $Cp_2SmCH{=}CH\text{-}CH_3$ + propane

Adduct of propene on $Cp_2SmCH_2CH_2CH_3$

C	2.736420	-0.148380	-6.150098
C	2.583386	-1.057592	-5.079485
C	1.366840	-1.761879	-5.275469
C	0.779045	-1.297721	-6.480025
C	1.617088	-0.293693	-7.014424
Sm	0.543710	0.772985	-4.661642
C	0.897244	2.200082	-2.289000
C	1.573582	0.967988	-2.112578
C	0.597602	-0.060441	-2.060547
C	-0.679399	0.539566	-2.203119
C	-0.494236	1.934420	-2.347687
C	0.852271	3.519989	-5.784866
C	2.134646	3.281684	-6.105504
C	3.319776	3.721391	-5.307106
C	-1.778098	0.544677	-5.508849
C	-2.989828	1.354284	-5.033205
H	-3.929695	0.970977	-5.466236
C	-2.902234	2.842838	-5.368080
H	1.360506	3.180154	-2.318044
H	2.642821	0.836929	-1.992753
H	0.792601	-1.113629	-1.896464
H	-1.631681	0.023812	-2.190355
H	-1.282899	2.669731	-2.452220
H	3.589581	0.500486	-6.311803
H	3.282383	-1.209017	-4.265599
H	0.982854	-2.555930	-4.645465
H	-0.148641	-1.649075	-6.913072
H	1.456505	0.233302	-7.948487
H	-1.722899	0.613215	-6.612586
H	-1.982031	-0.527334	-5.325765
H	0.037805	3.239597	-6.450725
H	-3.110949	1.249326	-3.945481
H	-3.800385	3.390415	-5.059411
H	-2.044358	3.312695	-4.870153
H	-2.781526	2.994922	-6.448458
H	0.585753	4.077416	-4.889241
H	2.348316	2.762639	-7.039571
H	3.923605	4.424501	-5.893824
H	3.026329	4.213897	-4.376579
H	3.974291	2.876409	-5.065495

E = -658.120974388
G = -657.835467

Transition state

C	2.870367	-0.294258	-5.937902
C	2.848278	-1.243878	-4.885147
C	1.674278	-2.027857	-5.027853
C	0.970511	-1.557957	-6.164851
C	1.708985	-0.486253	-6.725449
Sm	0.779662	0.466679	-4.289409
C	1.198924	1.414386	-1.732944
C	1.386974	0.011122	-1.655295
C	0.126859	-0.610299	-1.852695
C	-0.838299	0.410912	-2.045716
C	-0.175607	1.659967	-1.974160
C	0.855200	2.897661	-5.139429
C	1.619222	3.280706	-6.181803
C	2.328422	4.593232	-6.336505
C	-1.409559	1.141361	-5.567674
C	-2.578808	2.084609	-5.261670
H	-3.538815	1.569022	-5.412389
C	-2.569284	3.350339	-6.118285
H	1.966355	2.168346	-1.597836
H	2.320346	-0.497061	-1.442920
H	-0.069994	-1.675372	-1.811789
H	-1.902133	0.263394	-2.191416
H	-0.641980	2.633485	-2.064505
H	3.651803	0.433713	-6.122264
H	3.617015	-1.381063	-4.133449
H	1.388106	-2.864394	-4.401040
H	0.046776	-1.967452	-6.557405
H	1.444254	0.066965	-7.618599
H	-1.349808	0.946300	-6.647358
H	-1.640480	0.153098	-5.111775
H	-0.231617	2.050883	-5.365697
H	-2.558534	2.367979	-4.200125
H	-3.415444	4.001599	-5.874209
H	-1.649036	3.925355	-5.975302
H	-2.638289	3.100720	-7.183514
H	0.731097	3.647693	-4.347953
H	1.738949	2.597569	-7.028111
H	1.974616	5.126069	-7.229202
H	2.174642	5.238805	-5.466928
H	3.407694	4.447814	-6.472840

E = -658.091864736
G = -657.808867

Adduct of propane on $Cp_2SmCH=CH-CH_3$

C	2.929425	-0.338713	-5.952242
C	2.873365	-1.302600	-4.911476
C	1.649801	-2.010329	-5.034340
C	0.942472	-1.471045	-6.134862
C	1.734886	-0.436694	-6.702418
Sm	0.976473	0.540065	-4.223908
C	1.284996	1.380563	-1.623233
C	1.473573	-0.026016	-1.598728
C	0.220223	-0.640606	-1.852474
C	-0.737109	0.385223	-2.044633
C	-0.077323	1.634686	-1.903822
C	1.719188	2.808058	-4.795631
C	2.236920	3.239191	-5.967300
C	2.586759	4.655476	-6.336982
C	-1.762580	1.263602	-5.726277
C	-2.969163	2.121588	-5.345198
H	-3.864656	1.488839	-5.313708
C	-3.189980	3.282200	-6.312148
H	2.047865	2.129975	-1.450901
H	2.399466	-0.541221	-1.370549
H	0.024364	-1.706331	-1.862820
H	-1.798906	0.240657	-2.212455
H	-0.538610	2.612919	-1.970590
H	3.743786	0.349831	-6.138983
H	3.655321	-1.503987	-4.188321
H	1.325070	-2.833528	-4.408906
H	-0.011898	-1.822474	-6.511650
H	1.484676	0.150962	-7.578031
H	-1.869903	0.829556	-6.725527
H	-1.662075	0.420912	-5.022721
H	-0.851677	1.884732	-5.744066
H	-2.831180	2.509991	-4.328922
H	-4.058124	3.881111	-6.020054
H	-2.319393	3.946584	-6.337953
H	-3.362790	2.921433	-7.332243
H	1.568114	3.636238	-4.082173
H	2.448773	2.516212	-6.763703
H	2.039615	4.984424	-7.231083
H	2.357701	5.348236	-5.520949
H	3.654132	4.751941	-6.578958

E = -658.127442300
G = -657.844873

$Cp_2SmCH_2CH_2CH_3$ + SiH_4 : Si-H activation (Si at α position at the TS)

$Cp_2SmCH_2CH_2CH_3$ + SiH_4 → Cp_2SmSiH_3 + propane

Adduct of SiH_4 on $Cp_2SmCH_2CH_2CH_3$

C	1.765649	0.397114	-2.018578
C	1.246639	-0.776321	-2.625416
C	-0.135059	-0.576206	-2.847782
C	-0.471104	0.727194	-2.392602
C	0.703741	1.329272	-1.883913
Sm	0.178655	-0.701812	-0.091212
C	0.724082	-3.104245	-0.236896
C	0.191417	-4.053411	0.843420
C	0.432297	-5.541502	0.562593
C	-0.448831	0.438199	2.369669
C	0.618484	1.207748	1.847353
C	1.777444	0.389495	1.828710
C	1.426172	-0.882332	2.354066
C	0.051640	-0.854247	2.681096
Si	-3.681372	-0.477406	0.081399
H	-4.275131	-0.950430	1.360439
H	-4.537015	-0.831307	-1.083098
H	-3.414060	0.986190	0.123006
H	-2.372102	-1.196805	-0.102295
H	2.769929	0.700431	1.523346
H	0.567653	2.246811	1.544191
H	-1.455567	0.795278	2.558821
H	-0.511406	-1.668763	3.121640
H	2.094839	-1.722929	2.490658
H	-0.810074	-1.281280	-3.319760
H	-1.444203	1.200060	-2.470796
H	0.785915	2.335118	-1.489826
H	2.803154	0.574064	-1.758762
H	1.808858	-1.666533	-2.877531
H	1.816145	-3.242924	-0.328059
H	0.326967	-3.430445	-1.216995
H	0.641774	-3.805200	1.814965
H	-0.893245	-3.906940	0.984073
H	0.039415	-6.185980	1.359627
H	-0.044611	-5.842770	-0.377599
H	1.504660	-5.746443	0.463152

E = -546.532286564
G = -546.298756

Transition state

C	1.335567	1.129334	-1.987787
C	1.444552	-0.184490	-2.514775
C	0.140914	-0.642570	-2.825390
C	-0.776974	0.383734	-2.485671
C	-0.037710	1.479841	-1.969340
Sm	0.220183	-0.479920	-0.068450
C	0.043238	-3.023239	-0.218491
C	-0.421735	-4.141122	0.708966
C	0.263312	-5.488610	0.471286
C	0.147546	1.101011	2.173677
C	1.506497	1.086993	1.773672
C	2.012472	-0.221952	1.987940
C	0.967894	-1.012359	2.531691
C	-0.185043	-0.196936	2.643751
Si	-2.803238	-1.198823	0.216135
H	-3.430944	-1.715794	1.472308
H	-3.674756	-1.582017	-0.938893
H	-2.863099	0.308255	0.307237
H	-1.303668	-2.046790	0.004884
H	3.033980	-0.544195	1.818007
H	2.069166	1.934605	1.400754
H	-0.509959	1.962957	2.164131
H	-1.138660	-0.497001	3.061928
H	1.046984	-2.048185	2.837747
H	-0.109651	-1.597097	-3.271362
H	-1.848767	0.357076	-2.643935
H	-0.446859	2.432931	-1.653902
H	2.159996	1.768058	-1.693105
H	2.368613	-0.723880	-2.691683
H	1.147202	-2.898980	-0.097508
H	-0.105985	-3.317287	-1.266307
H	-0.277473	-3.842090	1.755923
H	-1.508065	-4.271020	0.591498
H	-0.116498	-6.262187	1.148901
H	0.101539	-5.834446	-0.555933
H	1.345964	-5.412578	0.625146

E = -546.520569708
G = -546.282468

Adduct of propane on Cp_2SmSiH_3

C	1.364818	0.940785	-1.939211
C	1.164646	-0.356170	-2.473702
C	-0.215154	-0.497538	-2.775073
C	-0.867997	0.711817	-2.432536
C	0.107577	1.598907	-1.907700
Sm	-0.089640	-0.348179	-0.029898
C	-0.080519	-3.478992	-0.275166
C	-0.117730	-4.717107	0.621087
C	1.099056	-5.619404	0.433672
C	0.432748	1.369982	2.002180
C	1.687350	0.778431	1.701807
C	1.634316	-0.580933	2.097705
C	0.348247	-0.827349	2.646190
C	-0.392656	0.378478	2.593784
Si	-3.082423	-0.419312	0.270047
H	-3.652669	-1.157021	1.466407
H	-3.910121	-0.971692	-0.874094
H	-3.670717	0.967716	0.445917
H	-0.992785	-2.876631	-0.123599
H	2.452206	-1.291012	2.039830
H	2.547280	1.285955	1.281813
H	0.167584	2.410215	1.851912
H	-1.399880	0.522936	2.962818
H	0.003483	-1.763006	3.071354
H	-0.686294	-1.364347	-3.224273
H	-1.919851	0.927144	-2.569984
H	-0.068248	2.618988	-1.585865
H	2.315614	1.368364	-1.644899
H	1.939476	-1.090949	-2.664260
H	0.831354	-2.895608	-0.054690
H	-0.039953	-3.746593	-1.335551
H	-0.192628	-4.405046	1.669382
H	-1.034334	-5.277667	0.403674
H	1.040240	-6.500319	1.079911
H	1.178311	-5.971101	-0.600915
H	2.028525	-5.091957	0.677138

E = -546.566856480
G = -546.326755

$Cp_2SmCH_2CH_2CH_3$ + SiH_4 : Si-H activation (Si at β position at the TS)

$Cp_2SmCH_2CH_2CH_3 + SiH_4 \rightarrow Cp_2SmH + SiH_3\text{-}CH_2\text{-}CH_2\text{-}CH_3$

Transition state

C	0.734768	-3.828079	-2.489900
C	1.819015	-2.979879	-2.150589
C	2.691296	-3.706868	-1.301318
C	2.150170	-5.006935	-1.126928
C	0.941347	-5.081229	-1.858413
Sm	0.380341	-3.286861	0.161244
C	-1.200738	-1.391576	-0.966655
C	-2.053093	-2.054515	-0.051149
C	-1.623921	-1.729734	1.261967
C	-0.502045	-0.871948	1.155888
C	-0.235683	-0.664311	-0.222339
Si	-1.449761	-5.008926	2.124746
C	0.423590	-4.167992	2.732023
C	1.857999	-4.694901	2.482182
Si	1.982800	-6.599879	2.664573
C	2.867113	-4.018163	3.427563
H	-2.813123	-5.003999	1.442371
H	-1.110703	-6.447974	2.361215
H	-1.966041	-4.441319	3.450546
H	-2.097152	-2.050976	2.182272
H	0.031479	-0.414965	1.982276
H	0.531690	-0.018586	-0.633467
H	-1.287141	-1.410257	-2.045755
H	-2.899536	-2.682909	-0.300383
H	3.637573	-3.350936	-0.907842
H	2.604822	-5.820041	-0.573957
H	0.301531	-5.950623	-1.943446
H	-0.084819	-3.580008	-3.153286
H	1.973482	-1.968811	-2.507952
H	-0.923613	-4.911681	0.486609
H	2.843891	-2.925872	3.320262
H	2.628075	-4.240038	4.473793
H	3.893691	-4.352172	3.240608
H	2.227075	-4.516975	1.452425
H	0.159724	-4.454636	3.755109
H	0.429281	-3.060256	2.804392
H	1.424641	-7.010969	3.988282
H	1.279484	-7.327495	1.569307
H	3.432651	-6.974821	2.618707

E = -551.605342753
G = -551.349882

SiH_3-CH_2-CH_2-CH_3 ('linear' hydrosilylation product)

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_2-CH=CH_2 (π-allylic complex)

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_2SmCH_2-CH=CH_2 + propene : 1,2 insertion

Cp_2SmCH_2-CH=CH_2 + propene → Cp2SmCH2CH(CH_3)CH_2CH=CH_2

Adduct of propene on Cp_2SmCH_2-CH=CH_2

C	1.483979	0.917882	-2.010703
C	2.387786	0.647641	-0.957611
C	2.540188	-0.761433	-0.865571
C	1.736024	-1.354231	-1.868112
C	1.070513	-0.319171	-2.568689
Sm	-0.008819	-0.297464	0.005590
C	-1.263271	2.497495	-0.525563
C	-2.168448	1.866800	-1.294109
C	-2.122809	1.788533	-2.788013
C	-2.441167	-1.307090	-0.806291
C	-1.517709	-2.330360	-1.028802
C	-0.691271	-2.906055	-0.062408
H	0.020704	-3.673457	-0.347231
C	0.425125	1.206170	2.292161
C	1.318399	0.111032	2.383856
C	0.556677	-1.061838	2.603487
C	-0.810982	-0.688170	2.666928
C	-0.892638	0.708220	2.476039
H	-1.018093	-2.927868	0.974897
H	-2.883308	-1.194209	0.185360
H	-3.045935	-0.944107	-1.630130
H	-1.268871	-2.537705	-2.072406
H	-0.396976	2.991291	-0.957652
H	-3.050417	1.443012	-0.817039
H	-1.415047	2.617109	0.541480
H	-1.204537	2.222721	-3.190834
H	-2.202305	0.754465	-3.137062
H	-2.973810	2.334907	-3.213765
H	0.950995	-2.061420	2.741090
H	2.398242	0.164429	2.317796
H	0.705958	2.245490	2.166067
H	-1.801941	1.297671	2.511739
H	-1.645260	-1.352072	2.860188
H	2.901633	1.385115	-0.352582
H	3.189803	-1.288823	-0.177110
H	1.655775	-2.414466	-2.070625
H	0.408280	-0.446307	-3.416692
H	1.199209	1.901137	-2.364125

E = -656.915969382
G = -656.648884

Transition state

C	2.031314	1.190756	-1.586038
C	2.763577	0.448562	-0.630112
C	2.590814	-0.930595	-0.916511
C	1.765294	-1.034632	-2.062996
C	1.412972	0.272074	-2.471895
Sm	0.141049	-0.068234	0.004622
C	-1.238792	1.903890	-0.769136
C	-2.332323	1.105638	-1.238364
C	-2.536015	1.041108	-2.739852
C	-2.513907	-0.862500	-0.741021
C	-1.603271	-1.913665	-1.148280
C	-0.817883	-2.664544	-0.318245
H	-0.118102	-3.391146	-0.716875
C	0.550658	1.262561	2.387479
C	1.338954	0.087508	2.482303
C	0.465475	-1.019228	2.597511
C	-0.865640	-0.526706	2.588708
C	-0.811206	0.880563	2.463127
H	-0.995792	-2.688376	0.754067
H	-2.741594	-0.866422	0.329206
H	-3.430422	-0.860205	-1.324574
H	-1.466863	-2.042595	-2.223815
H	-0.608017	2.355540	-1.532604
H	-3.259630	1.247466	-0.682989
H	-1.417146	2.530804	0.100772
H	-1.611482	0.761451	-3.253829
H	-3.318948	0.338436	-3.042382
H	-2.818027	2.036070	-3.103739
H	0.764568	-2.053896	2.719374
H	2.420956	0.044937	2.493892
H	0.924973	2.276950	2.312294
H	-1.661295	1.551931	2.453151
H	-1.764930	-1.119725	2.711614
H	3.375566	0.863018	0.161525
H	3.050708	-1.754560	-0.383425
H	1.476944	-1.955683	-2.555523
H	0.817777	0.529721	-3.339985
H	1.983378	2.271087	-1.650263

E = -656.890397354
G = -656.619369

$Cp_2SmCH_2CH(CH_3)CH_2CH{=}CH_2$

C	2.322730	1.434778	-1.216432
C	2.986153	0.298521	-0.685268
C	2.501935	-0.845365	-1.361550
C	1.549701	-0.414351	-2.323687
C	1.443669	0.993317	-2.238910
Sm	0.366645	0.100016	0.160761
C	-1.780104	1.170367	-0.583543
C	-2.750954	0.462314	-1.542894
C	-2.314081	0.569420	-3.005547
C	-2.951223	-1.008339	-1.110171
C	-1.684221	-1.806821	-1.128674
C	-1.156409	-2.475983	-0.087238
H	-0.260160	-3.085601	-0.197118
C	1.290087	1.170928	2.514614
C	1.557255	-0.215320	2.643672
C	0.318293	-0.888481	2.771425
C	-0.716239	0.083006	2.730535
C	-0.116687	1.353291	2.574881
H	-1.655435	-2.503761	0.878892
H	-3.383261	-1.036427	-0.102131
H	-3.672372	-1.499175	-1.782233
H	-1.161103	-1.855118	-2.084975
H	-1.598229	2.194996	-0.950242
H	-3.756280	0.916810	-1.491528
H	-2.301679	1.307457	0.379982
H	-1.302872	0.176677	-3.158332
H	-2.995692	0.035089	-3.679118
H	-2.296244	1.619355	-3.316449
H	0.187746	-1.952929	2.931881
H	2.538297	-0.674897	2.668954
H	2.032463	1.956927	2.437220
H	-0.639871	2.301014	2.525398
H	-1.778185	-0.109099	2.827569
H	3.741594	0.308219	0.091123
H	2.841441	-1.864393	-1.210547
H	1.040564	-1.047915	-3.040848
H	0.817476	1.624647	-2.855862
H	2.501323	2.465875	-0.932111

E = -656.918852885
G = -656.647130

Cp_2SmCH_2-CH=CH_2 + SiH_4 : Si-H activation (Si at α position at the TS)

Cp_2SmCH_2-CH=CH_2 + SiH_4 → Cp_2SmSiH_3 + propene

Transition state

C	1.624535	0.821719	-1.716559
C	1.271628	-0.538411	-1.537952
C	-0.136575	-0.647923	-1.674807
C	-0.651237	0.642698	-1.949903
C	0.439275	1.552244	-1.976935
Sm	0.737501	0.007805	-4.206252
C	0.393824	0.522116	-6.913440
C	0.511056	1.795202	-6.298873
C	-0.638275	1.999636	-5.495076
C	-1.462854	0.852583	-5.608208
C	-0.826555	-0.058837	-6.489396
Si	-0.596536	-2.829281	-4.339903
C	2.550368	-1.973620	-4.926712
C	3.318721	-0.906215	-4.349964
C	3.407330	0.378222	-4.834329
H	1.088943	0.090704	-7.624567
H	1.312962	2.507936	-6.451883
H	-0.862427	2.890533	-4.920281
H	-2.427671	0.710857	-5.135921
H	-1.230103	-1.007936	-6.821756
H	1.947648	-1.347133	-1.286464
H	2.622087	1.237648	-1.642244
H	0.371695	2.623586	-2.125781
H	-1.696772	0.897965	-2.074955
H	-0.721211	-1.549132	-1.535125
H	2.786187	-2.972076	-4.562942
H	2.426649	-1.943190	-6.011634
H	1.062455	-2.162469	-4.551482
H	3.728269	-1.090252	-3.355998
H	3.975803	1.133078	-4.302161
H	3.133684	0.605469	-5.862548
H	-1.966494	-2.267633	-4.078301
H	-0.338635	-3.842031	-3.262153
H	-0.696246	-3.589587	-5.631281

E = -545.313522788
G = -545.093326

Cp_2SmCH_2-CH=CH_2 + SiH_4 : Si-H activation (Si at β position at the TS)

Cp_2SmCH_2-CH=CH_2 + SiH_4 → Cp_2SmH + SiH_3-CH_2-CH=CH_2

Transition state

C	1.036774	-2.978281	2.947591
C	1.074109	-3.283212	1.561898
C	0.479000	-4.554538	1.376781
C	0.080389	-5.039530	2.650399
C	0.427886	-4.067485	3.619877
Sm	-1.606341	-2.964593	2.151204
C	-3.696799	-2.907464	0.337333
C	-4.322621	-2.902833	1.608352
C	-4.078452	-4.156735	2.222662
C	-3.294900	-4.933253	1.334799
C	-3.054486	-4.159252	0.168059
C	-0.958381	-0.452336	0.922264
C	-1.865760	-0.237386	1.910330
C	-1.599328	-0.153199	3.351891
Si	-1.960452	-1.367818	5.094352
H	-1.536986	-0.071155	5.794493
H	-1.063198	-2.294824	5.880354
H	-3.406299	-1.442869	5.492424
H	-2.523042	-4.489534	-0.716902
H	-3.734331	-2.110052	-0.396058
H	-4.921006	-2.101026	2.025296
H	-4.445363	-4.470162	3.192162
H	-2.969676	-5.953573	1.498126
H	1.521080	-2.674204	0.784730
H	0.386281	-5.083769	0.435909
H	-0.377267	-6.001170	2.850266
H	0.267304	-4.143869	4.687964
H	1.451190	-2.094320	3.418584
H	-2.241649	-2.763135	4.133191
H	-2.914100	-0.161529	1.614082
H	0.109038	-0.472226	1.128739
H	-1.262034	-0.480319	-0.120042
H	-0.569392	0.148295	3.562502
H	-2.279445	0.583820	3.787253

E = -545.301154788
G = -545.079480

$SiH_3-CH_2-CH=CH_2$

H	-0.335835	0.354396	1.684191
Si	-0.078010	0.021072	0.250693
H	-0.714056	1.067972	-0.610528
C	-0.778989	-1.704663	-0.164038
C	-0.065197	-2.784862	0.587726
C	-0.566464	-3.478773	1.611481
H	1.398657	0.048829	0.012137
H	-1.850246	-1.703541	0.067273
H	-0.678838	-1.848045	-1.247550
H	0.958697	-2.986415	0.269979
H	0.019966	-4.234521	2.125366
H	-1.580495	-3.316334	1.970560

E = -122.965540616
G = -122.899871

Cp_2SmSiH_3 (silyl complex)

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_2SmSiH_3 + propene : 1,2 insertion

Cp_2SmSiH_3 + propene → $Cp_2SmCH_2CH(CH_3)SiH_3$

Adduct of propene on Cp_2SmSiH_3

C	1.295378	2.602616	0.900099
C	1.438841	4.000836	0.723746
C	0.891853	4.345072	-0.540184
C	0.405386	3.159083	-1.143518
C	0.649182	2.083468	-0.251081
Sm	-1.281516	3.561786	0.966087
C	-3.230292	2.007595	-0.112414
C	-3.218907	3.175518	-0.918705
C	-3.713021	4.249013	-0.137302
C	-4.032074	3.744154	1.149600
C	-3.739107	2.358304	1.164790
C	-1.278756	6.381296	1.917003
C	-1.055857	5.919864	3.160632
C	-2.058172	5.905459	4.266767
Si	-0.997418	2.227590	3.655090
H	-0.776168	0.728062	3.619135
H	-4.461695	4.308428	1.969196
H	-3.899425	1.683665	1.995903
H	-2.945305	1.011800	-0.431741
H	-2.923555	3.228784	-1.959656
H	-3.866072	5.266097	-0.481703
H	-0.038143	3.081589	-2.128796
H	0.423329	1.039602	-0.435796
H	1.643987	2.028967	1.749234
H	1.928249	4.678607	1.414226
H	0.893333	5.331312	-0.991951
H	-3.036943	6.263173	3.936542
H	-1.711223	6.549404	5.084280
H	-2.166259	4.898751	4.684707
H	-0.059661	5.552873	3.414259
H	-2.244671	6.790984	1.629984
H	-0.470835	6.452200	1.188824
H	-2.144926	2.349644	4.643827
H	0.176300	2.692613	4.502423

E = -545.336626660
G = -545.119047

Transition state

C	1.351525	2.537120	0.987340
C	1.508028	3.907350	0.666337
C	0.953877	4.125030	-0.618745
C	0.456738	2.884586	-1.096153
C	0.698218	1.903432	-0.101223
Sm	-1.239841	3.526572	0.953441
C	-3.211313	2.319685	-0.516294
C	-3.411799	3.713358	-0.709046
C	-3.870376	4.262528	0.513537
C	-3.935665	3.216135	1.467586
C	-3.535011	2.013697	0.825853
C	-1.107398	5.940066	1.814485
C	-1.049595	5.506778	3.160870
C	-2.154121	5.916814	4.117365
Si	-1.132820	3.106994	3.815850
H	-1.086430	1.873900	2.870944
H	-4.293129	3.301201	2.486873
H	-3.509559	1.029602	1.279045
H	-2.894882	1.611894	-1.273325
H	-3.288943	4.249844	-1.643258
H	-4.156834	5.293795	0.678101
H	0.008140	2.709495	-2.067020
H	0.465080	0.847638	-0.177746
H	1.703977	2.049109	1.888374
H	1.997926	4.651354	1.283318
H	0.948904	5.063740	-1.160961
H	-3.142571	5.731593	3.687497
H	-2.069311	6.995860	4.301038
H	-2.106413	5.411086	5.086575
H	-0.056252	5.496643	3.609935
H	-2.012897	6.443272	1.481768
H	-0.183730	6.263411	1.340454
H	-2.315616	2.834739	4.698020
H	0.083968	2.949414	4.681798

E = -545.323492562
G = -545.098845

$Cp_2SmCH_2CH(CH_3)SiH_3$

C	1.311159	3.059110	1.015444
C	1.152504	4.368170	0.502083
C	0.657451	4.258942	-0.823328
C	0.527544	2.879941	-1.132716
C	0.922559	2.137991	0.005666
Sm	-1.424300	3.403352	0.733628
C	-3.188012	1.906148	-0.760464
C	-3.240606	3.212200	-1.310499
C	-3.864858	4.062483	-0.359949
C	-4.192803	3.285384	0.775411
C	-3.772105	1.952423	0.530309
C	-1.629699	5.303723	2.354482
C	-0.867139	5.052603	3.672723
C	-1.031150	6.133935	4.751242
Si	-1.443896	3.342588	4.234399
H	-1.301153	2.387899	3.043779
H	-4.695827	3.642018	1.665740
H	-3.919046	1.107448	1.194238
H	-2.799763	1.023118	-1.254946
H	-2.910141	3.498186	-2.302411
H	-4.076670	5.117596	-0.489947
H	0.202291	2.467903	-2.080611
H	0.968062	1.056748	0.076408
H	1.705208	2.801391	1.992036
H	1.387857	5.289636	1.019453
H	0.467793	5.083435	-1.501795
H	-2.082661	6.245046	5.040394
H	-0.700700	7.104613	4.361459
H	-0.451305	5.923711	5.659514
H	0.207378	4.943098	3.457308
H	-2.688744	5.496798	2.590326
H	-1.257872	6.237270	1.897071
H	-2.899653	3.308618	4.574495
H	-0.679488	2.656850	5.326702

E = -545.343148018
G = -545.119505

Cp_2SmSiH_3 + propene : 2,1 insertion

Cp_2SmSiH_3 + propene → $Cp_2SmCH(CH_3)CH_2SiH_3$

Adduct of propene on Cp_2SmSiH_3

C	-3.209095	2.093835	0.126699
C	-2.976270	3.162371	-0.778375
C	-3.336388	4.367837	-0.128452
C	-3.792480	4.044458	1.176418
C	-3.721140	2.639454	1.331938
Sm	-1.089102	3.419217	1.179513
C	0.480249	1.501127	0.073387
C	1.106598	1.775657	1.315928
C	1.656712	3.078870	1.247288
C	1.380288	3.607036	-0.039427
C	0.651849	2.632710	-0.766534
C	-1.169436	6.655140	1.577779
C	-0.333745	6.014318	2.412856
H	-0.693373	5.542082	3.327193
Si	-1.288736	2.357928	3.986195
H	-1.561181	0.867192	4.049457
H	-4.026157	2.080882	2.207396
H	-3.067313	1.040137	-0.083002
H	-2.626606	3.068073	-1.799436
H	-3.322617	5.356360	-0.573887
H	-4.174050	4.740666	1.914445
H	0.327604	2.716921	-1.796858
H	-0.002965	0.571521	-0.203314
H	1.174557	1.101613	2.160261
H	2.221800	3.566585	2.033024
H	1.709553	4.567395	-0.421123
H	0.741789	6.013915	2.249076
H	-2.232929	6.671997	1.817175
C	-0.753054	7.413771	0.357847
H	-2.389889	2.914249	4.871559
H	-0.070027	2.492779	4.881214
H	-1.006819	8.474365	0.474757
H	0.322106	7.336899	0.176008
H	-1.286622	7.064878	-0.533639

E = -545.335648235
G = -545.116546

Transition state

C	-3.415275	1.906947	0.782074
C	-3.205511	2.380068	-0.535567
C	-3.487316	3.772125	-0.551690
C	-3.881206	4.152891	0.753974
C	-3.829270	3.004582	1.582734
Sm	-1.187386	3.489850	0.937371
C	0.517619	1.736724	-0.301281
C	1.200901	2.083777	0.889931
C	1.585150	3.444617	0.796168
C	1.149453	3.937573	-0.459785
C	0.486680	2.883377	-1.137630
C	-1.106495	6.049646	1.611134
C	-1.292347	5.614189	2.934588
H	-2.300746	5.569374	3.338182
Si	-0.956114	3.299949	3.804848
H	-1.054885	1.943968	3.055764
H	-4.114301	2.957309	2.627080
H	-3.310600	0.880703	1.114622
H	-2.912667	1.780117	-1.388937
H	-3.456217	4.416628	-1.423237
H	-4.202745	5.141953	1.057959
H	0.071818	2.930197	-2.138004
H	0.123142	0.757764	-0.547476
H	1.414390	1.418438	1.717999
H	2.155052	3.994053	1.535947
H	1.330148	4.931010	-0.850923
H	-0.533247	5.864425	3.676286
H	-2.015749	6.304748	1.065034
C	0.142704	6.806539	1.216761
H	-2.042653	3.248582	4.837915
H	0.343905	3.226587	4.553502
H	0.117753	7.840925	1.591249
H	1.047843	6.342367	1.623748
H	0.266156	6.866760	0.131402

E = -545.319765258
G = -545.096801

$Cp_2SmCH(CH_3)CH_2SiH_3$

C	-3.440318	1.820389	0.745778
C	-3.252318	2.211237	-0.600802
C	-3.490737	3.607268	-0.689196
C	-3.847831	4.075372	0.601726
C	-3.810004	2.973681	1.488992
Sm	-1.170025	3.402861	0.754642
C	0.466968	1.664521	-0.613109
C	1.200653	1.985177	0.555449
C	1.588410	3.347994	0.471066
C	1.093589	3.868700	-0.746916
C	0.393892	2.830821	-1.417300
C	-1.022540	5.712593	1.771209
C	-1.640185	5.571967	3.184336
H	-2.713464	5.344310	3.131142
Si	-0.853408	4.150973	4.149157
H	-0.813415	2.933151	3.220392
H	-4.069631	2.993491	2.541469
H	-3.363262	0.810005	1.132152
H	-2.988993	1.557271	-1.423519
H	-3.464282	4.200811	-1.596466
H	-4.121829	5.091626	0.856125
H	-0.065925	2.899934	-2.396494
H	0.058905	0.692283	-0.864058
H	1.462263	1.297360	1.352215
H	2.182514	3.889011	1.197126
H	1.245177	4.876749	-1.114368
H	-1.558243	6.492615	3.791861
H	-1.706774	6.356581	1.192485
C	0.323758	6.435334	1.845494
H	-1.616331	3.670911	5.343625
H	0.572678	4.352868	4.541576
H	0.258808	7.407357	2.367242
H	1.088105	5.854792	2.380584
H	0.731205	6.638156	0.848367

E = -545.337694183
G = -545.113894

Cp_2SmSiH_3 + propene : allylic activation

Cp_2SmSiH_3 + propene → $Cp_2SmCH\text{-}CH_2{=}CH_2$ + SiH_4

Transition state

C	1.624535	0.821719	-1.716559
C	1.271628	-0.538411	-1.537952
C	-0.136575	-0.647923	-1.674807
C	-0.651237	0.642698	-1.949903
C	0.439275	1.552244	-1.976935
Sm	0.737501	0.007805	-4.206252
C	0.393824	0.522116	-6.913440
C	0.511056	1.795202	-6.298873
C	-0.638275	1.999636	-5.495076
C	-1.462854	0.852583	-5.608208
C	-0.826555	-0.058837	-6.489396
Si	-0.596536	-2.829281	-4.339903
C	2.550368	-1.973620	-4.926712
C	3.318721	-0.906215	-4.349964
C	3.407330	0.378222	-4.834329
H	1.088943	0.090704	-7.624567
H	1.312962	2.507936	-6.451883
H	-0.862427	2.890533	-4.920281
H	-2.427671	0.710857	-5.135921
H	-1.230103	-1.007936	-6.821756
H	1.947648	-1.347133	-1.286464
H	2.622087	1.237648	-1.642244
H	0.371695	2.623586	-2.125781
H	-1.696772	0.897965	-2.074955
H	-0.721211	-1.549132	-1.535125
H	2.786187	-2.972076	-4.562942
H	2.426649	-1.943190	-6.011634
H	1.062455	-2.162469	-4.551482
H	3.728269	-1.090252	-3.355998
H	3.975803	1.133078	-4.302161
H	3.133684	0.605469	-5.862548
H	-1.966494	-2.267633	-4.078301
H	-0.338635	-3.842031	-3.262153
H	-0.696246	-3.589587	-5.631281

E = -545.313522788
G = -545.093326

$Cp_2SmSiH_3 + SiH_4$: Si-H activation (Si at α position at the TS)

$Cp_2SmSiH_3 + SiH_4 \rightarrow Cp_2SmSiH_3 + SiH_4$

Transition state

Sm	-0.004736	-0.328300	-0.013216
Si	-2.736871	-1.382081	0.028548
H	-1.016412	-2.329166	0.053818
Si	0.470446	-3.387425	0.081031
H	-3.556055	-1.660258	1.251298
H	-2.605990	0.157416	-0.023961
H	-3.563786	-1.741811	-1.167423
C	1.730804	0.176175	2.021977
C	0.966966	1.366928	1.889245
C	-0.356642	1.085970	2.309236
C	-0.415823	-0.277234	2.698351
C	0.878092	-0.837854	2.527071
C	1.724863	0.039647	-2.082726
C	0.864073	-0.998191	-2.521599
C	-0.427344	-0.441397	-2.721350
C	-0.358646	0.942677	-2.416577
C	0.968518	1.240841	-2.020240
H	2.790784	0.074650	1.818954
H	1.342009	2.331033	1.566005
H	-1.173729	1.796789	2.356899
H	-1.279154	-0.784453	3.111995
H	1.174205	-1.846051	2.790303
H	2.785175	-0.056021	-1.878427
H	1.152825	-2.022552	-2.723319
H	-1.295397	-0.968010	-3.099387
H	-1.171674	1.654308	-2.504739
H	1.350404	2.220806	-1.758392
H	1.965019	-3.163557	0.070913
H	0.184876	-4.195113	1.312626
H	0.179688	-4.268793	-1.097707

E = -433.728606500
G = -433.555442

$Cp_2SmSiH_3 + SiH_4$: Si-H activation (Si at β position at the TS)

$Cp_2SmSiH_3 + SiH_4 \rightarrow Cp_2SmH + H_3Si\text{-}SiH_3$

Adduct of SiH_4 on Cp_2SmSiH_3

Sm	-0.156161	-0.519788	-0.254997
C	2.574637	-0.769010	-0.126421
C	2.180751	-1.527122	-1.258304
C	1.695588	-0.630402	-2.243309
C	1.799072	0.687830	-1.724205
C	2.344302	0.600810	-0.418970
C	-2.140347	-0.460832	-2.114363
C	-2.672510	-1.242440	-1.057837
C	-2.883757	-0.392457	0.056912
C	-2.492875	0.920521	-0.316505
C	-2.032780	0.879349	-1.656173
H	3.012995	-1.164446	0.781402
H	2.256652	-2.603357	-1.357032
H	1.354263	-0.897525	-3.236653
H	1.550922	1.600735	-2.253088
H	2.584857	1.438439	0.225771
H	-1.907598	-0.812114	-3.112858
H	-2.896269	-2.301694	-1.098037
H	-3.309078	-0.687374	1.008235
H	-2.576421	1.809072	0.298955
H	-1.701859	1.727493	-2.244199
H	1.144412	0.224887	3.621842
Si	-0.041864	0.954673	3.109845
Si	-0.209634	-2.589609	1.756442
H	0.018470	1.058068	1.600772
H	0.021565	2.388535	3.537425
H	-1.332762	0.360571	3.537060
H	-0.285396	-2.897931	0.199047
H	-1.420314	-3.373841	2.208933
H	0.931762	-3.510655	2.122716

E = -433.746570748
G = -433.572852

Transition state

Sm	-0.162119	-0.425941	-0.298036
C	2.553612	-0.774690	-0.136272
C	2.157245	-1.495606	-1.293050
C	1.720443	-0.562221	-2.264826
C	1.852007	0.740126	-1.710915
C	2.372283	0.607672	-0.399382
C	-2.118341	-0.453689	-2.186604
C	-2.643459	-1.241476	-1.133433
C	-2.895310	-0.387979	-0.027786
C	-2.538224	0.933207	-0.404958
C	-2.052847	0.893087	-1.735194
H	2.972142	-1.200982	0.767418
H	2.209304	-2.570790	-1.420756
H	1.387223	-0.795625	-3.269357
H	1.639067	1.672247	-2.221591
H	2.616728	1.420123	0.274129
H	-1.859608	-0.805196	-3.178587
H	-2.844759	-2.305651	-1.173007
H	-3.340217	-0.683486	0.914708
H	-2.648010	1.820518	0.206758
H	-1.734205	1.745493	-2.324012
H	1.514282	0.335020	3.013388
Si	0.026541	0.323782	2.890219
Si	-0.352489	-2.160999	2.009998
H	-0.159618	0.942137	1.399400
H	-0.528151	1.617503	3.445603
H	-0.465885	-0.606098	4.002089
H	-0.306440	-2.755106	0.555043
H	-1.662106	-2.644577	2.550660
H	0.728720	-2.887984	2.748508

E = -433.735479562
G = -433.558128

Adduct of SiH_3-SiH_3 on Cp_2SmH

Sm	-0.162823	-0.389068	-0.302297
C	2.544050	-0.812438	-0.136678
C	2.119078	-1.570184	-1.260093
C	1.703043	-0.665805	-2.267030
C	1.875243	0.654395	-1.768166
C	2.401187	0.562431	-0.455934
C	-2.110686	-0.335837	-2.205745
C	-2.634386	-1.175121	-1.192872
C	-2.896850	-0.373952	-0.049976
C	-2.544901	0.964261	-0.362691
C	-2.052528	0.988052	-1.690848
H	2.961550	-1.212303	0.779871
H	2.142356	-2.650608	-1.344578
H	1.356663	-0.931015	-3.259123
H	1.682938	1.570393	-2.314898
H	2.667271	1.394147	0.184526
H	-1.843873	-0.639410	-3.211310
H	-2.833056	-2.236709	-1.285106
H	-3.344328	-0.713774	0.876540
H	-2.654116	1.819484	0.292551
H	-1.733705	1.868676	-2.236584
H	1.316115	0.810013	3.138467
Si	-0.030940	0.227114	2.842408
Si	-0.249023	-2.097501	2.131766
H	-0.021333	1.010073	1.305250
H	-1.234118	1.030878	3.227994
H	-0.076114	-0.775511	4.060423
H	-0.334506	-2.610220	0.648346
H	-1.502297	-2.602396	2.762017
H	0.935171	-2.808820	2.692521

E = -433.738486018
G = -433.561621

$H_3Si-SiH_3$

Si	0.054504	-0.057069	-0.028662
H	-0.019671	0.029807	1.462234
H	1.493141	-0.011128	-0.433628
H	-0.514318	-1.372820	-0.454149
Si	-1.140894	1.720166	-1.020872
H	-0.572087	3.035881	-0.595397
H	-1.066730	1.633288	-2.511717
H	-2.579493	1.674223	-0.615907

E = -11.3961950618
G = -11.374637

$Cp_2SmCH_2CH(CH_3)SiH_3$

C	1.311159	3.059110	1.015444
C	1.152504	4.368170	0.502083
C	0.657451	4.258942	-0.823328
C	0.527544	2.879941	-1.132716
C	0.922559	2.137991	0.005666
Sm	-1.424300	3.403352	0.733628
C	-3.188012	1.906148	-0.760464
C	-3.240606	3.212200	-1.310499
C	-3.864858	4.062483	-0.359949
C	-4.192803	3.285384	0.775411
C	-3.772105	1.952423	0.530309
C	-1.629699	5.303723	2.354482
C	-0.867139	5.052603	3.672723
C	-1.031150	6.133935	4.751242
Si	-1.443896	3.342588	4.234399
H	-1.301153	2.387899	3.043779
H	-4.695827	3.642018	1.665740
H	-3.919046	1.107448	1.194238
H	-2.799763	1.023118	-1.254946
H	-2.910141	3.498186	-2.302411
H	-4.076670	5.117596	-0.489947
H	0.202291	2.467903	-2.080611
H	0.968062	1.056748	0.076408
H	1.705208	2.801391	1.992036
H	1.387857	5.289636	1.019453
H	0.467793	5.083435	-1.501795
H	-2.082661	6.245046	5.040394
H	-0.700700	7.104613	4.361459
H	-0.451305	5.923711	5.659514
H	0.207378	4.943098	3.457308
H	-2.688744	5.496798	2.590326
H	-1.257872	6.237270	1.897071
H	-2.899653	3.308618	4.574495
H	-0.679488	2.656850	5.326702

E = -545.343148018
G = -545.119505

$Cp_2SmCH_2CH(CH_3)SiH_3$ + propene : 1,2 insertion

$Cp_2SmCH_2CH(CH_3)SiH_3$ + propene → $Cp_2SmCH_2CH(CH_3)CH_2CH(CH_3)SiH_3$

Transition state

C	-3.894725	2.551219	1.109454
C	-3.589843	2.784594	2.470915
C	-2.626839	1.826325	2.874101
C	-2.338145	1.000770	1.760487
C	-3.115230	1.453073	0.664181
Sm	-1.238392	3.431096	1.091453
C	0.458273	1.678024	-0.200670
C	1.124031	2.003156	1.008565
C	1.551204	3.351492	0.922411
C	1.136535	3.865227	-0.327603
C	0.458641	2.828427	-1.023764
C	-0.635240	4.726764	3.157321
C	-1.068380	5.926511	2.526091
C	-0.025926	6.953930	2.149554
C	-2.254998	5.836805	0.758406
C	-2.126377	5.575858	-0.760899
C	-3.501326	5.542981	-1.459001
Si	-1.053018	6.904554	-1.619657
H	1.350231	4.855517	-0.710473
H	0.066079	2.886520	-2.032976
H	0.041792	0.712021	-0.458741
H	1.315488	1.325372	1.832523
H	2.125355	3.884074	1.670151
H	-1.661161	0.155225	1.755196
H	-3.148601	1.004116	-0.321889
H	-4.631815	3.086269	0.522190
H	-4.035303	3.543542	3.103494
H	-2.209218	1.721720	3.868411
H	0.816170	6.496042	1.622695
H	0.371493	7.402746	3.068604
H	-0.421168	7.760488	1.525730
H	-1.982982	6.357185	2.931257
H	0.435579	4.587977	3.289704
H	-1.255440	4.328020	3.956684
H	-2.371570	6.909418	0.914267
H	-3.188671	5.381753	1.129180
H	-1.627596	4.614460	-1.028861
H	-3.412848	5.332523	-2.531723
H	-4.015658	6.503565	-1.345840
H	-4.146534	4.774244	-1.020887
H	-0.922856	6.589069	-3.076857
H	-1.749747	8.221736	-1.476858
H	0.315543	7.030257	-1.038514

E = -663.193710110
G = -662.889668

$Cp_2SmCH_2CH(CH_3)SiH_3$ + propene : allylic activation

$Cp_2SmCH_2CH(CH_3)SiH_3$ + propene → Cp_2SmCH_2-CH=CH_2 + $SiH_3CH(CH_3)CH_3$

Transition state

C	2.013331	-1.835285	-5.923395
C	0.663877	-1.813183	-6.348445
C	-0.114704	-2.475210	-5.365452
C	0.753486	-2.899981	-4.331853
C	2.071119	-2.495366	-4.671543
Sm	0.714325	-0.174350	-4.097727
C	0.763120	1.386887	-1.797750
C	1.866745	0.503058	-1.671679
C	1.361856	-0.807783	-1.505466
C	-0.055215	-0.737444	-1.528961
C	-0.422523	0.620241	-1.699568
C	-1.734372	0.487906	-5.007179
C	-2.699545	1.660245	-5.244251
C	-4.070446	1.189892	-5.761402
C	0.566203	2.196098	-5.576014
C	1.906208	1.660778	-5.789747
C	2.886893	1.551217	-4.848760
H	-2.272066	2.327012	-6.011165
H	0.813891	2.464955	-1.896970
H	2.913600	0.783201	-1.664004
H	1.952762	-1.703355	-1.356309
H	-0.736547	-1.568858	-1.389799
H	-1.433169	1.006763	-1.718045
H	0.294179	-1.398211	-7.278811
H	2.861323	-1.439611	-6.469648
H	2.968717	-2.701565	-4.100408
H	0.467701	-3.463080	-3.451651
H	-1.183319	-2.648196	-5.409968
H	-1.745211	-0.151353	-5.902451
H	-2.122960	-0.134626	-4.183910
H	0.102108	2.559769	-6.495144
H	0.515923	2.959563	-4.794080
H	-0.425369	1.352077	-5.241399
Si	-2.942606	2.768136	-3.716215
H	-4.738261	2.028025	-5.994933
H	-3.952314	0.593327	-6.674636
H	-4.575923	0.555388	-5.023962
H	2.086471	1.185258	-6.755073
H	3.835360	1.078344	-5.081258
H	2.817416	2.075719	-3.898716
H	-3.868636	3.902541	-4.035488
H	-3.552647	1.988467	-2.590412
H	-1.656617	3.357809	-3.224836

E = -663.196649566
G = -662.896796

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

H	-0.099401	0.071614	1.834539
Si	-0.007402	-0.061514	0.345079
H	-0.728725	1.096430	-0.272652
C	1.817838	-0.098625	-0.203735
C	2.547667	-1.313875	0.382081
C	2.530174	1.213148	0.149574
H	-0.711666	-1.321300	-0.054938
H	1.799968	-0.199451	-1.298608
H	3.589427	-1.347145	0.038884
H	2.567857	-1.276468	1.477701
H	2.073707	-2.257643	0.092310
H	3.570781	1.198912	-0.198270
H	2.041469	2.081908	-0.304051
H	2.552447	1.374751	1.233803

E = -124.203530006
G = -124.114782

$Cp_2SmCH_2CH(CH_3)SiH_3 + SiH_4$: Si-H activation (Si at α position at the TS)

$Cp_2SmCH_2CH(CH_3)SiH_3$ + propene → Cp_2SmSiH_3 + $SiH_3CH(CH_3)CH_3$

Adduct of SiH4 on $Cp_2SmCH_2CH(CH_3)SiH_3$

C	2.307970	-0.780821	2.225301
C	1.175620	-0.182157	2.835749
C	1.099573	1.163069	2.399775
C	2.180555	1.394685	1.510043
C	2.930585	0.193545	1.405817
Sm	0.566440	-0.305862	0.151098
C	-0.576336	-3.144275	0.892068
C	-1.417813	-4.271551	0.279318
Si	-0.456118	-5.922096	0.269545
C	-0.203882	0.389496	-2.384008
C	1.093105	0.935933	-2.200236
C	2.020475	-0.137276	-2.145447
C	1.296076	-1.346944	-2.284868
C	-0.077956	-1.020175	-2.430040
Si	-2.167534	0.836078	0.682452
H	-2.730233	0.724624	2.086105
H	-3.318182	0.328402	-0.165999
H	-2.229534	2.330914	0.433162
H	-1.160779	-2.204103	0.879519
H	2.422045	2.338059	1.034072
H	0.358776	1.889260	2.709436
H	0.502220	-0.655786	3.540581
H	2.665292	-1.791029	2.393892
H	3.842918	0.058889	0.837381
H	3.096065	-0.046032	-2.053483
H	1.724790	-2.342424	-2.326706
H	-0.889397	-1.721363	-2.588512
H	-1.122834	0.950336	-2.495433
H	1.337897	1.991131	-2.160427
H	-0.324884	-3.344609	1.938944
H	0.374211	-3.032300	0.342925
C	-2.763235	-4.412485	1.002716
H	-1.610674	-4.024212	-0.773762
H	-1.258827	-6.988219	-0.402890
H	0.843436	-5.761522	-0.457180
H	-0.162250	-6.347269	1.674121
H	-3.385913	-5.187931	0.545675
H	-2.623664	-4.677902	2.056911
H	-3.327818	-3.473038	0.971242

E = -551.659058150
G = -551.409909

Transition state

C	2.584472	-0.753755	2.202700
C	1.350553	-0.523568	2.858426
C	0.913163	0.783786	2.523871
C	1.881197	1.362852	1.662793
C	2.914709	0.412771	1.463913
Sm	0.739717	-0.627357	0.166864
C	-0.379157	-2.833384	0.820930
C	-1.470886	-3.745654	0.247375
Si	-0.808211	-5.526064	0.064318
C	-0.285115	-0.327222	-2.372759
C	0.692516	0.693344	-2.235814
C	1.966175	0.074736	-2.178709
C	1.775965	-1.328651	-2.271322
C	0.384988	-1.575319	-2.397096
Si	-2.236212	0.067327	0.725737
H	-2.799731	0.185143	2.107205
H	-3.358806	-0.247709	-0.212593
H	-1.743134	1.443884	0.347530
H	-1.238499	-1.354128	0.758996
H	1.856186	2.369208	1.260465
H	0.025088	1.274471	2.904622
H	0.845035	-1.211212	3.525163
H	3.193134	-1.647525	2.285011
H	3.818734	0.566348	0.886304
H	2.919468	0.585344	-2.109929
H	2.561050	-2.076316	-2.297134
H	-0.079110	-2.545327	-2.525746
H	-1.351302	-0.174246	-2.491653
H	0.501766	1.760446	-2.222807
H	-0.294120	-2.986990	1.904454
H	0.615545	-3.131921	0.402862
C	-2.740023	-3.733239	1.109345
H	-1.739677	-3.411636	-0.766066
H	-1.822491	-6.460903	-0.527430
H	0.402565	-5.535052	-0.819483
H	-0.408674	-6.060226	1.405423
H	-3.535117	-4.344938	0.670295
H	-2.538343	-4.119324	2.115604
H	-3.139034	-2.718323	1.227833

E = -551.612781113
G = -551.364734

Adduct of $CH_3CH(CH_3)SiH_3$ on Cp_2SmSiH_3

C	2.321168	-1.185585	2.286842
C	1.224888	-0.550037	2.912888
C	1.143798	0.778006	2.415886
C	2.187853	0.959909	1.477553
C	2.912732	-0.256904	1.390676
Sm	0.515574	-0.847952	0.241720
C	0.244048	-3.284461	0.659746
C	-0.891472	-4.066119	-0.030054
Si	-0.785767	-5.910030	0.449579
C	-0.473293	-1.112723	-2.339494
C	-0.301527	0.286105	-2.161535
C	1.085426	0.548032	-2.058653
C	1.772355	-0.689258	-2.166353
C	0.806523	-1.713291	-2.350876
Si	-2.557556	1.336994	1.162889
H	-2.833266	1.428267	2.621790
H	-3.816572	1.274145	0.372374
H	-1.693449	2.459138	0.706895
H	-1.826684	0.042547	0.923999
H	2.416244	1.876479	0.946716
H	0.446462	1.540717	2.745328
H	0.582890	-0.990148	3.667320
H	2.652969	-2.200877	2.464927
H	3.799286	-0.426947	0.790829
H	1.544877	1.523167	-1.949211
H	2.848179	-0.820734	-2.167452
H	1.013910	-2.767161	-2.487837
H	-1.416683	-1.626583	-2.482771
H	-1.090072	1.030800	-2.164436
H	0.145815	-3.406177	1.753908
H	1.218815	-3.744858	0.418843
C	-2.272219	-3.488596	0.301350
H	-0.759942	-4.026162	-1.121496
H	-1.836438	-6.779395	-0.190113
H	0.549467	-6.469718	0.062696
H	-0.935252	-6.054400	1.935061
H	-3.089642	-4.032185	-0.186483
H	-2.460249	-3.510612	1.382128
H	-2.350072	-2.437457	-0.020382

E = -551.627667192
G = -551.382605

$Cp_2SmCH_2CH(CH_3)SiH_3 + SiH_4$: Si-H activation (Si at β position at the TS)

$Cp_2SmCH_2CH(CH_3)SiH_3$ + propene → $Cp_2SmH + SiH_3CH_2CH(CH_3)SiH_3$

Transition state

C	0.734768	-3.828079	-2.489900
C	1.819015	-2.979879	-2.150589
C	2.691296	-3.706868	-1.301318
C	2.150170	-5.006935	-1.126928
C	0.941347	-5.081229	-1.858413
Sm	0.380341	-3.286861	0.161244
C	-1.200738	-1.391576	-0.966655
C	-2.053093	-2.054515	-0.051149
C	-1.623921	-1.729734	1.261967
C	-0.502045	-0.871948	1.155888
C	-0.235683	-0.664311	-0.222339
Si	-1.449761	-5.008926	2.124746
C	0.423590	-4.167992	2.732023
C	1.857999	-4.694901	2.482182
Si	1.982800	-6.599879	2.664573
C	2.867113	-4.018163	3.427563
H	-2.813123	-5.003999	1.442371
H	-1.110703	-6.447974	2.361215
H	-1.966041	-4.441319	3.450546
H	-2.097152	-2.050976	2.182272
H	0.031479	-0.414965	1.982276
H	0.531690	-0.018586	-0.633467
H	-1.287141	-1.410257	-2.045755
H	-2.899536	-2.682909	-0.300383
H	3.637573	-3.350936	-0.907842
H	2.604822	-5.820041	-0.573957
H	0.301531	-5.950623	-1.943446
H	-0.084819	-3.580008	-3.153286
H	1.973482	-1.968811	-2.507952
H	-0.923613	-4.911681	0.486609
H	2.843891	-2.925872	3.320262
H	2.628075	-4.240038	4.473793
H	3.893691	-4.352172	3.240608
H	2.227075	-4.516975	1.452425
H	0.159724	-4.454636	3.755109
H	0.429281	-3.060256	2.804392
H	1.424641	-7.010969	3.988282
H	1.279484	-7.327495	1.569307
H	3.432651	-6.974821	2.618707

E = -551.605342753
G = -551.349882

$Cp_2SmCH(CH_3)CH_2SiH_3$

C	-3.440318	1.820389	0.745778
C	-3.252318	2.211237	-0.600802
C	-3.490737	3.607268	-0.689196
C	-3.847831	4.075372	0.601726
C	-3.810004	2.973681	1.488992
Sm	-1.170025	3.402861	0.754642
C	0.466968	1.664521	-0.613109
C	1.200653	1.985177	0.555449
C	1.588410	3.347994	0.471066
C	1.093589	3.868700	-0.746916
C	0.393892	2.830821	-1.417300
C	-1.022540	5.712593	1.771209
C	-1.640185	5.571967	3.184336
H	-2.713464	5.344310	3.131142
Si	-0.853408	4.150973	4.149157
H	-0.813415	2.933151	3.220392
H	-4.069631	2.993491	2.541469
H	-3.363262	0.810005	1.132152
H	-2.988993	1.557271	-1.423519
H	-3.464282	4.200811	-1.596466
H	-4.121829	5.091626	0.856125
H	-0.065925	2.899934	-2.396494
H	0.058905	0.692283	-0.864058
H	1.462263	1.297360	1.352215
H	2.182514	3.889011	1.197126
H	1.245177	4.876749	-1.114368
H	-1.558243	6.492615	3.791861
H	-1.706774	6.356581	1.192485
C	0.323758	6.435334	1.845494
H	-1.616331	3.670911	5.343625
H	0.572678	4.352868	4.541576
H	0.258808	7.407357	2.367242
H	1.088105	5.854792	2.380584
H	0.731205	6.638156	0.848367

E = -545.337694183
G = -545.113894

$Cp_2SmCH(CH_3)CH_2SiH_3 + SiH_4$: Si-H activation (Si at α position at the TS)

$Cp_2SmCH(CH_3)CH_2SiH_3 + SiH_4 \rightarrow Cp_2SmH + SiH_3\text{-}CH_2\text{-}CH_2\text{-}CH_3$

Adduct of SiH_4 on $Cp_2SmCH(CH_3)CH_2SiH_3$

C	1.915229	-0.456589	2.057215
C	0.785146	0.077522	2.723788
C	0.702532	1.456654	2.401898
C	1.774363	1.770667	1.525644
C	2.524318	0.587787	1.313596
Sm	2.915750	1.284969	3.950210
C	5.496779	-0.776355	5.026070
C	5.514428	-2.308672	5.106394
H	5.305072	-2.618868	6.137209
C	4.531088	3.471800	4.365539
C	4.355426	2.905742	5.655904
C	2.999036	3.070513	6.028925
C	2.332496	3.728864	4.963363
C	3.280480	3.982176	3.938273
Si	7.145832	-3.151644	4.606999
Si	1.595254	-0.220724	6.187177
H	2.276230	-0.240406	7.543034
H	1.297121	-1.690809	5.958506
H	0.224605	0.330488	6.528643
H	4.571232	-0.424056	5.518245
H	1.290530	4.026614	4.954340
H	2.556850	2.772142	6.970593
H	5.131716	2.465708	6.271354
H	5.467866	3.553983	3.824969
H	3.091456	4.509165	3.011070
H	1.960927	2.733503	1.065559
H	3.382932	0.489542	0.658106
H	2.227721	-1.494623	2.076346
H	0.093668	-0.475203	3.346459
H	-0.072370	2.139475	2.729780
H	6.315434	-0.356363	5.622545
C	5.592279	-0.231855	3.599207
H	4.703596	-2.731481	4.499087
H	7.058922	-4.617820	4.881362
H	7.452384	-2.967952	3.153467
H	8.281170	-2.575608	5.393809
H	6.524196	-0.527906	3.108111
H	4.788650	-0.618852	2.954313
H	5.600731	0.870943	3.578242

E = -551.659682555
G = -551.407079

Transition state

C	2.281941	-0.605501	2.081756
C	1.141738	-0.279420	2.858538
C	0.795058	1.068700	2.584631
C	1.716875	1.572840	1.632017
C	2.636982	0.539270	1.323412
Sm	3.173943	1.240302	3.929172
C	4.977415	-0.539068	4.634859
C	4.921704	-2.067070	4.711286
H	4.318819	-2.389360	5.572512
C	4.632196	3.542236	4.309262
C	4.640814	2.903093	5.575397
C	3.322018	2.938858	6.092583
C	2.496349	3.598274	5.145144
C	3.307125	3.974890	4.044917
Si	6.613970	-2.925395	4.886583
Si	2.041388	-0.414217	6.326818
H	2.583919	-0.303001	7.719442
H	1.493629	-1.799109	6.163438
H	0.858176	0.513577	6.258992
H	3.475412	-0.360752	5.333439
H	1.440788	3.814946	5.261959
H	3.009003	2.574257	7.063742
H	5.510121	2.497566	6.078754
H	5.495937	3.720169	3.678462
H	2.979830	4.528400	3.172660
H	1.698928	2.562330	1.190503
H	3.440443	0.600687	0.598049
H	2.764043	-1.574570	2.038515
H	0.599019	-0.956530	3.507379
H	-0.051787	1.604942	2.997012
H	5.505550	-0.140401	5.509876
C	5.660563	-0.035522	3.365210
H	4.414135	-2.479966	3.829127
H	6.461652	-4.407432	5.046735
H	7.481569	-2.682797	3.689894
H	7.332763	-2.392241	6.087533
H	6.742941	0.101504	3.480126
H	5.493448	-0.710420	2.519941
H	5.347756	0.979201	2.997618

E = -551.614894625
G = -551.364647

Adduct of $CH_3CH_2CH_2SiH_3$ on Cp_2SmSiH_3

C	2.697032	-0.411972	1.702364
C	1.737476	-0.744863	2.682628
C	0.901821	0.388132	2.882839
C	1.345020	1.415884	2.013919
C	2.463084	0.928497	1.291940
Sm	3.356349	1.173407	3.880701
C	5.082905	-0.492545	4.527561
C	4.816506	-2.002573	4.451698
H	4.020100	-2.305823	5.145099
C	4.750907	3.529035	4.104678
C	4.857429	2.941933	5.392476
C	3.574570	2.971083	5.989808
C	2.672179	3.572887	5.074462
C	3.401838	3.921439	3.910388
Si	6.349659	-3.051378	4.880501
Si	1.477322	-0.148256	6.783713
H	1.970465	0.031009	8.177242
H	0.753678	-1.441157	6.635032
H	0.593471	0.986892	6.397761
H	2.687916	-0.193216	5.885603
H	1.622391	3.776643	5.252293
H	3.336836	2.639278	6.994443
H	5.764793	2.569501	5.851535
H	5.567829	3.696164	3.411834
H	3.005027	4.428834	3.038868
H	0.894410	2.395178	1.904205
H	3.002550	1.461192	0.516852
H	3.463551	-1.070925	1.312371
H	1.638479	-1.706272	3.172685
H	0.032695	0.435106	3.529387
H	5.544845	-0.236104	5.488105
C	5.925652	0.059410	3.388730
H	4.460024	-2.292380	3.454752
H	6.104865	-4.532455	4.806866
H	7.492077	-2.740845	3.961018
H	6.797435	-2.735282	6.275904
H	6.827006	0.591170	3.709417
H	6.219584	-0.700794	2.655462
H	5.404437	0.830155	2.731470

E = -551.626443078
G = -551.378067