Supporting Information

A Combined Computational and Experimental Study of Rh-Catalyzed C–H Silylation with Silacyclobutanes: Insights Leading to a More Efficient Catalyst System

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S1. General Information

All air-sensitive manipulations were performed in a N_2-flushed glovebox. Toluene was purified following standard procedure prior to use. Substrates and diphosphine ligand TMS-segphos were prepared following literature procedures.[1,2] All other reagents were purchased from commercial sources and used as received. ^{1}H, ^{13}C, and ^{31}P NMR spectra were recorded in $CDCl_3$ or toluene-d_8 solution on Bruker Aescend^{TM} 400 MHz instrument and spectral data were reported in ppm relative to residual solvent peak. High-resolution mass spectral (HRMS) data were measured by means of ESI−IT−TOF and MALDI−TOF techniques.

S2. Benchmark of Density Functionals

Four density functionals, namely, B3LYP-D3(BJ), PBE0-D3(BJ), M06, and ωB97X-D, were adopted in computing the overall Gibbs free energy barriers for the [Rh]−Cl and [Rh]−H mechanisms, the Gibbs free energy difference between C(sp^2)−H and C(sp^3)−H bond activation (**TS14-sp^2** versus **TS14-sp^3**), and the competition between Si−C bond activation transition states **TS15-*S*** and **TS15-*R***. The computed activation Gibbs free energies [$\Delta G^{\ddagger}$([Rh]−Cl) and $\Delta G^{\ddagger}$([Rh]−H)] and Gibbs free energy differences [$\Delta\Delta G^{\ddagger}$(**TS14-sp^3** − **TS14-sp^2**) and $\Delta\Delta G^{\ddagger}$(**TS15-*R*** − **TS15-*S***)] were listed in Table S1. Different density functionals provided similar results and conclusions, suggesting that the results with B3LYP-D3(BJ) functional are reliable.

Table S1. Benchmark of Density Functionals[a]

DF	B3LYP-D3(BJ)	PBE0-D3(BJ)	M06	ωB97X-D
$\Delta G^{\ddagger}$([Rh]−Cl) (from **CAT1** to **TS4**)	49.0	50.8	51.0	52.7
$\Delta G^{\ddagger}$([Rh]−H) (from **CAT2** to **TS8**)	25.3	24.9	22.6	24.8
$\Delta\Delta G^{\ddagger}$(**TS14-sp^3** − **TS14-sp^2**)	0.4	1.6	1.4	1.2
$\Delta\Delta G^{\ddagger}$(**TS15-*R*** − **TS15-*S***)	2.2	2.1	2.5	2.6

[a]Reported in kcal/mol. Computed at the SMD(toluene)/DF/def2-TZVP-6-311++G(d,p)//B3LYP/LANL2DZ-6-31G(d) level.

S3. DFT Study on the [Rh]−Cl Mechanism

The reaction starts with the dissociation of [Rh(**L1**)Cl]$_2$ (**CAT1**). The resulting intermediate **INT0** then undergoes Si−C bond activation (via **TS1**) to form silametallacycle **INT1**. Subsequently, **INT1** proceeds through β-H elimination (via **TS2**) followed by reductive elimination (via **TS3**) to afford Rh^{I} intermediate **INT3** and HCl. **INT3** then undergoes C−H bond activation (via **TS4**) followed by reductive elimination (via **TS16**) to form **INT13**. Finally, alkene insertion (via **TS17**) and the subsequent protodemetallation with HCl (via **TS18** and **TS19**) occur to produce dibenzosilole **2a** and regenerate the [Rh]−Cl catalyst **CAT1**. DFT calculations indicate that the overall activation free energy is 49.0 kcal/mol (from **CAT1** to **TS4**), which is too high for a reaction that proceeds at 80 °C. In addition, the rate-limiting step of the [Rh]−Cl mechanism is the aryl C−H bond activation, which is inconsistent with the kinetic isotope effect (KIE) observed in our previous study.[1] Based on these results, we suggest that the [Rh]−Cl mechanism should not be feasible.

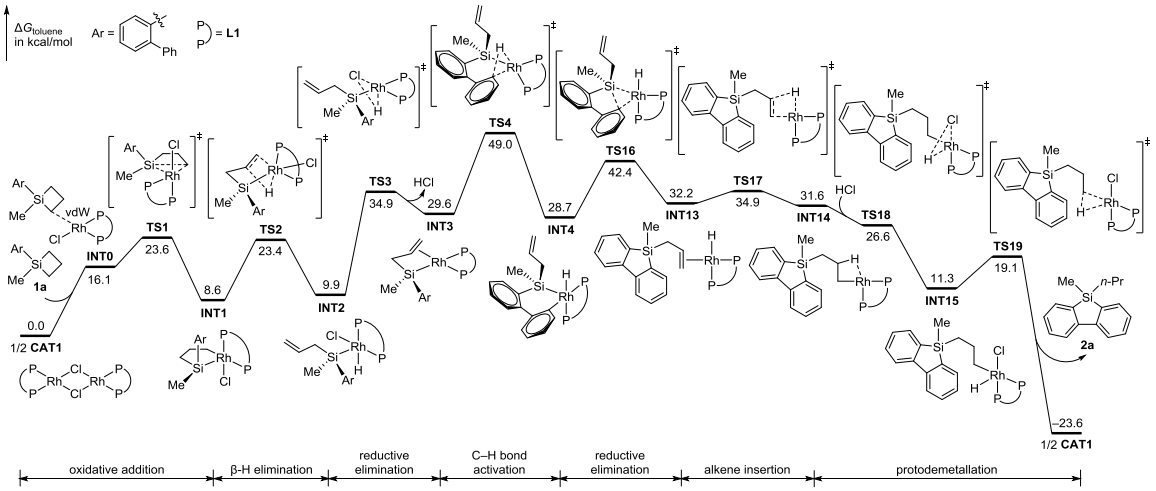

Figure S1. Free energy profile for the [Rh]−Cl mechanism. Computed at the SMD(toluene)/B3LYP-D3(BJ)/def2-TZVP-6-311++G(d,p)//B3LYP/LANL2DZ-6-31G(d) level.

S4. Energy Decomposition Analysis

To understand the origins of enantioselectivity in depth, we applied the distortion/interaction−activation strain model[3] on Si−C bond activation transition states (**TS15-*S*** and **TS15-*R***) and several non-stationary points along the intrinsic reaction coordinate (IRC) paths.[4] The energy change ΔE, $E - E$(SCB; minimum) − E(cat; minimum), is decomposed into three contributions: the distortion energy of the SCB substrate ΔE^{dist}(SCB), the distortion energy of the catalyst ΔE^{dist}(cat), and the interaction energy ΔE^{int} between the distorted substrate and catalyst. As depicted in Figure S2, the reason why the *S* pathway is favored over the *R* pathway lies in the lower extent of distortion of the catalyst and the smaller interaction energy.

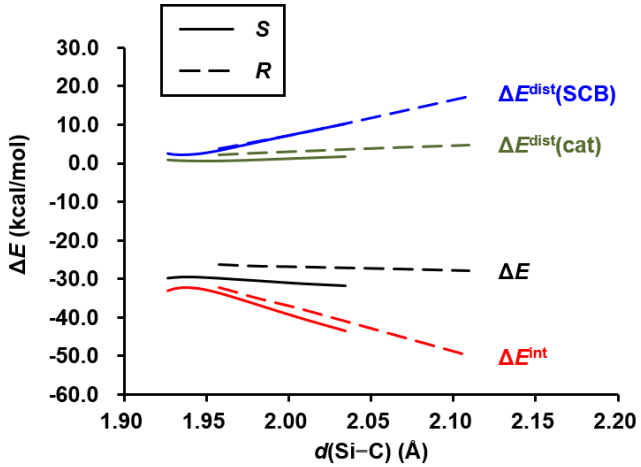

Figure S2. Activation strain diagram of Si−C bond activation. Computed at the B3LYP-D3(BJ)/LANL2DZ-6-31G(d)//B3LYP/LANL2DZ-6-31G(d) level. Si−C bond distances are 1.95 and 2.00 Å in **TS15-*S*** and **TS15-*R***, respectively.

Based on the generalized Kohn–Sham energy decomposition analysis (GKS-EDA),[5] the interaction energy ΔE^{int} can be further decomposed into steric interaction (ΔE^{steric}; the sum of electrostatic and exchange repulsion terms), polarization (ΔE^{pol}), and correlation/dispersion ($\Delta E^{corr/disp}$; the sum of correlation and dispersion terms). As shown in Figure S3, the steric interaction term determines the interaction energy difference between the two pathways. Therefore, we conclude that the steric interactions and the resulting distortion of the catalyst determine the enantioselectivity.

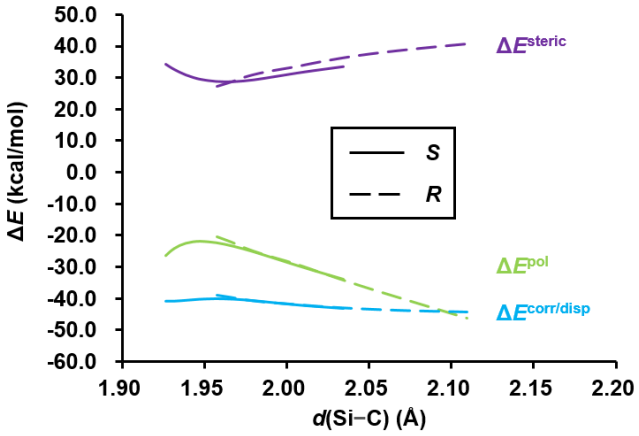

Figure S3. Generalized Kohn–Sham energy decomposition analysis (GKS-EDA) of the interaction energy. Computed at the B3LYP-D3(BJ)/LANL2DZ-6-31G(d)//B3LYP/LANL2DZ-6-31G(d) level. Si–C bond distances are 1.95 and 2.00 Å in **TS15-*S*** and **TS15-*R***, respectively.

Table S2. Energy Decomposition Analysis[a]

d(Si–C) (Å)	ΔE	ΔE^{dist}(SCB)	ΔE^{dist}(cat)	ΔE^{int}	ΔE^{steric}	ΔE^{pol}	$\Delta E^{corr/disp}$
S pathway							
1.927	−29.6	2.5	0.9	−33.0	34.2	−26.4	−40.8
1.929	−29.6	2.3	0.8	−32.7	33.3	−25.2	−40.8
1.932	−29.5	2.2	0.8	−32.5	32.5	−24.2	−40.8
1.935	−29.5	2.1	0.7	−32.3	31.7	−23.3	−40.7
1.939	−29.4	2.2	0.7	−32.3	30.8	−22.5	−40.6
1.943	−29.5	2.3	0.6	−32.4	30.1	−22.1	−40.4
1.948 (**TS15-*S***)	−29.5	2.6	0.6	−32.7	29.5	−22.0	−40.2
1.957	−29.8	3.2	0.6	−33.6	28.8	−22.4	−40.0
1.968	−30.0	4.2	0.7	−34.9	28.8	−23.5	−40.2
1.980	−30.4	5.4	0.9	−36.7	29.3	−25.3	−40.7
1.994	−30.8	6.6	1.1	−38.5	30.4	−27.5	−41.4
2.011	−31.2	8.1	1.3	−40.6	31.8	−30.2	−42.2
2.034	−31.6	10.2	1.7	−43.5	33.4	−33.8	−43.1

R pathway							
1.958	−26.2	3.9	2.2	−32.3	27.2	−20.5	−39.0
1.966	−26.4	4.5	2.4	−33.3	28.6	−22.2	−39.7
1.974	−26.6	5.2	2.5	−34.3	30.1	−24.0	−40.4
1.986	−26.8	6.2	2.7	−35.7	31.7	−26.2	−41.2
2.004 (**TS15-*R***)	−26.9	7.6	3.0	−37.5	33.3	−28.9	−41.9
2.022	−27.0	9.3	3.3	−39.6	35.2	−32.1	−42.7
2.044	−27.2	11.3	3.7	−42.2	37.1	−36.0	−43.3
2.074	−27.5	14.1	4.1	−45.7	38.9	−40.7	−43.9
2.109	−28.0	17.4	4.6	−50.0	40.7	−46.3	−44.4

[a]Energies are reported in kcal/mol. Computed at the B3LYP-D3(BJ)/LANL2DZ-6-31G(d)//B3LYP/LANL2DZ-6-31G(d) level. Corrections for basis set superposition error (BSSE) are considered by using the counterpoise method of Bernardi and Boys.[6]

S5. Discussion on H/D Scrambling

In our previous work,[1] we found that the C–H silylation of substrate **1a-d$_5$** gave product **2a-d$_5$** with deuterium incorporation at both C1 and C2 positions of the *n*-propyl group. Herein, we propose a possible mechanism for this phenomenon. As depicted in Figure S4, reductive elimination of intermediate **K** generates C1-deuterated Rh^{I} intermediate **L**. Alternatively, intermediate **K** may undergo endocyclic β-H elimination to give intermediate **M**, which could proceed through H/D scrambling followed by alkene insertion to furnish C2-deuterated Rh^{I} intermediate **N**. Finally, reductive elimination of intermediate **N** leads to the formation of C2-deuterated Rh^{I} intermediate **O**.

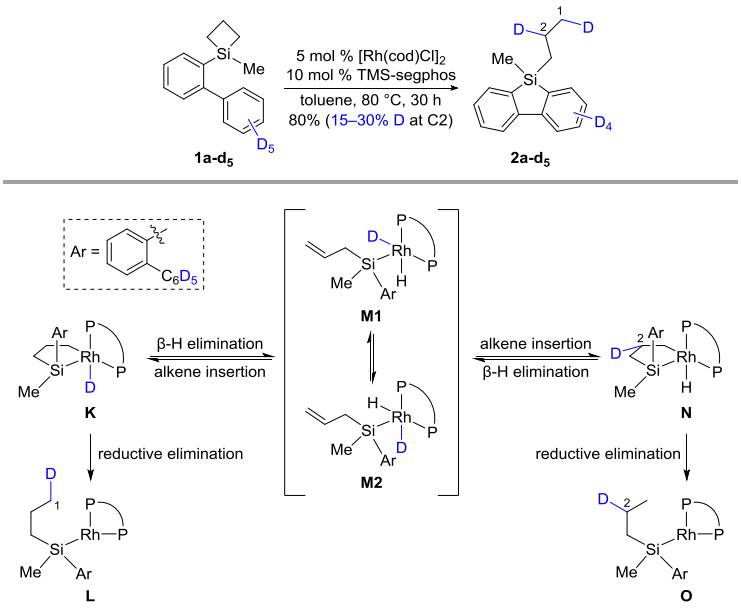

Figure S4. Rationalization of H/D scrambling. Diphosphine ligand = TMS-segphos.

S6. Computed Energies of the Stationary Points

Table S3. Thermal Corrections to Gibbs Energies (TCGs) and Single-Point Energies (SPEs)

	TCG[a,b] (a.u.)	SPE[a] (a.u.)	SPE[c] (a.u.)
HCl	−0.011223	−460.792269	−460.838415
1a	0.248930	−910.033394	−910.326646
2a	0.248596	−910.073709	−910.363900
6a	0.234324	−1369.677017	−1370.012247
CAT1	1.180834	−10687.560877	−10692.074439
CAT2	1.202314	−9768.245679	−9772.696646
INT0	0.843172	−6253.794593	−6256.340524
INT1	0.854863	−6253.788414	−6256.364119
INT2	0.847217	−6253.772700	−6256.354441
INT3	0.839194	−5792.953382	−5795.468374
INT4	0.837051	−5792.938152	−5795.467753
INT5	0.843871	−6253.805693	−6256.345041
INT6	0.841612	−6253.798087	−6256.340608
INT7	0.839258	−6253.780632	−6256.328782
INT8	0.848289	−5794.133919	−5796.634491
INT9	0.858977	−5794.153840	−5796.679850
INT10	0.860537	−5794.177804	−5796.698665
INT11	0.862251	−5794.172782	−5796.707526
INT12	0.856837	−5794.158493	−5796.672128
INT13	0.832381	−5792.960483	−5795.457488
INT14	0.833927	−5792.967687	−5795.460034
INT15	0.847400	−6253.794119	−6256.352425
TS1	0.855269	−6253.765020	−6256.340743
TS2	0.851780	−6253.753492	−6256.337478
TS3	0.844444	−6253.738706	−6256.311894
TS4	0.834887	−5792.907209	−5795.433198
TS5	0.854915	−6253.768973	−6256.337125
TS6	0.841535	−6253.794835	−6256.339257
TS7	0.847513	−6253.748435	−6256.317859
TS8	0.858939	−5794.118313	−5796.642052
TS9	0.860240	−5794.132032	−5796.662900
TS10	0.860505	−5794.140072	−5796.668352
TS11	0.861269	−5794.155151	−5796.684882
TS12	0.859473	−5794.152762	−5796.675530
TS13	0.857528	−5794.091743	−5796.621036
TS14-sp^2	0.885344	−5833.451823	−5836.004002
TS14-sp^3	0.884151	−5833.455532	−5836.002184
TS15-*S*	1.480802	−6698.645412	−6701.626004
TS15-*R*	1.481183	−6698.642287	−6701.622957
TS16	0.839318	−5792.922910	−5795.448162

TS17	0.831298	−5792.956334	−5795.452143
TS18	0.840580	−6253.766536	−6256.321215
TS19	0.845927	−6253.783738	−6256.338477

[a]Computed at the B3LYP/LANL2DZ-6-31G(d) level.

[b]A standard state at 1 atm and 298 K was used.

[c]Computed at the SMD(toluene)/B3LYP-D3(BJ)/def2-TZVP-6-311++G(d,p)//B3LYP/LANL2DZ-6-31G(d) level.

S7. Cartesian Coordinates of the Stationary Points

HCl

Cl	0.000000	0.000000	0.071638
H	0.000000	0.000000	−1.217840

1a

C	0.592946	1.296631	−0.134098
C	−0.790382	1.006410	−0.003043
C	−1.691919	2.086900	−0.028833
C	−1.264280	3.408572	−0.168649
C	0.097754	3.680007	−0.283780
C	1.014421	2.629132	−0.265177
C	1.634627	0.228215	−0.137717
C	2.707898	0.278049	0.768158
C	3.696733	−0.705970	0.762039
C	3.636406	−1.756769	−0.156345
C	2.582180	−1.812639	−1.069645
C	1.591872	−0.828695	−1.061768
H	−2.756394	1.892769	0.077037
H	−1.989992	4.217645	−0.183503
H	0.448364	4.702940	−0.394503
H	2.075850	2.836657	−0.374190
H	2.751935	1.087183	1.492404
H	4.513077	−0.653788	1.477812
H	4.406652	−2.523302	−0.161898
H	2.533328	−2.618390	−1.797464
H	0.789691	−0.865194	−1.792393
C	−3.411372	−0.876918	0.266864
C	−1.732748	−2.018923	−1.035607
C	−3.188672	−2.222965	−0.501800
H	−3.874296	−0.130027	−0.389450
H	−4.015465	−0.948176	1.176702
H	−1.740812	−1.567456	−2.035388
H	−1.108845	−2.917084	−1.071074
H	−3.933915	−2.428834	−1.280249
H	−3.215224	−3.064404	0.200594
Si	−1.508034	−0.717096	0.347451
C	−0.784246	−1.431443	1.943038
H	0.300058	−1.565022	1.871042
H	−0.986053	−0.766859	2.791748
H	−1.232794	−2.406880	2.166648

2a

Si	−0.935697	−0.205916	0.998838
C	−0.070038	1.359510	0.402494
C	−0.450665	2.702848	0.450791
C	0.382589	3.700193	−0.066403
C	1.608077	3.350438	−0.637838
C	2.006669	2.013563	−0.696952
C	1.176287	1.011238	−0.181252
C	1.488370	−0.445091	−0.184498
C	2.655984	−1.016618	−0.704182
C	2.841458	−2.399446	−0.649908
C	1.868728	−3.223270	−0.079160
C	0.700073	−2.657646	0.441258
C	0.495110	−1.276418	0.396965
C	−1.186675	−0.262768	2.874464
C	−2.586652	−0.551042	0.124834
C	−2.544163	−0.536918	−1.414781
C	−3.910641	−0.809508	−2.054867
H	−1.403653	2.986022	0.894256
H	0.078806	4.742954	−0.024162
H	2.258624	4.122666	−1.040670

H	2.964173	1.763289	−1.145934
H	3.425566	−0.393905	−1.152483
H	3.750982	−2.835221	−1.055730
H	2.020073	−4.298897	−0.040199
H	−0.051730	−3.308551	0.884028
H	−0.248350	−0.060087	3.401932
H	−1.549221	−1.246391	3.197318
H	−1.923166	0.482962	3.198018
H	−3.319917	0.189284	0.481470
H	−2.964056	−1.524156	0.475923
H	−1.821530	−1.284593	−1.767104
H	−2.166570	0.434207	−1.760855
H	−3.850448	−0.794190	−3.149708
H	−4.647738	−0.055888	−1.750247
H	−4.299152	−1.791063	−1.755388

6a

C	1.888731	−0.984483	−1.214706
C	2.922093	−3.263850	−0.897307
C	3.021907	−1.932327	−0.938538
H	2.168313	−0.261476	−1.994121
H	1.013926	−1.534346	−1.583129
H	1.981511	−3.776472	−1.090743
H	3.780148	−3.891534	−0.672715
H	3.987572	−1.469402	−0.736760
Si	1.340299	0.010688	0.314406
C	0.823498	−1.102943	1.735596
H	−0.052026	−1.707582	1.481396
H	1.649599	−1.778522	1.982201
H	0.585879	−0.511214	2.626039
C	0.096957	1.381934	−0.115502
C	0.572728	2.693372	−0.311836
C	−1.303450	1.168251	−0.208182
C	−0.285354	3.759962	−0.579201
H	1.637395	2.890507	−0.235003
C	−2.158930	2.252893	−0.455523
C	−1.659984	3.540747	−0.642767
H	0.120502	4.757458	−0.724946
H	−3.228766	2.071413	−0.516679
H	−2.341927	4.363734	−0.840202
Cl	3.092879	0.993777	0.986058
C	−1.934253	−0.180277	−0.060644
C	−2.740034	−0.472867	1.051274
C	−1.780892	−1.161782	−1.052284
C	−3.349305	−1.721466	1.182475
H	−2.874182	0.281442	1.822032
C	−2.391018	−2.411413	−0.922998
H	−1.200382	−0.931892	−1.941435
C	−3.172547	−2.696854	0.197976
H	−3.961333	−1.933252	2.055276
H	−2.263357	−3.157049	−1.703361
H	−3.646885	−3.669037	0.300487

CAT1

C	5.974956	−0.389066	−0.641566
C	5.009037	−1.366716	−1.036283
C	5.188240	−2.072275	−2.233955
C	6.284088	−1.868135	−3.089948
C	7.204646	−0.924686	−2.693338
C	7.047166	−0.215509	−1.505480
C	5.977220	0.388395	0.632370
C	5.012603	1.365765	1.030867
C	5.195685	2.070562	2.228390
C	6.294384	1.865992	3.080621
C	7.213771	0.922985	2.680284
C	7.052335	0.214436	1.492576
H	4.465085	−2.824746	−2.519524
H	6.399150	−2.430189	−4.010068
H	4.473325	2.822695	2.516814
H	6.412410	2.427405	4.000759
P	3.471558	−1.643895	−0.025314
P	3.472588	1.644756	0.024184
Rh	1.913643	0.001007	−0.000563
C	−5.976814	0.388907	−0.629560
C	−5.012665	1.366249	−1.029229
C	−5.197214	2.071242	−2.226404
C	−6.297034	1.866865	−3.077231
C	−7.215983	0.923895	−2.675788
C	−7.053106	0.215194	−1.488362
C	−5.972678	−0.389002	0.644129
C	−5.006251	−1.366954	1.036997
C	−5.183874	−2.073165	2.234494

C	−6.278495	−1.869363	3.092153
C	−7.199491	−0.925580	2.697378
C	−7.043625	−0.215796	1.509662
H	−4.475115	2.823326	−2.515628
H	−6.416222	2.428382	−3.997155
H	−4.460513	−2.825959	2.518682
H	−6.392350	−2.431937	4.012105
P	−3.471339	1.644987	−0.024566
P	−3.470592	−1.643667	0.023133
Rh	−1.912572	0.000899	−0.001852
O	8.344826	−0.514421	−3.334676
O	8.086982	0.678687	−1.374124
O	8.091652	−0.679808	1.357415
O	8.356072	0.512337	3.317610
O	−8.359095	0.513417	−3.311743
O	−8.092328	−0.678975	−1.352003
O	−8.083580	0.678489	1.380183
O	−8.338764	−0.515606	3.340495
C	−9.036937	−0.317545	−2.364201
H	−9.863019	0.247197	−1.908210
H	−9.396395	−1.219344	−2.862807
C	−9.022015	0.316663	2.397977
H	−9.851273	−0.247167	1.946660
H	−9.377820	1.218217	2.899654
C	9.035085	−0.318379	2.370684
H	9.861577	0.246578	1.915691
H	9.394120	−1.220201	2.869540
C	9.026832	0.317254	−2.390742
H	9.855360	−0.246933	−1.938520
H	9.383491	1.219017	−2.891434
C	2.824044	−3.244465	−0.709144
C	2.078424	−3.203919	−1.898909
C	3.026837	−4.481702	−0.087961
C	1.569072	−4.369977	−2.489107
H	1.884458	−2.237738	−2.357042
C	2.525230	−5.674114	−0.641283
H	3.574844	−4.523961	0.847648
C	1.806932	−5.595932	−1.843581
H	1.413666	−6.510627	−2.285007
C	4.144622	−2.130273	1.629450
C	5.334927	−2.856500	1.773562
C	3.419951	−1.774851	2.774949
C	5.809679	−3.237377	3.039732
C	3.860660	−2.135214	4.060028
H	2.505385	−1.200427	2.642718
C	5.053789	−2.869005	4.166042
C	2.826685	3.243785	0.712823
C	2.082834	3.199879	1.903861
C	3.037967	4.483803	0.100644
C	1.589653	4.365956	2.507214
H	1.885030	2.232161	2.356929
C	2.541429	5.675403	0.660904
H	3.597006	4.530278	−0.828232
C	1.836649	5.595112	1.870776
H	1.468741	6.511799	2.329517
C	4.142569	2.133169	−1.631265
C	5.332823	2.859285	−1.776574
C	3.416825	1.777717	−2.776084
C	5.806271	3.240444	−3.043130
H	5.901499	3.125517	−0.889179
C	3.856562	2.137810	−4.061591
H	2.502560	1.202994	−2.643064
C	5.049532	2.871734	−4.168726
H	5.402036	3.164710	−5.157598
C	−2.826041	3.243892	−0.713956
C	−2.082747	3.199664	−1.905335
C	−3.037249	4.484072	−0.102102
C	−1.589912	4.365589	−2.509250
H	−1.885024	2.231805	−2.358132
C	−2.541123	5.675552	−0.662991
H	−3.595863	4.530753	0.827025
C	−1.836798	5.594927	−1.873104
H	−1.469143	6.511511	−2.332259
C	−4.139216	2.133107	1.631801
C	−5.329173	2.859409	1.778680
C	−3.412458	1.776816	2.775716
C	−5.801358	3.239886	3.045907
H	−5.898691	3.126227	0.892002
C	−3.850952	2.136181	4.061860
H	−2.498465	1.201935	2.641508
C	−5.043681	2.870252	4.170568
H	−5.395251	3.162576	5.159967

C	−2.821635	−3.245144	0.703885
C	−2.077869	−3.206534	1.895897
C	−3.027371	−4.481233	0.083409
C	−1.579298	−4.374116	2.490431
H	−1.883638	−2.241034	2.355223
C	−2.527496	−5.675496	0.636244
H	−3.583654	−4.522184	−0.847617
C	−1.821290	−5.600486	1.845173
H	−1.448289	−6.518871	2.295894
C	−4.147766	−2.128756	−1.630362
C	−5.338267	−2.855303	−1.771623
C	−3.426632	−1.772024	−2.777625
C	−5.816604	−3.235343	−3.036666
H	−5.903217	−3.122715	−0.882197
C	−3.871024	−2.131457	−4.061738
H	−2.512070	−1.197134	−2.647616
C	−5.064257	−2.865482	−4.164889
H	−5.420496	−3.157760	−5.152631
Si	2.885927	1.630513	−5.593465
H	2.546458	2.818911	−6.424080
H	3.684103	0.705916	−6.446433
H	1.635161	0.945601	−5.179903
Si	7.413776	4.199586	−3.214382
H	8.517131	3.346915	−3.743195
H	7.251198	5.338789	−4.158347
H	7.825539	4.716581	−1.882779
Si	2.804737	7.326905	−0.198687
H	2.781179	8.423387	0.807428
H	4.115757	7.335472	−0.903615
H	1.745094	7.607879	−1.207772
Si	0.592130	4.283247	4.099575
H	0.891552	5.476370	4.939270
H	−0.872805	4.267264	3.839968
H	0.951100	3.052386	4.852626
Si	0.551935	−4.288880	−4.069165
H	0.768284	−5.530333	−4.862873
H	−0.904905	−4.173024	−3.791176
H	0.970715	−3.112808	−4.877411
Si	2.835493	−7.328001	0.197872
H	1.744737	−8.279807	−0.146796
H	4.125426	−7.937650	−0.233662
H	2.889400	−7.149855	1.673993
Si	−2.904748	−1.624824	−5.596596
H	−2.562773	−2.814130	−6.424896
H	−3.707492	−0.704965	−6.450391
H	−1.655488	−0.934906	−5.186823
Si	−7.424643	−4.194607	−3.202582
H	−8.529733	−3.342057	−3.727862
H	−7.264966	−5.333894	−4.146966
H	−7.831866	−4.711633	−1.869599
Si	−2.797824	−7.324680	−0.226313
H	−2.443396	−8.426830	0.708313
H	−4.219832	−7.477914	−0.641388
H	−1.957760	−7.456125	−1.449150
Si	−0.580320	−4.297147	4.082233
H	−0.861515	−5.505342	4.906564
H	0.883707	−4.255821	3.821238
H	−0.956484	−3.081600	4.851728
Si	−0.592824	4.282415	−4.101872
H	−0.894651	5.473733	−4.943276
H	0.872228	4.269544	−3.842709
H	−0.949858	3.049793	−4.852942
Si	−2.804347	7.327331	0.196103
H	−2.780421	8.423500	−0.810340
H	−4.115509	7.336314	0.900768
H	−1.744873	7.608405	1.205334
Si	−7.408536	4.199212	3.219188
H	−8.510988	3.346850	3.750386
H	−7.244501	5.339090	4.162088
H	−7.822422	4.715311	1.887899
Si	−2.879032	1.627670	5.592523
H	−2.538194	2.815474	6.423427
H	−3.676893	0.703069	6.445792
H	−1.629008	0.942382	5.177399
Cl	0.000426	1.610219	−0.000895
Cl	0.000286	−1.606823	−0.001924
H	5.406896	−3.162616	5.154494
H	5.902438	−3.123031	0.885466
Si	7.417244	−4.196469	3.210182
H	8.525380	−3.341199	3.724390
H	7.258180	−5.326778	4.165368
H	7.820354	−4.726502	1.880914

Si	2.890353	−1.629565	5.592666
H	2.558781	−2.818209	6.426079
H	3.685151	−0.699073	6.442416
H	1.635333	−0.951856	5.180113

CAT2

H	−0.000008	1.157412	−0.000159
C	5.454042	−0.424325	−0.614947
C	4.489729	−1.424663	−0.956660
C	4.660029	−2.182629	−2.123017
C	5.750509	−2.017233	−2.994503
C	6.674681	−1.058885	−2.644439
C	6.523366	−0.294624	−1.490089
C	5.454040	0.424656	0.614878
C	4.489660	1.424934	0.956612
C	4.659934	2.182915	2.122957
C	5.750452	2.017599	2.994416
C	6.674673	1.059305	2.644343
C	6.523381	0.295021	1.489999
H	3.931479	−2.943834	−2.371480
H	5.859680	−2.618384	−3.890384
H	3.931329	2.944062	2.371445
H	5.859602	2.618759	3.890293
P	2.952380	−1.646327	0.069557
P	2.952267	1.646437	−0.069561
Rh	1.376858	−0.000017	−0.000067
H	0.000004	−1.157417	−0.000154
C	−5.454188	0.424349	−0.614920
C	−4.489863	1.424689	−0.956594
C	−4.660154	2.182687	−2.122935
C	−5.750637	2.017327	−2.994423
C	−6.674816	1.058974	−2.644393
C	−6.523502	0.294669	−1.490072
C	−5.454169	−0.424660	0.614876
C	−4.489777	−1.424929	0.956570
C	−4.660035	−2.182940	2.122906
C	−5.750548	−2.017658	2.994372
C	−6.674795	−1.059379	2.644319
C	−6.523516	−0.295065	1.490001
H	−3.931590	2.943878	−2.371393
H	−5.859799	2.618502	−3.890289
H	−3.931418	−2.944074	2.371385
H	−5.859677	−2.618834	3.890241
P	−2.952483	1.646268	0.069591
P	−2.952369	−1.646408	−0.069591
Rh	−1.376946	−0.000005	−0.000049
O	7.812298	−0.678381	−3.310194
O	7.564408	0.604769	−1.406909
O	7.564472	−0.604307	1.406805
O	7.812326	0.678889	3.310074
O	−7.812432	0.678500	−3.310161
O	−7.564533	−0.604736	−1.406928
O	−7.564616	0.604249	1.406818
O	−7.812458	−0.679007	3.310058
C	−8.502011	−0.187135	−2.403653
H	−9.323242	0.365273	−1.923858
H	−8.869921	−1.060985	−2.943903
C	−8.502038	0.186702	2.403620
H	−9.323363	−0.365621	1.923893
H	−8.869829	1.060575	2.943919
C	8.501925	−0.186723	2.403559
H	9.323170	0.365692	1.923800
H	8.869823	−1.060586	2.943800
C	8.501901	0.187153	−2.403614
H	9.323068	−0.365340	−1.923807
H	8.869898	1.061003	−2.943802
C	2.327582	−3.295366	−0.521434
C	1.456974	−3.307506	−1.623772
C	2.712657	−4.517527	0.042667
C	1.009287	−4.510164	−2.193394
H	1.133248	−2.354258	−2.034379
C	2.262191	−5.744140	−0.478308
H	3.375235	−4.521389	0.901870
C	1.429547	−5.717039	−1.606938
H	1.100412	−6.659611	−2.042566
C	3.648147	−2.019129	1.747684
C	4.832607	−2.747007	1.931887
C	2.965298	−1.539545	2.873946
C	5.333081	−3.021017	3.215522
C	3.439432	−1.779853	4.175618
H	2.060544	−0.956160	2.711558
C	4.617578	−2.530246	4.321086

C	2.327263	3.295374	0.521484	C	−2.262038	−5.744143	0.478549
C	1.456773	3.307381	1.623921	H	−3.375153	−4.521548	−0.901701
C	2.712054	4.517588	−0.042690	C	−1.429340	−5.716921	1.607152
C	1.008924	4.509968	2.193557	H	−1.100225	−6.659449	2.042893
H	1.133270	2.354090	2.034599	C	−3.647936	−2.019209	−1.747799
C	2.261392	5.744131	0.478286	C	−4.832339	−2.747128	−1.932188
H	3.374513	4.521544	−0.901985	C	−2.964931	−1.539602	−2.873960
C	1.428875	5.716905	1.607004	C	−5.332573	−3.021222	−3.215904
H	1.099605	6.659435	2.042627	H	−5.381223	−3.093996	−1.060326
C	3.647953	2.019360	−1.747699	C	−3.438830	−1.779963	−4.175706
C	4.832373	2.747301	−1.931892	H	−2.060219	−0.956189	−2.711428
C	2.965138	1.539745	−2.873970	C	−4.616878	−2.530475	−4.321356
C	5.332891	3.021285	−3.215518	H	−4.992774	−2.733923	−5.324053
H	5.381091	3.094203	−1.059940	Si	2.541248	1.087500	−5.678607
C	3.439295	1.780046	−4.175638	H	2.219250	2.170358	−6.649188
H	2.060425	0.956292	−2.711595	H	3.388651	0.091016	−6.391893
C	4.617451	2.530427	−4.321083	H	1.284982	0.426907	−5.243607
H	4.993664	2.733650	−5.323709	Si	6.924368	3.997343	−3.432904
C	−2.327648	3.295297	−0.521390	H	8.036590	3.140694	−3.935523
C	−1.457008	3.307397	−1.623692	H	6.743104	5.098958	−4.417572
C	−2.712783	4.517486	0.042628	H	7.333367	4.571483	−2.124101
C	−1.009367	4.510035	−2.193399	Si	2.759995	7.372997	−0.318301
H	−1.133246	2.354133	−2.034233	H	2.774149	8.449923	0.708795
C	−2.262353	5.744073	−0.478419	H	4.113054	7.252289	−0.925628
H	−3.375340	4.521384	0.901847	H	1.812502	7.781797	−1.393458
C	−1.429706	5.716929	−1.607057	Si	−0.110129	4.523499	3.706535
H	−1.100638	6.659482	−2.042780	H	0.338391	5.587667	4.647412
C	−3.648108	2.019014	1.747785	H	−1.527351	4.803516	3.353359
C	−4.832538	2.746898	1.932154	H	−0.036895	3.207141	4.391246
C	−2.965081	1.539467	2.873955	Si	−0.109923	−4.523875	−3.706256
C	−5.332743	3.021061	3.215865	H	0.337556	−5.589317	−4.646181
H	−5.381437	3.093714	1.060281	H	−1.527405	−4.802175	−3.352779
C	−3.438969	1.779873	4.175698	H	−0.035490	−3.208182	−4.392135
H	−2.060339	0.956096	2.711438	Si	2.761271	−7.372857	0.318283
C	−4.617003	2.530407	4.321332	H	2.776159	−8.449777	−0.708806
H	−4.992842	2.733964	5.324027	H	4.114118	−7.251511	0.925956
C	−2.327427	−3.295373	0.521432	H	1.813670	−7.782133	1.393162
C	−1.456743	−3.307391	1.623700	Si	−2.540771	−1.087154	−5.678545
C	−2.712544	−4.517597	−0.042521	H	−2.223381	−2.169303	−6.651431
C	−1.009022	−4.509993	2.193430	H	−3.386081	−0.086813	−6.388922
H	−1.132995	−2.354099	2.034184	H	−1.282019	−0.430953	−5.244091

Si	−6.923980	−3.997331	−3.433564
H	−8.036489	−3.140530	−3.935290
H	−6.742753	−5.098201	−4.419069
H	−7.332589	−4.572437	−2.125061
Si	−2.760983	−7.373060	−0.317720
H	−2.775961	−8.449678	0.709688
H	−4.113756	−7.251997	−0.925609
H	−1.813210	−7.782545	−1.392371
Si	0.110317	−4.523383	3.706200
H	−0.337104	−5.588507	4.646512
H	1.527741	−4.801861	3.352644
H	0.035980	−3.207470	4.391667
Si	0.109977	4.523598	−3.706161
H	−0.337207	5.589132	−4.646118
H	1.527477	4.801597	−3.352529
H	0.035352	3.207915	−4.392049
Si	−2.761381	7.372886	0.318012
H	−2.777166	8.449505	−0.709383
H	−4.113835	7.251402	0.926521
H	−1.813230	7.782674	1.392213
Si	−6.924138	3.997183	3.433554
H	−8.036845	3.140259	3.934632
H	−6.743031	5.097583	4.419602
H	−7.332417	4.572889	2.125212
Si	−2.540920	1.087033	5.678526
H	−2.225109	2.168964	6.652166
H	−3.385507	0.085401	6.387947
H	−1.281322	0.432326	5.244275
H	5.381357	−3.093874	1.059942
H	4.993721	−2.733553	5.323719
Si	6.924566	−3.997071	3.432930
H	8.036820	−3.140358	3.935366
H	6.743343	−5.098555	4.417752
H	7.333482	−4.571384	2.124177
Si	2.541449	−1.087224	5.678592
H	2.221696	−2.169781	6.650249
H	3.387905	−0.088934	6.390484
H	1.283973	−0.428713	5.243928

INT0

C	−5.578004	−2.553707	−2.416884
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C	−4.224565	−2.036524	−3.014732
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H	−3.700682	−0.418008	−1.600976
H	−2.435339	−1.667515	−1.664942
H	−4.345935	−1.291954	−3.811478
H	−3.650077	−2.869452	−3.436729
Si	−4.689932	−2.613263	−0.725772
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H	−4.583795	−5.042523	−0.050727
H	−3.511910	−4.681967	−1.410754
C	−5.544865	−2.075182	0.891990
C	−5.227574	−2.807355	2.054271
C	−6.534856	−1.064650	1.009847
C	−5.855864	−2.575293	3.279203
H	−4.474315	−3.587920	2.004016
C	−7.177806	−0.852136	2.239487
C	−6.845260	−1.597411	3.370084
H	−5.581468	−3.164895	4.150137
H	−7.938536	−0.078303	2.305966
H	−7.354416	−1.412387	4.312627
C	2.745740	2.067659	0.629890
C	1.490807	2.068320	1.315077
C	1.388182	2.605067	2.602961
C	2.487400	3.162405	3.280623
C	3.690031	3.155978	2.609653
C	3.807588	2.624727	1.325450
C	2.950867	1.637542	−0.786763
C	2.793889	0.317460	−1.320214
C	3.021887	0.085992	−2.684201
C	3.417778	1.095064	−3.578114
C	3.580814	2.354668	−3.046567
C	3.350342	2.607476	−1.695439
H	0.427818	2.601122	3.105054
H	2.391723	3.577789	4.277579
H	2.896164	−0.914466	−3.078136
H	3.587195	0.890087	−4.629212
P	0.044873	1.232881	0.531016
P	2.203323	−1.094644	−0.276250

Rh	0.153045	−1.007639	0.524865	C	−1.547172	0.729205	2.763973
Cl	−0.233415	−3.278096	1.111546	C	−2.365232	2.546460	1.393109
C	−6.938274	−0.180951	−0.127276	C	−2.643164	0.856692	3.633928
C	−8.227534	−0.265251	−0.675438	H	−0.793589	−0.036836	2.948391
C	−6.060854	0.793208	−0.628725	C	−3.475287	2.705586	2.238120
C	−8.620809	0.583216	−1.711955	H	−2.259326	3.187284	0.522646
H	−8.918066	−1.011803	−0.292039	C	−3.595491	1.847152	3.346188
C	−6.454204	1.645454	−1.662812	H	−4.461600	1.946361	3.997742
H	−5.070814	0.888575	−0.191969	O	3.533406	3.949220	−1.450857
C	−7.734144	1.539931	−2.210919	O	3.932729	3.513261	−3.684637
H	−9.620139	0.495460	−2.130540	O	5.114776	2.730109	0.910592
H	−5.761034	2.394747	−2.036380	O	4.907725	3.618784	3.033771
H	−8.039871	2.200872	−3.017576	C	5.759395	3.559132	1.885320
C	3.499992	−1.297947	1.025924	H	5.890562	4.570070	1.474170
C	3.182032	−2.050849	2.165324	H	6.715706	3.112922	2.163453
C	4.797149	−0.783617	0.883228	C	4.118248	4.480174	−2.644821
C	4.141673	−2.302523	3.160924	H	3.610004	5.407552	−2.915817
H	2.172995	−2.446956	2.259939	H	5.193461	4.642877	−2.485405
C	5.780343	−1.008077	1.860872	Si	3.711242	−3.328765	4.683008
H	5.044496	−0.199752	0.001023	H	4.889309	−3.329039	5.593479
C	5.430502	−1.772118	2.988145	H	2.545453	−2.750439	5.402951
H	6.182932	−1.962688	3.751868	H	3.387490	−4.733268	4.318442
C	2.460652	−2.577551	−1.353939	Si	7.510466	−0.301457	1.662949
C	3.730655	−3.143670	−1.541046	H	7.706623	0.937460	2.470141
C	1.358193	−3.147609	−2.001818	H	8.529117	−1.286298	2.117141
C	3.916401	−4.258704	−2.373388	H	7.752976	0.038969	0.235840
H	4.586862	−2.713871	−1.029286	Si	5.626986	−5.007474	−2.608968
C	1.501169	−4.265821	−2.841110	H	5.990020	−5.059461	−4.052465
H	0.376917	−2.716713	−1.825500	H	6.623423	−4.167040	−1.892143
C	2.787787	−4.797894	−3.016555	H	5.696098	−6.395665	−2.076498
H	2.915472	−5.659906	−3.670595	Si	0.000396	−5.053496	−3.663897
C	−0.299632	2.251938	−0.969774	H	−1.044362	−4.022081	−3.897150
C	−0.882637	1.632299	−2.081790	H	0.410764	−5.640562	−4.969807
C	−0.015269	3.624924	−1.022499	H	−0.580616	−6.141134	−2.832783
C	−1.198986	2.360363	−3.242735	Si	0.129738	6.214222	−2.233735
H	−1.081532	0.563603	−2.032199	H	1.371300	6.455864	−3.023601
C	−0.304531	4.385496	−2.165999	H	−0.964344	6.990171	−2.877127
H	0.450632	4.101389	−0.163533	H	0.355635	6.718980	−0.853825
C	−0.899663	3.732143	−3.260855	Si	−2.001861	1.527943	−4.731785
H	−1.130759	4.307548	−4.156189	H	−1.812974	2.402843	−5.920845
C	−1.392604	1.566644	1.645165	H	−1.376076	0.204510	−4.986158

H	−3.461329	1.328224	−4.524741
Si	−4.752551	4.052387	1.912826
H	−6.099450	3.595240	2.342065
H	−4.424848	5.293875	2.669363
H	−4.763408	4.387615	0.464351
Si	−2.818654	−0.255231	5.148266
H	−2.690069	−1.687990	4.785687
H	−1.761232	0.068059	6.147052
H	−4.144449	−0.002372	5.771621

INT1

C	−3.766294	0.496421	−2.197056
C	−1.541253	1.493982	−2.824256
C	−2.880021	0.982000	−3.351031
H	−4.054997	1.347347	−1.564317
H	−4.692927	0.031496	−2.553173
H	−1.695184	2.436010	−2.289766
H	−0.836855	1.668882	−3.644868
H	−3.386170	1.784539	−3.913952
H	−2.703978	0.164142	−4.056251
Si	−2.729115	−0.725238	−1.161037
C	−2.814715	−2.488644	−1.863999
H	−2.011563	−3.125401	−1.478559
H	−3.776862	−2.945462	−1.604671
H	−2.704675	−2.461608	−2.950860
C	−3.382331	−0.857842	0.651516
C	−2.491484	−0.681537	1.725832
C	−4.722379	−1.211206	0.980105
C	−2.873723	−0.816945	3.062889
H	−1.456452	−0.442555	1.510232
C	−5.098893	−1.347622	2.326878
C	−4.191534	−1.147816	3.367154
H	−2.142258	−0.665959	3.852021
H	−6.127775	−1.615247	2.553608
H	−4.513678	−1.256612	4.399610
C	1.623350	0.816001	1.947160
C	0.388134	1.500095	1.696064
C	−0.407942	1.907462	2.775423
C	−0.069307	1.675455	4.118670
C	1.112953	1.008493	4.343958
C	1.922883	0.600463	3.286826
C	2.707839	0.479492	0.966989
C	2.725722	−0.559386	−0.019390
C	3.900028	−0.790223	−0.750532
C	5.080044	−0.047714	−0.580002
C	5.046630	0.942184	0.374623
C	3.896922	1.182545	1.121645
H	−1.325154	2.446678	2.585355
H	−0.700903	2.017309	4.930971
H	3.924336	−1.594629	−1.472178
H	5.971894	−0.257950	−1.159760
P	−0.190842	1.820626	−0.045878
P	1.192692	−1.556903	−0.393644
Rh	−0.516292	0.096802	−1.582048
Cl	−0.338440	−1.147530	−3.641589
C	−5.801156	−1.498223	−0.024578
C	−6.160690	−2.827679	−0.300759
C	−6.542775	−0.470443	−0.624240
C	−7.211735	−3.120605	−1.171314
H	−5.608127	−3.634894	0.173087
C	−7.597795	−0.761103	−1.491887
H	−6.295781	0.563731	−0.404641
C	−7.933042	−2.086849	−1.771694
H	−7.467986	−4.156590	−1.377195
H	−8.159924	0.051141	−1.945396
H	−8.753033	−2.312840	−2.448057
C	0.925661	−2.499650	1.183840
C	1.958972	−2.726598	2.104025
C	−0.311040	−3.127369	1.392856
C	1.776360	−3.557968	3.221661
H	2.925141	−2.260000	1.939804
C	−0.532792	−3.975776	2.490950
H	−1.112235	−2.964542	0.679052
C	0.525590	−4.174695	3.391892
H	0.375311	−4.834482	4.246031
C	1.828936	−2.934792	−1.478242
C	1.855352	−4.269097	−1.051387
C	2.258466	−2.649365	−2.787459
C	2.305645	−5.307688	−1.887599
H	1.525946	−4.513732	−0.047655
C	2.723137	−3.653601	−3.649174
H	2.226488	−1.626347	−3.141142

C	2.740354	−4.977609	−3.178918
H	3.101129	−5.768779	−3.833921
C	1.234390	2.803534	−0.721439
C	1.855828	3.797129	0.054491
C	1.694042	2.581185	−2.024243
C	2.905578	4.573998	−0.454049
H	1.510300	3.965162	1.071059
C	2.757787	3.326035	−2.568240
H	1.215867	1.814533	−2.628835
C	3.341496	4.318624	−1.768586
H	4.158977	4.909062	−2.179453
C	−1.510109	3.128809	0.144673
C	−1.323934	4.435973	−0.327433
C	−2.753590	2.801294	0.713528
C	−2.326024	5.416233	−0.215167
H	−0.382336	4.702702	−0.793871
C	−3.770498	3.757149	0.869983
H	−2.929615	1.786781	1.056847
C	−3.532857	5.061590	0.404156
H	−4.306398	5.817247	0.528192
O	1.686557	0.660705	5.536959
O	3.041440	−0.021502	3.796547
O	4.142218	2.217274	1.998858
O	6.040047	1.808427	0.751127
C	3.012561	0.236086	5.204412
H	3.723326	1.040196	5.442807
H	3.247942	−0.680969	5.746070
C	5.557272	2.428066	1.945817
H	6.029361	1.955588	2.819663
H	5.763757	3.498555	1.910121
Si	−2.051053	7.157707	−0.879222
Si	−5.411855	3.323341	1.689798
Si	3.699272	5.913915	0.600291
Si	3.373414	3.007323	−4.322651
H	2.319409	3.316489	−5.324892
H	3.781423	1.588273	−4.492268
Si	3.253494	−3.239833	−5.407119
Si	2.333669	−7.087509	−1.282238
Si	−2.185121	−4.850250	2.734236
Si	3.178119	−3.859064	4.438131
H	4.548055	3.886988	−4.568192
H	5.115346	5.584542	0.928782
H	3.704969	7.220744	−0.110987
H	2.940034	6.047364	1.871096
H	3.176272	−7.231831	−0.061752
H	0.967706	−7.571543	−0.939533
H	2.894782	−7.954217	−2.353486
H	4.318635	−4.190668	−5.833743
H	2.129150	−3.347946	−6.374178
H	3.793443	−1.854496	−5.458512
H	−2.030638	−6.318155	2.530341
H	−2.685390	−4.644186	4.120408
H	−3.172752	−4.332428	1.756313
H	4.476936	−3.500933	3.810326
H	3.025434	−3.043765	5.678078
H	3.203232	−5.286962	4.855027
H	−5.196177	2.356298	2.796573
H	−6.016360	4.571958	2.228061
H	−6.372605	2.727690	0.722779
H	−2.153637	7.201248	−2.363268
H	−3.082634	8.061932	−0.304553
H	−0.698478	7.648933	−0.499035

INT2

H	1.914768	−0.927801	−1.637512
Si	2.229139	−2.350970	0.119195
C	−2.221619	1.770284	0.845830
C	−2.440294	0.404475	1.217455
C	−3.031661	0.109832	2.450498
C	−3.410067	1.104472	3.373010
C	−3.175097	2.410241	3.004160
C	−2.606814	2.724584	1.770604
C	−1.779510	2.196816	−0.514865
C	−0.488686	2.010695	−1.094027
C	−0.284277	2.305783	−2.452880
C	−1.282923	2.852431	−3.273733
C	−2.502463	3.093436	−2.677515
C	−2.734477	2.771697	−1.343112
H	−3.236402	−0.920552	2.711518
H	−3.874755	0.852748	4.320016
H	0.688460	2.121039	−2.893818
H	−1.103520	3.071472	−4.320199

P	−1.907613	−0.916530	0.015054
P	0.943150	1.252259	−0.185829
Rh	0.552550	−0.928070	−0.845832
Cl	−0.186561	−2.806678	−2.160026
O	−3.634938	3.613461	−3.238724
O	−4.034530	3.069614	−1.020890
O	−2.486166	4.088993	1.659370
O	−3.431074	3.560687	3.702791
C	−4.639305	3.579307	−2.215780
H	−5.006345	4.595193	−2.032890
H	−5.451784	2.913776	−2.525802
C	−3.203792	4.628320	2.774968
H	−4.169271	5.025075	2.431224
H	−2.601659	5.403317	3.253453
C	2.363594	2.272454	−0.830711
C	2.179512	3.630617	−1.152879
C	3.644339	1.721326	−0.964410
C	3.233485	4.435043	−1.605157
H	1.187928	4.064302	−1.075862
C	4.734535	2.498680	−1.407087
H	3.792777	0.675199	−0.718515
C	4.503334	3.845494	−1.722995
H	5.335950	4.451504	−2.077082
C	0.836864	1.853948	1.571655
C	0.960330	3.210260	1.912355
C	0.660524	0.920736	2.598376
C	0.900839	3.641294	3.245182
H	1.106112	3.947591	1.131218
C	0.610510	1.305595	3.950529
H	0.549044	−0.124201	2.324950
C	0.730067	2.670962	4.248462
H	0.687129	2.987799	5.289547
C	−3.180266	−0.661602	−1.319086
C	−4.520090	−0.423844	−0.968234
C	−2.830499	−0.698161	−2.673055
C	−5.509077	−0.222208	−1.941434
H	−4.792201	−0.389893	0.083250
C	−3.794191	−0.501189	−3.681418
H	−1.800231	−0.907005	−2.940805
C	−5.120878	−0.263739	−3.294637
H	−5.873482	−0.108572	−4.066832
C	−2.446755	−2.522961	0.761274
C	−3.201483	−3.429443	0.004020
C	−2.010203	−2.920960	2.037051
C	−3.546693	−4.698300	0.500833
H	−3.517928	−3.146388	−0.993928
C	−2.353835	−4.168721	2.580519
H	−1.388259	−2.248865	2.620622
C	−3.125057	−5.041630	1.793207
H	−3.395778	−6.017116	2.194425
Si	−7.289142	0.116381	−1.439197
H	−7.686397	1.513988	−1.778325
H	−8.232887	−0.794826	−2.141517
H	−7.426796	−0.064472	0.029819
Si	−3.316366	−0.576680	−5.502489
H	−3.061309	−1.971975	−5.948857
H	−4.439638	−0.021129	−6.307025
H	−2.092193	0.227918	−5.758781
Si	−1.817874	−4.664108	4.317424
H	−2.962774	−4.575282	5.268702
H	−1.331194	−6.068807	4.329637
H	−0.749008	−3.749662	4.791270
Si	−4.530707	−5.911822	−0.551218
H	−5.097141	−6.965198	0.334744
H	−5.643537	−5.208934	−1.246021
H	−3.682501	−6.567027	−1.582379
Si	0.408250	0.042995	5.333558
H	1.694508	−0.640138	5.641042
H	−0.055557	0.746575	6.559083
H	−0.584240	−0.993620	4.950185
Si	1.025725	5.471095	3.663515
H	−0.295905	6.026840	4.073256
H	1.970972	5.694861	4.790173
H	1.491792	6.216302	2.464825
Si	2.940697	6.233393	−2.077800
H	4.036213	7.093328	−1.554456
H	2.887114	6.409344	−3.555549
H	1.642969	6.681693	−1.505076
Si	6.489513	1.826628	−1.593300
H	6.489340	0.457694	−2.160350
H	7.214604	2.744419	−2.515359
H	7.214665	1.819718	−0.295333

C	3.887897	−1.540827	0.657655
C	3.852492	−0.802174	1.858690
C	5.164407	−1.748651	0.065458
C	4.996514	−0.307096	2.482562
H	2.894753	−0.615511	2.335143
C	6.316385	−1.264570	0.715584
C	6.243735	−0.553197	1.910750
H	4.912918	0.255644	3.408702
H	7.284117	−1.435296	0.251628
H	7.152202	−0.186937	2.381668
C	5.386584	−2.446682	−1.237018
C	4.763099	−2.016000	−2.418443
C	6.294782	−3.515869	−1.317327
C	5.028608	−2.640328	−3.637823
H	4.066292	−1.183817	−2.386399
C	6.556729	−4.145401	−2.534225
H	6.782364	−3.866766	−0.411452
C	5.924640	−3.708989	−3.700400
H	4.532789	−2.289202	−4.538864
H	7.252100	−4.980083	−2.569969
H	6.127633	−4.198245	−4.649240
C	2.560644	−3.929343	−0.869846
H	2.700983	−3.748823	−1.935400
H	3.447620	−4.437048	−0.475223
H	1.697983	−4.592712	−0.758333
C	1.430579	−2.988625	1.761677
H	0.516025	−3.508401	1.458556
H	1.130074	−2.149559	2.400062
C	2.332335	−3.917513	2.520822
H	3.166380	−3.449827	3.044922
C	2.207406	−5.248569	2.575231
H	1.402366	−5.770247	2.061317
H	2.911312	−5.864611	3.128763

INT3

C	2.614733	2.499319	2.414288
C	0.044073	2.458837	2.567283
C	1.289895	1.923426	2.883947
H	2.489130	3.531771	2.069953
H	3.386739	2.475900	3.190292
H	−0.026325	3.412996	2.050611
H	−0.831898	2.178992	3.146571
H	1.345980	1.162102	3.660939
Si	2.751236	1.238839	0.991888
C	4.075231	−0.060857	1.416759
H	4.097276	−0.877409	0.686387
H	5.072179	0.391050	1.450822
H	3.867024	−0.506616	2.395956
C	3.195184	2.104750	−0.674232
C	2.215067	2.150456	−1.686914
C	4.460639	2.678752	−0.975591
C	2.444008	2.731136	−2.936775
H	1.248532	1.693031	−1.488666
C	4.687812	3.247929	−2.240589
C	3.692698	3.283713	−3.216516
H	1.654980	2.738952	−3.684723
H	5.662611	3.681717	−2.449383
H	3.894561	3.737689	−4.183393
C	−1.867974	−0.893595	−1.766151
C	−1.888603	0.527887	−1.598354
C	−1.845157	1.364779	−2.719177
C	−1.769787	0.870707	−4.035268
C	−1.741342	−0.497901	−4.178401
C	−1.801736	−1.347330	−3.073168
C	−2.047579	−1.885934	−0.661203
C	−1.089748	−2.224846	0.346381
C	−1.414838	−3.187276	1.311371
C	−2.649227	−3.862154	1.339920
C	−3.545159	−3.545415	0.344384
C	−3.243777	−2.586065	−0.620626
H	−1.871672	2.438915	−2.581444
H	−1.744710	1.534882	−4.892239
H	−0.684861	−3.448546	2.066600
H	−2.874443	−4.603665	2.098538
P	−1.800728	1.220447	0.120021
P	0.585236	−1.394038	0.365122
Rh	0.389417	0.785221	1.089483
C	5.609072	2.710082	−0.015606
C	5.573122	3.487000	1.152260
C	6.785965	2.001216	−0.308213
C	6.671795	3.536747	2.012106
H	4.685570	4.068972	1.377600

C	7.884056	2.047387	0.551905
H	6.828938	1.398865	−1.211942
C	7.829404	2.813815	1.717954
H	6.624773	4.148645	2.909361
H	8.781617	1.483386	0.311105
H	8.683675	2.851657	2.388719
C	−2.091520	3.040783	−0.139286
C	−3.329826	3.668277	0.052427
C	−0.993022	3.836228	−0.508354
C	−3.490751	5.054781	−0.122282
H	−4.186455	3.070963	0.347855
C	−1.114405	5.219062	−0.718851
H	−0.024273	3.357953	−0.627359
C	−2.374599	5.808711	−0.516567
H	−2.485601	6.881335	−0.664604
C	−3.404341	0.669772	0.875093
C	−4.599186	0.561406	0.145326
C	−3.419289	0.362823	2.240332
C	−5.799873	0.173641	0.759708
H	−4.586082	0.778366	−0.919920
C	−4.600692	−0.025634	2.897868
H	−2.482051	0.418888	2.790312
C	−5.777772	−0.108501	2.138547
H	−6.701583	−0.406211	2.632230
C	1.477768	−2.381689	1.675513
C	2.337909	−3.451321	1.406890
C	1.291272	−1.996661	3.014563
C	3.014228	−4.133298	2.437452
H	2.499816	−3.755081	0.377208
C	1.924097	−2.662512	4.073863
H	0.644778	−1.143851	3.211672
C	2.792484	−3.725444	3.760297
H	3.314146	−4.239181	4.565894
C	1.314992	−2.113792	−1.196194
C	0.927448	−3.379661	−1.667373
C	2.301285	−1.413209	−1.900854
C	1.507192	−3.952382	−2.810126
H	0.163280	−3.931072	−1.127941
C	2.908770	−1.948501	−3.052586
H	2.600007	−0.430589	−1.551418
C	2.502040	−3.220613	−3.483479
H	2.977862	−3.655890	−4.361607
O	−4.806402	−4.039211	0.131736
O	−4.322761	−2.440457	−1.463339
O	−1.822536	−2.652085	−3.506486
O	−1.708892	−1.237661	−5.331998
C	−5.195475	−3.529539	−1.148474
H	−5.082864	−4.318799	−1.905818
H	−6.223598	−3.167677	−1.098369
C	−1.545291	−2.595604	−4.910117
H	−2.255048	−3.231149	−5.445488
H	−0.509963	−2.913757	−5.090433
Si	0.951817	−5.645440	−3.412689
H	0.132742	−5.540954	−4.654693
H	2.123713	−6.507234	−3.727628
H	0.125167	−6.295884	−2.362555
Si	4.224753	−0.995243	−4.008197
H	5.063051	−1.974650	−4.754402
H	3.621649	−0.063984	−4.999570
H	5.083365	−0.216361	−3.080839
Si	4.184746	−5.554691	2.048244
H	4.817737	−6.018742	3.311973
H	3.457860	−6.699735	1.432065
H	5.248848	−5.133131	1.096916
Si	1.618429	−2.153555	5.859603
H	1.275346	−0.707408	5.921395
H	0.493164	−2.919029	6.466164
H	2.836571	−2.410573	6.674377
Si	−4.603573	−0.418517	4.738913
H	−4.401910	0.808091	5.558656
H	−5.914362	−1.021056	5.101747
H	−3.513827	−1.374068	5.075732
Si	−7.384597	0.024763	−0.241907
H	−7.728554	−1.398151	−0.525229
H	−8.531035	0.615696	0.500254
H	−7.217365	0.727322	−1.541016
Si	0.359856	6.262268	−1.258382
H	0.667507	6.069827	−2.701904
H	0.025452	7.696605	−1.042156
H	1.570202	5.914252	−0.470198
Si	−5.155163	5.878519	0.183454
H	−5.400960	6.110637	1.633994

H	−5.187883	7.193815	−0.511072
H	−6.257829	5.022093	−0.332731

INT4

C	0.535140	−4.862461	−1.031970
C	1.325698	−7.047673	−0.038222
C	0.349296	−6.209494	−0.403558
H	1.573902	−4.732764	−1.366023
H	−0.107610	−4.755985	−1.915825
H	2.375289	−6.812621	−0.207305
H	1.112017	−8.003082	0.434108
H	−0.684349	−6.501748	−0.212948
Si	0.111856	−3.402125	0.158829
C	1.391304	−3.499173	1.563526
H	1.118514	−2.873039	2.420287
H	1.490328	−4.534182	1.914248
H	2.376398	−3.176022	1.207920
C	−1.617644	−3.730642	0.853216
C	−1.784424	−4.280198	2.135907
C	−2.769974	−3.451338	0.078770
C	−3.049705	−4.543416	2.665410
H	−0.908383	−4.522160	2.733243
C	−4.039459	−3.686564	0.637601
C	−4.182119	−4.226557	1.914602
H	−3.148982	−4.983680	3.654387
H	−4.929028	−3.431207	0.068470
H	−5.176186	−4.398665	2.320009
C	0.937431	2.335820	−1.265558
C	1.820553	1.255682	−1.596669
C	2.335969	1.150567	−2.894288
C	2.019040	2.058990	−3.919274
C	1.151216	3.076706	−3.592269
C	0.641095	3.209393	−2.301191
C	0.474521	2.698561	0.112663
C	−0.532643	2.054848	0.897691
C	−0.851350	2.563141	2.165412
C	−0.236044	3.699506	2.717388
C	0.708268	4.325276	1.934872
C	1.044691	3.831560	0.676449
H	3.014099	0.340891	−3.132787
H	2.441331	1.965324	−4.913631
H	−1.621765	2.079306	2.751420
H	−0.503816	4.070528	3.700495
P	2.072987	−0.123049	−0.373727
P	−1.467257	0.593677	0.218532
Rh	−0.037285	−1.237464	−0.732020
C	−2.650394	−2.969516	−1.328781
C	−3.605710	−3.421645	−2.266846
C	−1.601413	−2.122129	−1.765296
C	−3.554284	−3.050900	−3.606913
H	−4.383124	−4.107023	−1.940716
C	−1.559833	−1.781946	−3.132635
H	0.840868	−2.339586	−1.458273
C	−2.520419	−2.219547	−4.045288
H	−4.297827	−3.426261	−4.305208
H	−0.754952	−1.144302	−3.495694
H	−2.454676	−1.925775	−5.090525
C	3.553207	−1.070231	−1.003854
C	4.793299	−1.053562	−0.351447
C	3.419122	−1.888000	−2.141720
C	5.886976	−1.810692	−0.812232
H	4.917504	−0.443337	0.536381
C	4.486635	−2.646082	−2.644407
H	2.454580	−1.933011	−2.638652
C	5.716748	−2.589301	−1.965084
H	6.558934	−3.166612	−2.342610
C	2.794770	0.727618	1.106436
C	3.724357	1.773278	0.979275
C	2.455419	0.276559	2.385333
C	4.322685	2.360676	2.102930
H	3.983284	2.127031	−0.015483
C	3.027330	0.841274	3.541250
H	1.735707	−0.533433	2.475700
C	3.961042	1.874564	3.374092
H	4.423142	2.311698	4.257805
C	−2.713805	1.438525	−0.879190
C	−2.846685	2.834910	−0.906303
C	−3.595640	0.664386	−1.652550
C	−3.830791	3.468019	−1.683762
H	−2.183296	3.442148	−0.301349
C	−4.602636	1.260098	−2.433191
H	−3.506684	−0.416191	−1.628957

C	−4.703042	2.661215	−2.431698
H	−5.490691	3.133326	−3.016976
C	−2.507007	0.105978	1.674959
C	−3.843072	0.495153	1.821248
C	−1.906894	−0.641944	2.701680
C	−4.587486	0.154740	2.966230
H	−4.313821	1.076222	1.034419
C	−2.600827	−0.968859	3.874494
H	−0.877166	−0.966463	2.577764
C	−3.943785	−0.564466	3.982766
H	−4.503932	−0.822085	4.880363
O	1.460442	5.436060	2.214871
O	2.039070	4.617891	0.137671
O	−0.126259	4.349321	−2.234909
O	0.712050	4.110133	−4.376066
C	2.082762	5.779637	0.971711
H	1.518966	6.594154	0.494190
H	3.121011	6.060213	1.150907
C	−0.260522	4.803416	−3.587317
H	−0.065268	5.877737	−3.629703
H	−1.267833	4.567927	−3.954432
Si	−3.978049	5.341807	−1.703042
H	−3.204893	5.950285	−2.824794
H	−5.400713	5.740829	−1.877934
H	−3.453192	5.908764	−0.432619
Si	−5.813463	0.238501	−3.456527
H	−5.240156	−0.165879	−4.767627
H	−6.236204	−0.979314	−2.719740
H	−7.008567	1.087213	−3.724243
Si	−6.396192	0.648769	3.126874
H	−7.259848	−0.114590	2.184675
H	−6.849843	0.373155	4.516698
H	−6.576931	2.097414	2.834517
Si	−1.763265	−1.907304	5.274265
H	−1.502037	−1.006041	6.432319
H	−2.623265	−3.018685	5.760422
H	−0.462599	−2.448415	4.802750
Si	4.266986	−3.738480	−4.164423
H	5.543120	−3.784841	−4.929014
H	3.901959	−5.131913	−3.791650
H	3.191646	−3.182260	−5.027511
Si	7.534308	−1.777289	0.099142
H	8.546873	−2.507246	−0.709374
H	7.995258	−0.377172	0.309017
H	7.430945	−2.424578	1.435762
Si	5.575479	3.750589	1.909256
H	4.997401	5.072492	2.282182
H	6.753381	3.518589	2.787977
H	6.018188	3.819250	0.492013
Si	2.561397	0.237933	5.263777
H	1.151206	0.579241	5.593536
H	2.714134	−1.237549	5.369501
H	3.454534	0.896962	6.253899

INT5

C	3.888514	0.328682	−0.796288
C	1.902282	−1.325862	−1.158647
C	2.565799	−0.026798	−1.506117
H	4.101435	1.401042	−0.909432
H	3.782421	0.146647	0.280421
H	2.357112	−1.873473	−0.329509
H	1.701426	−1.988331	−2.003608
H	2.648340	0.119292	−2.587372
H	1.854336	0.861402	−1.209250
Si	5.428404	−0.619408	−1.384457
C	5.468603	−2.418551	−0.839522
H	5.490029	−2.508409	0.251430
H	4.581689	−2.941488	−1.212306
H	6.356139	−2.919669	−1.241492
C	7.044848	0.306559	−0.995279
C	7.733080	0.956195	−2.038768
C	7.636587	0.328165	0.295119
C	8.956530	1.595040	−1.835858
H	7.311304	0.949410	−3.038536
C	8.877237	0.957159	0.483149
C	9.536932	1.589040	−0.569484
H	9.454838	2.085504	−2.667890
H	9.316214	0.960145	1.477428
H	10.493746	2.075143	−0.397309
C	−3.302407	−0.156353	1.213083
C	−2.337932	−1.202587	1.381529
C	−2.211926	−1.831263	2.627978

C	−2.990185	−1.489636	3.747314
C	−3.914358	−0.486105	3.566833
C	−4.058153	0.150577	2.336583
C	−3.648314	0.565784	−0.052600
C	−2.832708	1.518248	−0.741521
C	−3.337787	2.186815	−1.864055
C	−4.635273	1.974903	−2.362538
C	−5.411673	1.064760	−1.681771
C	−4.926432	0.389630	−0.563722
H	−1.490740	−2.629449	2.747645
H	−2.871949	−1.996058	4.698885
H	−2.713561	2.909730	−2.374555
H	−5.005873	2.506888	−3.231806
P	−1.165416	−1.658157	0.005647
P	−1.062828	1.754693	−0.232437
Rh	0.322131	−0.092263	−0.583299
Cl	5.286092	−0.684931	−3.498806
C	6.999598	−0.283808	1.503381
C	7.559790	−1.423047	2.103983
C	5.879963	0.308872	2.107935
C	7.003050	−1.966765	3.262330
H	8.432551	−1.885905	1.651050
C	5.323231	−0.232305	3.269135
H	5.462161	1.215528	1.679574
C	5.881798	−1.373526	3.847936
H	7.446759	−2.852552	3.709206
H	4.462404	0.247487	3.727649
H	5.452056	−1.792130	4.753826
O	−6.696418	0.662754	−1.948153
O	−5.900544	−0.467414	−0.098450
O	−5.031461	1.121008	2.444747
O	−4.788684	0.051283	4.476970
C	−7.089658	−0.105657	−0.807733
H	−7.730366	0.507269	−0.156771
H	−7.604209	−1.009593	−1.137691
C	−5.659775	0.886537	3.708596
H	−6.617130	0.368730	3.550381
H	−5.801349	1.837421	4.225241
C	−0.434167	−3.261038	0.612179
C	0.666554	−3.188772	1.482774
C	−0.900521	−4.525093	0.233214
C	1.280005	−4.340394	1.998043
H	1.039335	−2.203729	1.755986
C	−0.301178	−5.707008	0.708243
H	−1.746186	−4.596319	−0.443869
C	0.776287	−5.591918	1.598481
H	1.234731	−6.497411	1.992670
C	−2.307704	−2.226307	−1.339262
C	−3.535950	−2.852718	−1.075570
C	−1.913102	−2.046335	−2.669927
C	−4.363594	−3.306750	−2.114137
H	−3.851599	−2.981461	−0.043489
C	−2.709538	−2.490793	−3.740950
H	−0.968972	−1.536257	−2.852911
C	−3.926983	−3.120294	−3.438890
H	−4.553897	−3.471533	−4.257104
C	−1.204879	2.478941	1.468698
C	−2.303699	3.236094	1.900289
C	−0.142170	2.265262	2.355953
C	−2.350364	3.791159	3.189931
H	−3.136877	3.390583	1.219488
C	−0.146170	2.804815	3.653990
H	0.694612	1.658077	2.013761
C	−1.256027	3.571416	4.045366
H	−1.268644	4.009357	5.042679
C	−0.539918	3.228952	−1.244821
C	−0.643775	4.557638	−0.814251
C	0.019721	2.978128	−2.508851
C	−0.198939	5.628180	−1.611415
H	−1.070210	4.764984	0.163014
C	0.451369	4.016722	−3.348734
H	0.116733	1.942526	−2.830931
C	0.338044	5.335918	−2.875097
H	0.681296	6.155245	−3.504756
Si	−0.299687	7.401004	−0.986871
H	−0.249403	8.335405	−2.143513
H	−1.568479	7.611261	−0.237823
H	0.828690	7.730623	−0.072243
Si	1.145170	3.653787	−5.061656
H	0.072406	3.656404	−6.095493
H	2.138385	4.698485	−5.430478
H	1.795657	2.317457	−5.070656

Si	−3.846348	4.781098	3.752188
H	−4.736926	3.983511	4.643328
H	−3.420732	5.983975	4.518274
H	−4.638834	5.202599	2.567159
Si	1.276020	2.480758	4.841825
H	1.103902	1.196390	5.576446
H	2.561599	2.407921	4.094938
H	1.350891	3.577838	5.844208
Si	−2.159607	−2.247663	−5.525064
H	−3.237086	−2.734414	−6.428730
H	−1.898191	−0.811177	−5.813536
H	−0.912132	−3.005347	−5.816968
Si	−6.014159	−4.121924	−1.734930
H	−7.161660	−3.211920	−2.015549
H	−6.206406	−5.338854	−2.570248
H	−6.062832	−4.497459	−0.297298
Si	−0.927049	−7.395023	0.159580
H	−0.487522	−7.723781	−1.224678
H	−0.394536	−8.435244	1.080575
H	−2.414949	−7.434039	0.184249
Si	2.748954	−4.223197	3.167754
H	2.674857	−2.956838	3.944014
H	2.726849	−5.376469	4.109271
H	4.046226	−4.253473	2.439482

INT6

C	3.380751	−0.875797	0.086945
C	1.958439	0.759595	1.442505
C	2.435267	−0.523286	1.214397
H	3.152810	−1.878130	−0.291007
H	3.252274	−0.182394	−0.754260
H	2.243009	1.576875	0.787044
H	1.610993	1.044179	2.432684
H	2.430720	−1.224829	2.043370
H	0.768022	−1.912527	0.617567
Si	5.215247	−0.816669	0.606856
C	5.612876	0.835143	1.410000
H	5.633883	1.628708	0.652499
H	4.830713	1.082098	2.135749
H	6.577259	0.829888	1.922188
C	6.299106	−1.244298	−0.888666
C	5.661069	−1.878491	−1.973915
C	7.667405	−0.894558	−1.042350
C	6.320656	−2.150269	−3.172464
H	4.617161	−2.164949	−1.890152
C	8.315283	−1.156292	−2.260731
C	7.655010	−1.777495	−3.319109
H	5.792343	−2.643946	−3.983621
H	9.362753	−0.885418	−2.362722
H	8.184699	−1.975980	−4.247252
C	−3.287712	0.862925	−1.156874
C	−2.042212	1.509316	−1.434590
C	−1.783029	1.983325	−2.727265
C	−2.696010	1.858882	−3.789651
C	−3.892561	1.243257	−3.501586
C	−4.170103	0.765752	−2.222752
C	−3.756350	0.391940	0.181933
C	−3.233935	−0.711620	0.927399
C	−3.822576	−1.060729	2.150922
C	−4.925294	−0.379492	2.695047
C	−5.424263	0.669520	1.956361
C	−4.852799	1.033990	0.739757
H	−0.847330	2.487058	−2.931071
H	−2.470844	2.238509	−4.780172
H	−3.423792	−1.896940	2.710921
H	−5.362461	−0.671003	3.643623
P	−0.755605	1.662994	−0.093234
P	−1.702766	−1.606516	0.366320
Rh	0.217779	−0.398345	0.566521
Cl	5.422426	−2.319444	2.087506
C	8.481888	−0.261451	0.037600
C	8.705721	−0.915339	1.259570
C	9.090768	0.986215	−0.176494
C	9.498774	−0.327349	2.246644
H	8.263007	−1.890924	1.433807
C	9.880992	1.574963	0.810966
H	8.927194	1.501701	−1.119425
C	10.085739	0.920644	2.027854
H	9.660823	−0.849796	3.185675
H	10.334460	2.546222	0.630635
H	10.701387	1.378144	2.797671
C	0.492375	2.789216	−0.892571

C	1.408477	2.207474	−1.787502
C	0.604592	4.157678	−0.622778
C	2.396225	2.965173	−2.434644
H	1.338233	1.135753	−1.968360
C	1.599583	4.950296	−1.226668
H	−0.089631	4.618374	0.073657
C	2.476784	4.337648	−2.133744
H	3.245995	4.939697	−2.614052
C	−1.602929	2.780940	1.121125
C	−2.488080	3.800063	0.734580
C	−1.348946	2.588578	2.483761
C	−3.108281	4.628968	1.681497
H	−2.701265	3.938206	−0.322343
C	−1.940589	3.403560	3.466563
H	−0.688305	1.772786	2.769568
C	−2.813810	4.416316	3.041519
H	−3.283396	5.052755	3.790132
C	−2.175825	−2.316760	−1.277636
C	−1.150546	−2.571645	−2.196268
C	−3.496170	−2.637312	−1.628849
C	−1.412479	−3.161873	−3.445560
H	−0.136545	−2.292282	−1.915827
C	−3.802340	−3.218816	−2.869492
H	−4.297180	−2.420570	−0.926720
C	−2.743590	−3.479294	−3.758581
H	−2.962242	−3.937065	−4.722165
C	−1.718199	−3.112716	1.464549
C	−2.475509	−4.259553	1.191124
C	−0.943172	−3.084212	2.632400
C	−2.465715	−5.370520	2.052380
H	−3.076166	−4.297543	0.287493
C	−0.926047	−4.160053	3.535394
H	−0.337096	−2.199761	2.817279
C	−1.691487	−5.295608	3.222256
H	−1.679528	−6.144010	3.904637
O	−5.418394	0.181335	−2.222713
O	−4.951304	0.986216	−4.335129
O	−6.472246	1.504184	2.248950
O	−5.526986	2.122841	0.232738
C	−6.683087	2.275446	1.062177
H	−7.566864	1.893781	0.530822
H	−6.802758	3.327798	1.327553
C	−6.008720	0.563003	−3.469374
H	−6.516930	−0.296529	−3.908659
H	−6.702001	1.400497	−3.302819
Si	−5.579121	−3.627284	−3.326515
H	−6.143109	−2.650202	−4.301543
H	−5.662042	−4.972544	−3.957891
H	−6.426234	−3.602385	−2.105078
Si	−0.019308	−3.518292	−4.659482
H	−0.605966	−3.969206	−5.950451
H	0.802214	−2.300141	−4.899273
H	0.889339	−4.583932	−4.153761
Si	−3.440857	−6.923593	1.632425
H	−3.885824	−7.594984	2.883964
H	−4.632637	−6.564109	0.816727
H	−2.628331	−7.899283	0.853633
Si	0.090887	−4.079414	5.117917
H	−0.570392	−3.228902	6.147592
H	0.235092	−5.451871	5.674274
H	1.436352	−3.507066	4.849415
Si	−1.576516	3.142250	5.295325
H	−2.495427	3.997080	6.094346
H	−1.774066	1.718292	5.677641
H	−0.173576	3.513491	5.628833
Si	−4.325683	5.955216	1.139600
H	−5.732659	5.565133	1.443141
H	−4.062194	7.238561	1.845783
H	−4.208668	6.163788	−0.327560
Si	3.565862	2.177487	−3.683308
H	2.949438	2.105506	−5.037570
H	4.804553	2.995387	−3.781393
H	3.911622	0.795684	−3.260288
Si	1.753198	6.781809	−0.818006
H	2.635016	7.432182	−1.824064
H	0.415971	7.435053	−0.842309
H	2.339460	6.997214	0.533683

INT7

C	−4.547839	4.272159	−0.730736
C	−6.854940	4.560548	−1.722203
C	−6.048926	4.336309	−0.679722

H	−4.170688	4.685689	−1.674868	C	−5.911759	−0.138924	0.073726
H	−4.111291	4.870624	0.080500	C	−6.956195	0.447971	−0.657467
H	−6.463847	4.744648	−2.721003	C	−5.522147	−1.449652	−0.241998
H	−7.935815	4.579952	−1.612134	C	−7.587575	−0.253151	−1.686611
H	−6.494672	4.163543	0.300673	H	−7.278125	1.457233	−0.415089
H	−2.038701	−0.151979	−0.228561	C	−6.151437	−2.149768	−1.273070
Si	−3.895387	2.488681	−0.571728	H	−4.710998	−1.911377	0.313545
C	−4.103042	1.535193	−2.167154	C	−7.186111	−1.553760	−1.998377
H	−3.743106	0.510269	−2.051500	H	−8.397365	0.215438	−2.239891
H	−5.149409	1.506880	−2.483231	H	−5.829813	−3.160475	−1.509078
H	−3.511731	2.023394	−2.950604	H	−7.678265	−2.100941	−2.797962
C	−4.457914	1.729710	1.062127	O	5.321142	−2.529108	−2.947382
C	−3.975275	2.361283	2.226764	O	5.356035	−1.429128	−0.915581
C	−5.276759	0.585094	1.217408	O	4.386105	−2.824717	1.710968
C	−4.261116	1.880661	3.502621	O	4.994321	−1.910769	3.741577
H	−3.341024	3.240228	2.138376	C	6.172419	−2.099492	−1.880601
C	−5.541000	0.097202	2.508058	H	6.644979	−2.976400	−1.414340
C	−5.040760	0.732180	3.642771	H	6.919501	−1.404521	−2.268748
H	−3.871068	2.394067	4.377217	C	5.300328	−2.947438	2.804809
H	−6.165428	−0.785847	2.613308	H	6.328701	−2.815832	2.436923
H	−5.267773	0.337315	4.629476	H	5.167007	−3.919634	3.281410
C	3.125752	−0.868382	0.858049	C	−1.092900	−2.765208	−1.151473
C	2.726252	0.457983	1.214651	C	−1.280751	−4.109926	−0.811231
C	3.106571	0.987381	2.454808	C	−1.776799	−2.254108	−2.265555
C	3.874511	0.273578	3.391713	C	−2.135078	−4.947019	−1.553017
C	4.253836	−0.999255	3.030982	H	−0.760781	−4.515810	0.051406
C	3.887669	−1.542125	1.801708	C	−2.609009	−3.062399	−3.056268
C	2.921212	−1.529747	−0.468564	H	−1.650473	−1.198839	−2.497104
C	1.688058	−1.996508	−1.026014	C	−2.779116	−4.406121	−2.676763
C	1.698521	−2.653738	−2.265309	H	−3.431703	−5.045109	−3.269911
C	2.870181	−2.892283	−3.003396	C	0.167420	−2.458309	1.432195
C	4.046878	−2.445234	−2.446715	C	0.985536	−3.572794	1.671312
C	4.060237	−1.788604	−1.219294	C	−0.627288	−1.965444	2.475466
H	2.813179	1.997003	2.712142	C	1.012505	−4.206144	2.924740
H	4.159880	0.708331	4.343338	H	1.617690	−3.946356	0.869800
H	0.765540	−3.006257	−2.685332	C	−0.636754	−2.576090	3.742314
H	2.846318	−3.405362	−3.958462	H	−1.233989	−1.083708	2.276157
P	1.613525	1.423948	0.078659	C	0.188325	−3.694570	3.942899
P	0.048989	−1.619710	−0.219106	H	0.192694	−4.176533	4.919500
Rh	−0.556591	0.500956	−0.190991	C	2.680715	1.703488	−1.409844
Cl	−1.771849	2.810014	−0.375976	C	4.078192	1.815761	−1.351620

C	2.043043	1.819083	−2.650757
C	4.841501	2.048863	−2.506287
H	4.574724	1.710711	−0.390139
C	2.768583	2.064027	−3.830871
H	0.960796	1.699575	−2.680271
C	4.164361	2.176378	−3.733602
H	4.740681	2.362771	−4.638593
C	1.587323	3.104169	0.876529
C	2.364716	4.189651	0.453202
C	0.699132	3.294832	1.948411
C	2.281925	5.445807	1.080924
H	3.049537	4.055388	−0.378860
C	0.600973	4.525010	2.617293
H	0.079323	2.455035	2.257455
C	1.405493	5.587298	2.168304
H	1.347663	6.546639	2.679465
Si	6.715053	2.157732	−2.407171
H	7.369855	0.911564	−2.899840
H	7.224674	3.280312	−3.241260
H	7.126665	2.365324	−0.993636
Si	1.895613	2.231909	−5.489752
H	1.066886	3.467797	−5.549082
H	2.918980	2.297990	−6.568263
H	0.998606	1.071382	−5.740214
Si	−0.584584	4.758802	4.058129
H	−0.557209	3.576694	4.961091
H	−0.191381	5.971918	4.824638
H	−1.990194	4.942448	3.597912
Si	3.311920	6.898338	0.472442
H	3.377275	7.934572	1.538397
H	4.691781	6.453490	0.135336
H	2.724797	7.520427	−0.746794
Si	−1.722588	−1.921183	5.132550
H	−3.163986	−2.207526	4.891913
H	−1.323807	−2.585748	6.403835
H	−1.568290	−0.449777	5.285365
Si	2.129901	−5.685342	3.229627
H	3.354711	−5.316479	3.995794
H	1.416477	−6.724491	4.021790
H	2.558375	−6.266426	1.929746
Si	−2.414358	−6.736015	−1.043511
H	−3.371231	−6.847881	0.092936
H	−2.972880	−7.494272	−2.195839
H	−1.132930	−7.362901	−0.618723
Si	−3.447936	−2.382313	−4.597304
H	−2.576676	−2.529508	−5.797957
H	−4.703849	−3.137578	−4.858296
H	−3.756220	−0.939257	−4.429148

INT8

C	5.126765	1.103117	1.222070
C	2.948182	0.066170	1.061888
C	3.606133	1.455185	1.358732
H	5.514440	1.361995	0.230688
H	5.783286	1.558592	1.969034
H	2.637365	−0.033015	0.004928
H	2.124114	−0.220476	1.744849
H	3.274694	2.259710	0.693784
H	3.377154	1.766397	2.384817
Si	4.659311	−0.740004	1.352671
C	4.791784	−1.486921	3.088471
H	4.227466	−2.425613	3.148236
H	5.826996	−1.700961	3.376374
H	4.373801	−0.797406	3.832102
C	5.205775	−1.951573	0.002639
C	4.216705	−2.835040	−0.474530
C	6.479154	−1.976920	−0.619586
C	4.464125	−3.719646	−1.524995
H	3.220849	−2.813384	−0.034797
C	6.710362	−2.857429	−1.689509
C	5.716943	−3.726034	−2.138366
H	3.680106	−4.390485	−1.866745
H	7.691932	−2.870719	−2.156413
H	5.923279	−4.405458	−2.961504
C	−3.014122	1.089714	−1.046088
C	−1.746351	1.629135	−1.428657
C	−1.554534	2.095547	−2.735511
C	−2.563326	2.067709	−3.714821
C	−3.781577	1.558576	−3.325918
C	−3.990358	1.087887	−2.031342
C	−3.403136	0.653097	0.330349
C	−2.929852	−0.498979	1.036114

C	−3.438374	−0.783522	2.311965
C	−4.412733	0.005536	2.946668
C	−4.867008	1.100159	2.246295
C	−4.372451	1.404116	0.980805
H	−0.594779	2.511162	−3.015247
H	−2.391860	2.437912	−4.719554
H	−3.073841	−1.652693	2.844540
H	−4.788515	−0.239237	3.933960
P	−0.346041	1.635967	−0.206077
P	−1.536109	−1.543482	0.379694
Rh	0.427749	−0.535008	0.391378
C	7.598309	−1.092001	−0.183750
C	8.066781	−1.106372	1.139865
C	8.236610	−0.245240	−1.105684
C	9.127958	−0.289704	1.534375
H	7.616385	−1.788436	1.855344
C	9.296469	0.572260	−0.712686
H	7.882463	−0.219027	−2.132896
C	9.745190	0.554555	0.609902
H	9.478957	−0.322336	2.562574
H	9.770287	1.226664	−1.439913
H	10.571448	1.190591	0.915982
H	0.967367	−2.052362	0.531808
O	−5.793211	2.037530	2.624848
O	−4.973132	2.557241	0.526338
O	−5.281549	0.616374	−1.927641
O	−4.927388	1.410017	−4.065922
C	−6.017679	2.841484	1.462307
H	−6.988468	2.578482	1.018279
H	−5.980842	3.897938	1.737130
C	−5.940131	1.070007	−3.114526
H	−6.537428	1.963655	−2.880971
H	−6.560031	0.266703	−3.514783
C	0.981203	2.560081	−1.122755
C	1.768050	1.826856	−2.031180
C	1.273635	3.914167	−0.928795
C	2.818875	2.419710	−2.745289
H	1.544120	0.771372	−2.175369
C	2.326092	4.547919	−1.618175
H	0.675194	4.487651	−0.226638
C	3.079586	3.785290	−2.522057
H	3.890434	4.266041	−3.067210
C	−0.916105	2.865290	1.057892
C	−1.742199	3.959532	0.756733
C	−0.495926	2.679496	2.379984
C	−2.144218	4.866958	1.748951
H	−2.080877	4.097306	−0.266960
C	−0.864106	3.571782	3.403300
H	0.119023	1.808876	2.602317
C	−1.685952	4.657578	3.063346
H	−1.981859	5.356633	3.844146
C	−1.657108	−3.063068	1.455926
C	−0.750669	−3.206930	2.513297
C	−2.634887	−4.051749	1.272108
C	−0.807641	−4.302139	3.393058
H	0.015231	−2.443621	2.628852
C	−2.717969	−5.171080	2.116450
H	−3.342246	−3.953875	0.454273
C	−1.799841	−5.271176	3.176533
H	−1.859332	−6.124850	3.849775
C	−2.155467	−2.179947	−1.247891
C	−3.516503	−2.349475	−1.544383
C	−1.203185	−2.548864	−2.206027
C	−3.935734	−2.894975	−2.768627
H	−4.260584	−2.043410	−0.813473
C	−1.580205	−3.104340	−3.441521
H	−0.154109	−2.386192	−1.965276
C	−2.950139	−3.272856	−3.698282
H	−3.257466	−3.706922	−4.648495
Si	−5.763819	−3.106521	−3.149640
H	−6.270685	−2.051592	−4.073466
H	−6.012289	−4.419032	−3.805989
H	−6.548985	−3.029439	−1.889241
Si	−0.286738	−3.605629	−4.713586
H	−0.980477	−4.126250	−5.923002
H	0.561197	−2.447300	−5.106414
H	0.612401	−4.667872	−4.184651
Si	−4.008973	−6.507410	1.821489
H	−3.469670	−7.634977	1.011138
H	−4.472756	−7.063403	3.122042
H	−5.169850	−5.928897	1.092047
Si	0.422663	−4.470759	4.807072

H	0.416047	−3.258646	5.671619
H	0.049140	−5.651695	5.632116
H	1.810860	−4.660691	4.304106
Si	2.711458	6.368569	−1.333352
H	3.186003	6.614628	0.056027
H	3.774016	6.790773	−2.284893
H	1.502125	7.208936	−1.553079
Si	3.860373	1.414714	−3.951780
H	3.216659	0.094537	−4.173712
H	3.976704	2.130945	−5.252352
H	5.238686	1.201859	−3.431295
Si	−0.282653	3.311635	5.174881
H	−0.878674	4.368809	6.035596
H	−0.699435	1.977626	5.685578
H	1.200622	3.393743	5.274388
Si	−3.291414	6.295818	1.328853
H	−4.684095	6.038482	1.796840
H	−2.832684	7.552959	1.980144
H	−3.327353	6.484680	−0.145296

INT9

Rh	0.707450	0.352909	1.212452
P	−0.129924	−1.780632	0.391610
P	−0.965256	1.702777	0.086866
Si	3.086808	0.164240	1.005562
Si	0.635102	−3.172237	5.811182
Si	1.484927	−7.119582	1.763037
Si	−1.565779	−5.660370	−3.529328
Si	3.304636	−2.704462	−4.051288
Si	−2.547075	7.156203	−0.619407
Si	2.925643	5.630725	−1.186453
Si	−6.598362	2.619842	0.466159
Si	−3.434074	1.827940	5.162716
O	−5.036233	−0.517726	−1.283355
O	−6.130777	−1.808950	0.281310
O	−3.044541	−1.806562	−3.353583
O	−2.418059	−0.612431	−5.235819
C	−1.993748	−1.802882	0.407768
C	−2.684258	−2.562554	1.361686
C	−4.087513	−2.634319	1.418466
C	−4.775680	−1.919686	0.464625
C	−4.106781	−1.148588	−0.484257
C	−2.725651	−1.037067	−0.555044
C	−2.162576	−0.217198	−1.676335
C	−2.399143	−0.654181	−2.972355
C	−2.027552	0.060727	−4.109612
C	−1.397793	1.281083	−4.016318
C	−1.146307	1.757815	−2.717661
C	−1.508997	1.053193	−1.562096
C	0.302829	−3.104388	1.631151
C	0.307427	−2.752188	2.991877
C	0.624923	−3.678080	3.997196
C	0.960113	−4.986908	3.607135
C	0.989280	−5.373043	2.258693
C	0.647527	−4.416577	1.284496
C	0.209153	−2.657799	−1.217076
C	−0.668519	−3.630312	−1.723864
C	−0.378212	−4.345781	−2.896130
C	0.824466	−4.056733	−3.566042
C	1.719764	−3.080951	−3.101500
C	1.393854	−2.395470	−1.916421
C	−0.565114	3.484909	−0.268191
C	−1.544775	4.488828	−0.317633
C	−1.217757	5.824009	−0.601394
C	0.129595	6.135364	−0.853051
C	1.138974	5.161219	−0.813426
C	0.770978	3.839038	−0.503328
C	−2.528394	1.852203	1.070937
C	−3.780601	2.099074	0.485623
C	−4.932070	2.277502	1.267880
C	−4.803147	2.194449	2.666525
C	−3.572223	1.934630	3.287004
C	−2.442098	1.765054	2.466461
C	−6.274456	−1.172924	−0.992256
C	−2.948283	−1.862280	−4.781917
C	3.569555	0.883718	−0.732383
C	2.576013	0.963772	−1.729579
C	2.826661	1.437166	−3.019273
C	4.109317	1.867302	−3.353598
C	5.116188	1.808161	−2.391165
C	4.872841	1.319321	−1.095649
C	6.060154	1.298506	−0.177482

C	6.839031	0.141019	−0.032512
C	7.985901	0.144442	0.764714
C	8.379529	1.310910	1.422505
C	7.623157	2.475218	1.271842
C	6.477331	2.469362	0.474463
C	3.872839	−1.572059	1.103286
C	3.696059	1.290674	2.412165
C	2.710477	2.467376	2.458145
C	1.247224	1.996286	2.463983
H	−2.122608	−3.145655	2.080507
H	−4.597120	−3.234903	2.163791
H	−1.119348	1.850041	−4.896466
H	−0.651453	2.715988	−2.618579
H	0.060907	−1.727679	3.260331
H	1.201395	−5.721811	4.373298
H	0.652437	−4.704797	0.238363
H	−1.588648	−3.840153	−1.186117
H	1.074812	−4.614147	−4.468008
H	2.075591	−1.643469	−1.533167
H	−2.580965	4.231596	−0.123863
H	0.400690	7.165266	−1.080995
H	1.531729	3.067161	−0.441672
H	−3.857739	2.144834	−0.597582
H	−5.686046	2.333364	3.288550
H	−1.472514	1.565579	2.916865
H	−6.473386	−1.934008	−1.761057
H	−7.074076	−0.433591	−0.941434
H	−2.271147	−2.674838	−5.071461
H	−3.945569	−2.010636	−5.207058
H	1.567037	0.651374	−1.475766
H	2.021626	1.471980	−3.749111
H	4.328089	2.244615	−4.349309
H	6.121004	2.139333	−2.641619
H	6.549548	−0.762619	−0.561524
H	8.574945	−0.763620	0.864955
H	9.271883	1.314749	2.042836
H	7.925478	3.390762	1.773836
H	5.891853	3.377645	0.357920
H	4.962669	−1.516640	1.010665
H	3.503958	−2.244689	0.319997
H	3.636658	−2.033219	2.069475
H	4.734781	1.621878	2.320160
H	3.621838	0.707723	3.342841
H	2.881668	3.106976	1.580484
H	2.906099	3.106244	3.335742
H	0.589393	2.858757	2.304032
H	1.003212	1.577920	3.455478
H	1.698976	−0.478163	2.161449
H	0.435474	−4.380346	6.657213
H	−0.457183	−2.198053	6.076835
H	1.925140	−2.540483	6.201923
H	2.906109	−7.189861	1.323694
H	0.636911	−7.597124	0.636623
H	1.311825	−8.028838	2.927997
H	−0.826327	−6.885511	−3.936890
H	−2.327291	−5.185587	−4.720901
H	−2.542540	−5.998767	−2.461313
H	4.386506	−2.306588	−3.115418
H	3.104328	−1.615607	−5.045388
H	3.714002	−3.929257	−4.792945
H	−2.557993	7.946171	0.642936
H	−3.880550	6.516657	−0.781949
H	−2.315146	8.101919	−1.745239
H	3.074954	7.100114	−0.998450
H	3.296944	5.305819	−2.590051
H	3.859612	4.921137	−0.275849
H	−6.399186	2.955142	−0.968414
H	−7.284543	3.751713	1.146168
H	−7.506357	1.440914	0.547958
H	−4.803129	1.862887	5.744340
H	−2.651498	2.966501	5.715867
H	−2.761039	0.565794	5.571526

INT10

Rh	0.935907	0.688480	0.212437
P	0.758087	−1.529222	0.204460
P	−1.439567	1.130343	−0.071083
Si	3.310339	0.645148	−0.162515
Si	3.865872	−1.829944	4.897183
Si	4.372549	−5.943121	0.958415
Si	−0.299027	−6.154872	−2.967536
Si	1.489082	−1.295856	−5.403597

Si	−3.965892	6.278765	−0.240728	C	−4.465301	1.055977	3.462555
Si	0.128154	4.888389	−3.983857	C	−3.087974	1.115468	3.723223
Si	−6.826410	0.868090	1.830412	C	−2.210405	1.126852	2.622995
Si	−2.437921	1.174545	5.489170	C	−5.223918	−3.201349	1.628560
O	−4.511988	−2.403937	0.677807	C	−3.893414	−3.863816	−3.081873
O	−4.362690	−3.410613	2.752591	C	3.570077	2.203957	−1.272408
O	−3.141960	−3.553607	−1.903602	C	4.056722	2.068950	−2.587692
O	−3.754753	−2.765182	−3.987750	C	4.373465	3.170914	−3.383938
C	−0.819876	−2.161214	0.996454	C	4.220038	4.461141	−2.875256
C	−0.763068	−2.770662	2.258064	C	3.728589	4.632010	−1.581589
C	−1.897808	−3.233354	2.946983	C	3.384184	3.524798	−0.789022
C	−3.109058	−3.070511	2.313971	C	2.824313	3.769485	0.566776
C	−3.190420	−2.468783	1.061417	C	3.516916	4.542763	1.511477
C	−2.091966	−1.988220	0.362020	C	2.993783	4.752352	2.788325
C	−2.356933	−1.392661	−0.982367	C	1.755671	4.210221	3.142387
C	−2.901614	−2.199862	−1.969390	C	1.038405	3.465388	2.205083
C	−3.272280	−1.730177	−3.227887	C	1.573810	3.241508	0.933569
C	−3.130946	−0.403947	−3.569250	C	4.208399	−0.765431	−1.102525
C	−2.599257	0.445608	−2.582158	C	4.390795	0.895163	1.417424
C	−2.214269	−0.010431	−1.315825	C	5.829261	1.398514	1.192955
C	2.041014	−2.472253	1.174550	C	6.623494	1.545674	2.497958
C	2.443824	−1.923116	2.404528	H	0.196691	−2.913950	2.735650
C	3.365715	−2.571738	3.239495	H	−1.818173	−3.702072	3.921635
C	3.916264	−3.787586	2.793806	H	−3.425209	−0.029665	−4.543575
C	3.572545	−4.347242	1.555007	H	−2.503158	1.497152	−2.821915
C	2.619382	−3.677811	0.763309	H	2.024772	−0.963573	2.699831
C	0.705415	−2.393387	−1.438118	H	4.634712	−4.308109	3.425741
C	0.296074	−3.730700	−1.570613	H	2.335945	−4.105105	−0.192940
C	0.258375	−4.365575	−2.821175	H	−0.012865	−4.280035	−0.685062
C	0.629967	−3.617834	−3.954142	H	0.604063	−4.092712	−4.933933
C	1.020748	−2.273386	−3.864248	H	1.326757	−0.632659	−2.470889
C	1.050017	−1.678183	−2.589674	H	−3.263708	3.475468	0.483449
C	−1.693125	2.810137	−0.823264	H	−1.985694	6.334883	−2.453530
C	−2.618054	3.745568	−0.346678	H	−0.111865	2.470475	−2.245987
C	−2.730358	5.029084	−0.915675	H	−4.436047	0.987866	0.063359
C	−1.898967	5.349876	−1.997444	H	−5.158012	1.038643	4.302795
C	−0.953163	4.439695	−2.506297	H	−1.133183	1.135448	2.779824
C	−0.854595	3.183361	−1.892649	H	−5.476264	−4.171378	1.176418
C	−2.683212	1.098158	1.306409	H	−6.120473	−2.668068	1.951131
C	−4.068384	1.031802	1.085469	H	−3.490517	−4.768176	−3.541508
C	−4.978678	1.005767	2.152369	H	−4.953286	−3.987528	−2.816061

H	4.218921	1.074958	−2.995526
H	4.752341	3.021560	−4.392239
H	4.472523	5.327951	−3.480617
H	3.585580	5.633978	−1.183706
H	4.485341	4.958099	1.246794
H	3.554669	5.342032	3.508890
H	1.345519	4.381845	4.133737
H	0.055398	3.076589	2.449943
H	0.944547	2.798707	0.145946
H	5.239180	−0.472268	−1.339763
H	3.722739	−1.054932	−2.040335
H	4.261834	−1.662223	−0.475918
H	4.431201	−0.081873	1.920573
H	3.872843	1.569085	2.111653
H	5.806663	2.366507	0.675371
H	6.364762	0.711768	0.523125
H	7.643819	1.905591	2.313337
H	6.698316	0.586759	3.026618
H	6.134785	2.257440	3.175355
H	3.055547	−0.611600	5.155471
H	5.310033	−1.471822	4.917872
H	3.631323	−2.809560	5.994962
H	4.914807	−6.687197	2.127253
H	5.491208	−5.682262	0.011084
H	3.369526	−6.790817	0.257620
H	−0.515813	−6.713207	−1.607171
H	0.714435	−6.979508	−3.680805
H	−1.573854	−6.269640	−3.732685
H	1.233142	−2.140964	−6.601513
H	2.928065	−0.915008	−5.389611
H	0.687533	−0.047233	−5.509599
H	−3.996152	7.463451	−1.139614
H	−3.596177	6.727927	1.129812
H	−5.330945	5.688265	−0.168913
H	1.106619	3.801077	−4.227275
H	0.837741	6.174799	−3.749992
H	−0.714677	5.061367	−5.201558
H	−7.088044	1.056191	0.379462
H	−7.582658	1.887756	2.607179
H	−7.348607	−0.470066	2.231197
H	−3.558943	0.890529	6.424806
H	−1.877972	2.515316	5.816913
H	−1.359846	0.170247	5.691634

INT11

Rh	−0.105634	−1.540126	0.672361
P	1.951666	−0.448779	0.078403
P	−1.447301	0.581802	0.254611
Si	−0.526485	−3.302228	−0.808016
Si	4.652681	−5.428018	0.240691
Si	7.295334	−0.844922	−1.936138
Si	5.583976	3.328538	2.370523
Si	2.233259	0.096062	5.692303
Si	−7.124322	1.224589	0.350554
Si	−4.265908	−0.052944	5.131232
Si	−3.363981	4.820919	−2.989909
Si	−2.081847	−0.212698	−5.359960
O	0.554696	4.160402	−2.215453
O	1.312421	3.559046	−4.315731
O	2.332694	4.366294	0.341705
O	1.542206	5.413049	2.238776
C	1.831008	0.811031	−1.269852
C	2.248748	0.456109	−2.560917
C	2.120903	1.310246	−3.668794
C	1.557627	2.544390	−3.428593
C	1.107968	2.902491	−2.160068
C	1.185113	2.068060	−1.052348
C	0.626533	2.575722	0.239953
C	1.209526	3.706506	0.791512
C	0.742649	4.338900	1.941530
C	−0.360464	3.867650	2.615156
C	−0.989299	2.733079	2.071522
C	−0.538825	2.082278	0.915864
C	3.457220	−1.456237	−0.371128
C	3.487045	−2.813214	−0.032260
C	4.633456	−3.605267	−0.236907
C	5.761860	−2.997419	−0.802946
C	5.773335	−1.635889	−1.160481
C	4.614564	−0.882262	−0.927463
C	2.661895	0.456509	1.538713
C	3.657961	1.437706	1.422392
C	4.245886	2.020716	2.553423

C	3.809130	1.595515	3.822577	H	4.264248	2.029391	4.711524
C	2.808560	0.625626	3.979155	H	1.482849	−0.706370	2.898505
C	2.249008	0.063538	2.816489	H	−4.292664	1.125309	−0.525727
C	−3.065367	0.619945	1.166583	H	−6.402149	0.626174	3.176509
C	−4.283156	0.898332	0.534470	H	−2.156525	0.019059	3.027091
C	−5.501007	0.888208	1.239269	H	−2.439833	3.182252	−0.697254
C	−5.469856	0.609929	2.612824	H	−2.928819	2.577596	−4.921516
C	−4.271754	0.304651	3.282065	H	−1.486693	−0.616534	−2.428681
C	−3.084683	0.292552	2.534852	H	1.671923	5.405829	−3.441635
C	−1.923193	1.221512	−1.421342	H	−0.031024	5.094418	−3.966617
C	−2.382454	2.540801	−1.572486	H	3.381949	5.812881	1.383079
C	−2.759738	3.048297	−2.823573	H	1.938524	6.398779	0.457165
C	−2.654152	2.196578	−3.938244	H	−2.073057	−3.250708	−3.404222
C	−2.198976	0.874519	−3.827018	H	−4.443128	−2.929398	−3.987015
C	−1.838511	0.401773	−2.550408	H	−6.115887	−2.518596	−2.179195
C	0.866489	4.661928	−3.519919	H	−5.395420	−2.489380	0.176874
C	2.358395	5.593521	1.077632	H	−4.796255	−3.881558	1.742728
C	−2.354526	−3.081673	−1.268702	H	−4.253700	−4.109831	4.133575
C	−2.792154	−3.089089	−2.605177	H	−1.999070	−3.400515	4.957156
C	−4.134035	−2.906163	−2.945093	H	−0.356876	−2.485550	3.378427
C	−5.070178	−2.686654	−1.933445	H	−0.625879	−5.811310	−0.869897
C	−4.662015	−2.679621	−0.601208	H	−0.813124	−5.215911	0.792293
C	−3.316710	−2.890745	−0.245461	H	0.791600	−5.268545	0.046116
C	−2.921033	−2.963604	1.188292	H	1.564193	−2.869582	−2.081618
C	−3.837389	−3.521149	2.104979	H	0.186152	−2.275315	−2.976979
C	−3.530780	−3.665891	3.453969	H	−0.380036	−4.713351	−3.587529
C	−2.270482	−3.273897	3.911353	H	1.059202	−5.216737	−2.728504
C	−1.346064	−2.748437	3.006759	H	1.516350	−5.054860	−5.181113
C	−1.644252	−2.546884	1.643585	H	2.489131	−3.858973	−4.307055
C	−0.269938	−5.068302	−0.145405	H	1.033843	−3.349477	−5.177339
C	0.545532	−3.134491	−2.392673	H	0.765914	−2.775637	1.135267
C	0.626293	−4.383480	−3.296626	H	3.647801	−6.200548	−0.538500
C	1.462394	−4.150726	−4.562136	H	4.348777	−5.604536	1.686193
H	2.700967	−0.514949	−2.722782	H	6.006333	−5.976298	−0.042774
H	2.455934	1.015956	−4.657206	H	8.525568	−1.245953	−1.201518
H	−0.738526	4.352934	3.508126	H	7.151704	0.634807	−1.888366
H	−1.883594	2.378646	2.566539	H	7.461361	−1.255325	−3.358328
H	2.597313	−3.252141	0.410534	H	6.715371	3.056684	3.297995
H	6.657144	−3.595660	−0.964907	H	5.075606	4.694445	2.683955
H	4.610663	0.170670	−1.191634	H	6.083073	3.331358	0.969894
H	3.972968	1.758228	0.433544	H	2.279044	−1.384078	5.834417

H	0.836307	0.538026	5.955071
H	3.127071	0.714666	6.707964
H	−6.877004	2.077759	−0.843087
H	−8.068607	1.920333	1.267117
H	−7.779035	−0.032135	−0.108873
H	−2.876014	−0.310906	5.586134
H	−5.130834	−1.212869	5.473705
H	−4.794815	1.126746	5.875114
H	−3.463990	5.432096	−1.639056
H	−4.692468	4.879733	−3.658098
H	−2.423330	5.638495	−3.809349
H	−1.691538	0.630007	−6.523712
H	−3.381082	−0.860238	−5.688165
H	−1.062484	−1.274789	−5.163599

INT12

Rh	0.480573	0.733898	0.768242
P	0.130960	−1.578613	0.315526
P	−1.516463	1.434547	0.004195
Si	3.549891	1.049055	1.048509
Si	1.974834	−1.811476	5.642899
Si	3.450628	−5.957657	1.993735
Si	−0.790780	−6.012302	−3.178020
Si	3.318882	−2.222642	−4.334313
Si	−4.186811	6.448432	−0.853517
Si	1.258321	5.727142	−2.421348
Si	−7.163085	1.283086	0.898263
Si	−3.507894	1.545632	5.289243
O	−5.128312	−1.810633	−0.475071
O	−5.559590	−3.165771	1.342652
O	−3.251206	−2.768743	−2.810446
O	−3.162982	−1.684819	−4.851198
C	−1.612406	−2.119276	0.674727
C	−1.901626	−2.933752	1.777044
C	−3.206417	−3.346068	2.102157
C	−4.211943	−2.918612	1.264703
C	−3.943785	−2.105943	0.164990
C	−2.671884	−1.666121	−0.170541
C	−2.507170	−0.860947	−1.418872
C	−2.845567	−1.466448	−2.620830
C	−2.791808	−0.820682	−3.853402
C	−2.396581	0.494133	−3.954285
C	−2.058813	1.141572	−2.753022
C	−2.103066	0.509833	−1.502391
C	1.104401	−2.511695	1.599655
C	1.195288	−1.943969	2.882541
C	1.914614	−2.562247	3.917246
C	2.577987	−3.769085	3.629617
C	2.526592	−4.358765	2.356866
C	1.773953	−3.717143	1.355698
C	0.515215	−2.552106	−1.225348
C	−0.165454	−3.730065	−1.569541
C	0.167581	−4.461585	−2.720512
C	1.222902	−3.990670	−3.521411
C	1.924798	−2.814128	−3.213504
C	1.548208	−2.103739	−2.058857
C	−1.552392	3.205096	−0.589862
C	−2.685750	4.027126	−0.524242
C	−2.665883	5.350210	−0.998479
C	−1.475503	5.833762	−1.566109
C	−0.317099	5.043121	−1.648119
C	−0.375439	3.734711	−1.139018
C	−2.987808	1.384014	1.136638
C	−4.310457	1.338110	0.668222
C	−5.402127	1.354426	1.550838
C	−5.136968	1.419817	2.930818
C	−3.828303	1.456292	3.436534
C	−2.763589	1.431348	2.517673
C	−6.090955	−2.700726	0.098708
C	−3.653102	−2.850866	−4.181741
C	3.994779	1.484452	−0.748904
C	2.949764	1.490656	−1.694595
C	3.173598	1.746674	−3.048983
C	4.472283	1.987235	−3.497691
C	5.526034	1.980988	−2.585277
C	5.307531	1.747251	−1.217681
C	6.496914	1.791270	−0.313816
C	7.533912	0.855451	−0.458163
C	8.655855	0.898743	0.370205
C	8.766255	1.885887	1.352374
C	7.751342	2.834291	1.493569
C	6.628333	2.788616	0.664983

C	4.730285	−0.208526	1.823555
C	3.232564	2.527809	2.175436
C	1.988920	3.340056	1.775295
C	0.679963	2.540424	1.865110
H	−1.092631	−3.281295	2.407361
H	−3.406441	−3.978794	2.959885
H	−2.354417	1.007540	−4.908551
H	−1.758848	2.180192	−2.811101
H	0.688433	−0.995680	3.058835
H	3.150789	−4.257405	4.415800
H	1.711418	−4.164385	0.367852
H	−0.967283	−4.080594	−0.925950
H	1.509027	−4.556311	−4.406901
H	2.065882	−1.183707	−1.797372
H	−3.601024	3.636916	−0.090679
H	−1.447265	6.852243	−1.949556
H	0.508704	3.102646	−1.152262
H	−4.489558	1.279207	−0.402249
H	−5.971819	1.437201	3.630011
H	−1.734867	1.441049	2.869494
H	−6.243253	−3.555847	−0.576340
H	−7.021854	−2.161619	0.279118
H	−3.215622	−3.742985	−4.635044
H	−4.750797	−2.871307	−4.240042
H	1.936526	1.272590	−1.349501
H	2.340916	1.746417	−3.747698
H	4.665820	2.181011	−4.549568
H	6.538622	2.179611	−2.926867
H	7.446793	0.080788	−1.215474
H	9.443205	0.159055	0.250345
H	9.639786	1.919702	1.997863
H	7.836324	3.616972	2.242896
H	5.855140	3.545661	0.757784
H	5.692220	0.244405	2.083249
H	4.923092	−1.046377	1.144420
H	4.283643	−0.616584	2.737731
H	4.124509	3.166581	2.211823
H	3.098536	2.137041	3.196018
H	2.123280	3.746872	0.762543
H	1.922897	4.220760	2.437145
H	−0.151713	3.242858	1.740400
H	0.589196	2.133397	2.890888
H	2.243523	0.248962	0.936025
H	0.711633	−2.058968	6.392017
H	2.179480	−0.340136	5.566104
H	3.096017	−2.427216	6.403009
H	3.878308	−6.575885	3.277648
H	4.661571	−5.717622	1.160556
H	2.577632	−6.912798	1.257822
H	−1.494277	−6.540224	−1.979331
H	0.125420	−7.054589	−3.716140
H	−1.814424	−5.740515	−4.228473
H	3.689456	−3.341169	−5.244828
H	4.510987	−1.824979	−3.540788
H	2.904560	−1.063747	−5.171018
H	−4.238736	7.159917	0.454111
H	−5.421034	5.625616	−0.975474
H	−4.169296	7.472363	−1.933412
H	1.062446	7.179246	−2.683559
H	1.565650	5.055944	−3.714410
H	2.425815	5.547818	−1.519176
H	−7.161972	1.550600	−0.564177
H	−8.018962	2.290265	1.582950
H	−7.790394	−0.050289	1.125935
H	−2.476713	0.552301	5.694488
H	−4.775899	1.257516	6.013045
H	−3.028348	2.894053	5.700233

INT13

C	3.450704	1.395032	0.943518
C	2.235581	−0.754933	1.613469
C	2.536836	0.582530	1.831215
H	3.349588	1.096104	−0.106470
H	3.191032	2.459843	0.997563
H	2.626788	−1.275561	0.742491
H	1.933882	−1.385731	2.443276
H	2.424539	0.959799	2.844340
Si	5.296332	1.219683	1.420811
C	5.543091	1.590242	3.259301
H	6.603575	1.532134	3.527283
H	5.185196	2.595408	3.514186
H	4.997476	0.874957	3.886004

C	6.418791	2.216927	0.281605	O	−3.497629	−1.574551	−3.485395
C	6.529841	3.592301	0.061693	O	−5.468651	−0.458441	−1.341011
C	7.260081	1.327694	−0.436583	O	−6.537993	−1.885166	0.122716
C	7.457457	4.095027	−0.856813	C	−3.679476	−1.372813	−4.890655
H	5.893492	4.287125	0.606257	H	−4.726401	−1.100909	−5.088248
C	8.185768	1.836713	−1.355616	H	−3.397829	−2.281359	−5.427122
C	8.280753	3.214252	−1.562037	C	−6.699211	−1.143987	−1.090358
H	7.539050	5.166524	−1.020293	H	−6.905027	−1.838408	−1.918298
H	8.837272	1.169011	−1.912989	H	−7.501883	−0.415936	−0.967694
H	9.002611	3.601352	−2.276827	C	−0.091580	−3.084043	1.431966
C	−2.588447	−0.102165	−1.713566	C	0.394697	−4.321791	0.998104
C	−1.875957	1.122602	−1.517835	C	−0.199981	−2.855881	2.815854
C	−1.474043	1.873236	−2.631663	C	0.767584	−5.329134	1.909096
C	−1.743341	1.488951	−3.956489	H	0.491056	−4.507544	−0.067475
C	−2.440426	0.313838	−4.124973	C	0.132640	−3.840931	3.757302
C	−2.846569	−0.448274	−3.032834	H	−0.545051	−1.879379	3.151910
C	−3.148651	−0.988530	−0.648682	C	0.620474	−5.071875	3.279898
C	−2.399480	−1.796822	0.262586	H	0.898458	−5.843707	3.995484
C	−3.075758	−2.647182	1.147738	C	−0.088833	−2.344678	−1.380310
C	−4.476840	−2.757822	1.190168	C	−0.833623	−3.336757	−2.036135
C	−5.180580	−1.982985	0.296650	C	1.042204	−1.818059	−2.016468
C	−4.527447	−1.130202	−0.589714	C	−0.464034	−3.810760	−3.304943
H	−0.933632	2.798739	−2.479571	H	−1.722584	−3.733807	−1.553003
H	−1.422306	2.090480	−4.799693	C	1.458070	−2.275619	−3.279508
H	−2.506980	−3.269321	1.826050	H	1.587718	−1.022502	−1.513728
H	−4.973278	−3.427560	1.883658	C	0.688127	−3.269597	−3.903948
P	−1.317819	1.657911	0.176314	H	0.987798	−3.625693	−4.889050
P	−0.538615	−1.682658	0.293511	C	−0.889685	3.448886	−0.119960
Rh	0.375579	0.397095	1.027519	C	−1.845646	4.474288	−0.137967
C	7.070839	−0.115731	−0.122964	C	0.448932	3.779072	−0.369412
C	7.790949	−1.164841	−0.707079	C	−1.490628	5.809079	−0.396093
C	6.078107	−0.398445	0.852210	H	−2.885995	4.234925	0.058591
C	7.534747	−2.484130	−0.328965	C	0.845629	5.097249	−0.654736
H	8.552929	−0.963905	−1.455399	H	1.184512	2.979020	−0.333557
C	5.840078	−1.725648	1.220455	C	−0.141629	6.096076	−0.664175
H	0.649315	1.807781	1.747459	H	0.147484	7.121711	−0.887565
C	6.563544	−2.769130	0.633396	C	−2.882332	1.799833	1.160008
H	8.098261	−3.292990	−0.787296	C	−4.133450	2.092713	0.595263
H	5.085721	−1.956552	1.968988	C	−2.788038	1.638103	2.547606
H	6.371411	−3.798324	0.925430	C	−5.279445	2.240395	1.392920
O	−2.825041	−0.297056	−5.290959	H	−4.215763	2.196630	−0.483835

C	−3.909768	1.784144	3.383471
H	−1.813904	1.387205	2.963835
C	−5.142240	2.088404	2.784971
H	−6.019733	2.205956	3.419007
Si	2.646585	5.520120	−0.999470
H	2.724165	6.922478	−1.491606
H	3.476674	5.411150	0.232124
H	3.222927	4.609727	−2.023894
Si	−2.785828	7.173401	−0.364559
H	−2.909210	7.792863	0.984392
H	−2.413224	8.245328	−1.327575
H	−4.114056	6.615606	−0.737505
Si	−6.949703	2.619833	0.618818
H	−7.838035	1.422911	0.591643
H	−7.659262	3.674090	1.393790
H	−6.758216	3.084001	−0.780763
Si	−3.760609	1.577740	5.248251
H	−5.120490	1.636762	5.849877
H	−3.136046	0.270705	5.590695
H	−2.926264	2.652180	5.852961
Si	−1.510173	−5.102192	−4.183615
H	−2.266828	−4.511012	−5.325017
H	−0.659678	−6.191110	−4.737095
H	−2.489559	−5.679003	−3.225637
Si	3.003502	−1.579425	−4.101184
H	2.844602	−1.631209	−5.580307
H	3.213029	−0.172148	−3.671431
H	4.215754	−2.365445	−3.742237
Si	1.461722	−6.970149	1.302088
H	2.870665	−6.834276	0.838988
H	1.426224	−7.956133	2.415514
H	0.657364	−7.487735	0.161698
Si	−0.078614	−3.531319	5.602815
H	0.881368	−4.378056	6.361271
H	0.168338	−2.097913	5.911437
H	−1.454429	−3.872233	6.061234

INT14

C	3.746479	1.529642	0.833963
C	2.225459	−0.507764	1.390819
C	2.577360	0.929385	1.638206
H	3.612567	1.312714	−0.233907
H	3.741372	2.626291	0.925223
H	2.787296	−0.988787	0.585771
H	2.191398	−1.140563	2.279581
H	2.676184	1.150808	2.707152
Si	5.489392	0.941115	1.337665
C	5.677147	0.961737	3.220820
H	6.699352	0.693640	3.508946
H	5.459472	1.954027	3.634837
H	4.995964	0.245844	3.696067
C	6.810509	1.930234	0.426553
C	7.108076	3.295263	0.428309
C	7.576201	1.052877	−0.383972
C	8.151439	3.799029	−0.355409
H	6.528567	3.981532	1.043304
C	8.619028	1.562315	−1.167230
C	8.902522	2.929342	−1.149416
H	8.377688	4.862126	−0.346962
H	9.214364	0.903658	−1.793883
H	9.714000	3.317111	−1.760171
C	−2.882812	−0.098922	−1.550072
C	−2.099273	1.098239	−1.560632
C	−1.845179	1.753895	−2.771957
C	−2.330879	1.293859	−4.008747
C	−3.090842	0.146583	−3.980281
C	−3.354730	−0.519228	−2.785263
C	−3.332036	−0.855549	−0.339105
C	−2.519868	−1.637989	0.543593
C	−3.123008	−2.343363	1.594316
C	−4.507406	−2.331515	1.836853
C	−5.273944	−1.584626	0.971733
C	−4.695230	−0.874775	−0.077674
H	−1.254522	2.661605	−2.768669
H	−2.123581	1.820220	−4.933927
H	−2.506513	−2.940870	2.253394
H	−4.946453	−2.889326	2.656622
P	−1.297593	1.691846	0.006635
P	−0.664108	−1.654657	0.374816
Rh	0.391546	0.274659	0.782230
C	7.176828	−0.379988	−0.315485
C	7.799142	−1.419633	−1.017179

C	6.082361	−0.664410	0.543635
C	7.347221	−2.732101	−0.869288
H	8.636800	−1.216517	−1.678996
C	5.650106	−1.986209	0.683303
H	1.652634	1.603689	1.366860
C	6.276632	−3.020381	−0.020053
H	7.835822	−3.533328	−1.418081
H	4.816974	−2.220159	1.341814
H	5.931566	−4.044723	0.093900
O	−3.678638	−0.520281	−5.025663
O	−4.117208	−1.636024	−3.051241
O	−5.683918	−0.197593	−0.759729
O	−6.631620	−1.388829	0.975575
C	−4.526282	−1.497543	−4.415773
H	−5.569250	−1.150001	−4.450293
H	−4.407312	−2.453598	−4.928474
C	−6.914354	−0.733658	−0.264520
H	−7.308531	−1.466995	−0.983417
H	−7.622011	0.079105	−0.093740
C	−0.646372	3.370408	−0.475099
C	0.659324	3.436794	−0.990270
C	−1.369167	4.562126	−0.339000
C	1.241648	4.652414	−1.382194
H	1.220942	2.509355	−1.089128
C	−0.819871	5.804974	−0.704207
H	−2.379044	4.525179	0.058803
C	0.479928	5.825300	−1.232903
H	0.909408	6.777588	−1.540297
C	−2.739017	2.132203	1.086659
C	−3.985271	2.541388	0.587741
C	−2.555977	2.066131	2.473022
C	−5.037837	2.894593	1.446872
H	−4.135649	2.576469	−0.488324
C	−3.579995	2.420177	3.369870
H	−1.592682	1.719434	2.844805
C	−4.809665	2.834256	2.834084
H	−5.612027	3.113698	3.515107
C	−0.177276	−3.043374	1.518771
C	0.012262	−4.367322	1.107070
C	0.033010	−2.727745	2.871910
C	0.405227	−5.372670	2.011222
H	−0.140231	−4.623925	0.062816
C	0.396348	−3.702989	3.812593
H	−0.083924	−1.690304	3.178825
C	0.584200	−5.021081	3.357400
H	0.884709	−5.789121	4.068076
C	−0.407054	−2.406904	−1.300374
C	−1.304828	−3.324718	−1.865721
C	0.745948	−2.060909	−2.017292
C	−1.067055	−3.902293	−3.123892
H	−2.208332	−3.584760	−1.320532
C	1.029233	−2.625754	−3.272965
H	1.417454	−1.325403	−1.579731
C	0.108240	−3.541891	−3.806250
H	0.307753	−3.981237	−4.783005
Si	2.604062	−2.176862	−4.203186
H	3.730539	−3.081914	−3.844419
H	2.366537	−2.300497	−5.667632
H	3.003613	−0.781930	−3.880589
Si	−2.304173	−5.101699	−3.874838
H	−3.086452	−4.473805	−4.978124
H	−1.609509	−6.285858	−4.450280
H	−3.258367	−5.551269	−2.827268
Si	0.616529	−3.262020	5.629051
H	−0.652866	−3.423642	6.392329
H	1.635196	−4.155336	6.244432
H	1.053743	−1.846280	5.757887
Si	0.697265	−7.137272	1.425548
H	1.953086	−7.254641	0.633686
H	0.801869	−8.031959	2.609656
H	−0.425564	−7.597341	0.563121
Si	−1.798636	7.396786	−0.477988
H	−1.770165	7.865756	0.935301
H	−1.209415	8.461187	−1.334463
H	−3.222153	7.189358	−0.859627
Si	2.996599	4.721691	−2.063327
H	3.988564	5.013202	−0.992106
H	3.346398	3.420579	−2.690170
H	3.091455	5.805677	−3.079037
Si	−6.706103	3.412927	0.753374
H	−7.711110	2.314889	0.840773
H	−7.252880	4.570739	1.512192

H	−6.555848	3.785941	−0.678045
Si	−3.313543	2.335107	5.231209
H	−4.571401	2.738572	5.915976
H	−2.950820	0.957026	5.661529
H	−2.219079	3.247405	5.663193

INT15

C	4.144552	−2.063582	−1.050031
C	2.415574	−0.881343	0.475292
C	2.743990	−1.407081	−0.923623
H	4.207782	−2.911686	−0.355601
H	4.238207	−2.497198	−2.058149
H	2.731836	−1.585808	1.247552
H	2.882327	0.089183	0.660308
H	2.655805	−0.596593	−1.660917
Si	5.675708	−0.964098	−0.795993
C	5.435677	0.726578	−1.618297
H	6.346100	1.329709	−1.531439
H	5.209885	0.612912	−2.686214
H	4.613364	1.287747	−1.160497
C	7.255833	−1.811838	−1.385891
C	7.630667	−2.291760	−2.643138
C	8.161608	−1.929135	−0.300802
C	8.883903	−2.881516	−2.838347
H	6.945965	−2.211933	−3.485940
C	9.415616	−2.519205	−0.500795
C	9.771506	−2.991506	−1.765500
H	9.166662	−3.253550	−3.819836
H	10.119637	−2.617111	0.321287
H	10.746435	−3.449554	−1.912853
C	−3.148528	1.184061	−0.832811
C	−3.356009	0.237508	0.221922
C	−4.394284	0.442190	1.139777
C	−5.272031	1.539205	1.073542
C	−5.069916	2.426215	0.040210
C	−4.038934	2.244500	−0.879745
C	−2.118493	1.075706	−1.910391
C	−0.701095	1.184440	−1.748787
C	0.148883	0.974100	−2.847537
C	−0.328237	0.733832	−4.145687
C	−1.697718	0.704336	−4.298221
C	−2.555506	0.864248	−3.211148
H	−4.545424	−0.275199	1.936739
H	−6.067904	1.674981	1.797387
H	1.222681	0.996814	−2.700718
H	0.344541	0.578853	−4.981517
P	−2.216184	−1.220479	0.407309
P	0.091727	1.339648	−0.092420
Rh	0.326612	−0.831651	0.583667
C	7.662868	−1.396078	0.996567
C	8.382490	−1.412481	2.197800
C	6.352943	−0.848621	0.964259
C	7.812995	−0.895230	3.362383
H	9.385438	−1.829257	2.235496
C	5.799813	−0.341385	2.143050
H	2.005486	−2.169551	−1.212356
C	6.522786	−0.361344	3.340596
H	8.377609	−0.914201	4.291239
H	4.789885	0.061262	2.140833
H	6.079261	0.031693	4.251778
Cl	0.505114	−3.170068	1.225801
H	0.548898	−0.322413	2.007947
O	−5.748459	3.582211	−0.246867
O	−4.032220	3.298293	−1.764934
O	−3.854658	0.730792	−3.638320
O	−2.421910	0.483800	−5.436238
C	−5.261205	3.994106	−1.527990
H	−5.991642	3.720270	−2.302755
H	−5.073766	5.068941	−1.516225
C	−3.789840	0.699630	−5.069490
H	−4.127092	1.665126	−5.471144
H	−4.401326	−0.123766	−5.442594
C	−2.713294	−2.294269	−1.025039
C	−3.934678	−2.130065	−1.696824
C	−1.850965	−3.324726	−1.428706
C	−4.305480	−2.970665	−2.758914
H	−4.606928	−1.335126	−1.388269
C	−2.189024	−4.188284	−2.486043
H	−0.917425	−3.464722	−0.888625
C	−3.417693	−3.993537	−3.136008
H	−3.691414	−4.658646	−3.953692
C	−2.902960	−2.128152	1.863476

C	−4.060755	−2.913745	1.787627
C	−2.222879	−2.039884	3.086342
C	−4.565581	−3.585749	2.914039
H	−4.572911	−3.011121	0.833881
C	−2.688396	−2.701322	4.233722
H	−1.297035	−1.474191	3.125989
C	−3.864260	−3.462179	4.125131
H	−4.238858	−3.984127	5.004597
C	1.555780	2.466519	−0.285928
C	1.792563	3.294376	−1.388973
C	2.392406	2.588235	0.838604
C	2.862611	4.209576	−1.404526
H	1.131686	3.239950	−2.248547
C	3.453621	3.503155	0.873847
H	2.193421	1.967012	1.708358
C	3.677465	4.295956	−0.267120
H	4.504012	5.004638	−0.266017
C	−0.937769	2.494615	0.926868
C	−1.274528	3.765135	0.433102
C	−1.274826	2.166828	2.242518
C	−1.947585	4.702265	1.227611
H	−1.001603	4.027616	−0.585735
C	−1.943762	3.081499	3.077722
H	−1.005845	1.182735	2.617046
C	−2.263198	4.341145	2.551706
H	−2.765248	5.065825	3.190961
Si	3.190291	5.285091	−2.916078
H	1.932716	5.939049	−3.370742
H	4.189145	6.327377	−2.561833
H	3.718409	4.480393	−4.051704
Si	4.524995	3.694304	2.415015
H	5.967030	3.620580	2.065784
H	4.274827	5.015424	3.055835
H	4.176100	2.622269	3.381783
Si	−2.411478	6.388188	0.534302
H	−3.861131	6.464992	0.197599
H	−2.124702	7.460415	1.524486
H	−1.635335	6.635699	−0.709636
Si	−2.412988	2.619666	4.843119
H	−2.642657	3.865328	5.623041
H	−3.660780	1.808422	4.879526
H	−1.325898	1.826333	5.473826
Si	−6.141717	−4.607810	2.803414
H	−6.150188	−5.632687	3.881243
H	−7.358050	−3.761074	2.964219
H	−6.227338	−5.275673	1.476956
Si	−1.723972	−2.619478	5.849524
H	−2.673668	−2.546493	6.994920
H	−0.865145	−3.817986	6.043851
H	−0.863807	−1.406895	5.851326
Si	−1.028045	−5.579164	−3.008508
H	−1.592640	−6.221934	−4.227329
H	0.325365	−5.050499	−3.326435
H	−0.891990	−6.608006	−1.944161
Si	−5.939838	−2.718033	−3.650479
H	−5.761512	−2.005736	−4.949898
H	−6.582769	−4.025028	−3.953390
H	−6.849820	−1.899638	−2.805915

TS1

C	−3.021244	0.590487	0.090882
C	−2.572311	−0.532942	0.854434
C	−3.312415	−0.943994	1.969924
C	−4.492845	−0.305539	2.390960
C	−4.916384	0.763028	1.634942
C	−4.195347	1.188494	0.521873
C	−2.392473	1.092240	−1.163497
C	−1.077393	1.636391	−1.284461
C	−0.610004	2.052175	−2.539784
C	−1.386806	1.976202	−3.708230
C	−2.660712	1.470727	−3.567809
C	−3.142918	1.052094	−2.331380
H	−3.002883	−1.816990	2.526332
H	−5.045998	−0.651282	3.257068
H	0.391128	2.456790	−2.623826
H	−1.003138	2.301098	−4.668874
P	−1.061867	−1.483577	0.279899
P	0.105715	1.671459	0.144182
O	−3.608154	1.263846	−4.535150
O	−4.417960	0.562772	−2.481882
O	−4.817338	2.291567	−0.019757
O	−6.014488	1.563184	1.811735

C	−4.776551	0.801820	−3.847100
H	−5.555517	1.574360	−3.890936
H	−5.121189	−0.131859	−4.300383
C	−6.101156	2.338211	0.611325
H	−6.851940	1.892843	−0.057376
H	−6.344644	3.370811	0.862154
C	−1.188894	−3.079186	1.232939
C	−1.036198	−3.062612	2.632602
C	−1.328239	−4.320680	0.600935
C	−1.076346	−4.235276	3.399307
H	−0.867140	−2.111222	3.130381
C	−1.350421	−5.526098	1.329159
H	−1.414316	−4.356802	−0.480135
C	−1.233647	−5.459851	2.724359
H	−1.250038	−6.383859	3.299571
C	−1.722211	−1.997374	−1.391768
C	−3.019039	−2.531918	−1.498518
C	−0.978122	−1.822221	−2.558920
C	−3.561414	−2.907223	−2.734680
H	−3.618094	−2.645343	−0.599043
C	−1.478354	−2.188971	−3.823768
H	0.001976	−1.368351	−2.481859
C	−2.768752	−2.732312	−3.885588
H	−3.172932	−3.016341	−4.856299
C	1.271191	3.034638	−0.377262
C	2.632024	2.808599	−0.617746
C	0.767197	4.338366	−0.522457
C	3.494911	3.867412	−0.966064
H	3.026546	1.807701	−0.498845
C	1.587836	5.413773	−0.888321
H	−0.284300	4.527619	−0.337639
C	2.954550	5.155057	−1.088025
H	3.617692	5.984118	−1.333070
C	−0.810438	2.515495	1.524416
C	−1.856864	3.424972	1.304089
C	−0.375326	2.292163	2.837356
C	−2.456001	4.124311	2.363414
H	−2.218677	3.586940	0.292447
C	−0.953389	2.969988	3.926222
H	0.442153	1.595543	3.000564
C	−1.985686	3.883205	3.666739
H	−2.434180	4.422185	4.499965
Si	−3.836474	5.359922	2.049756
H	−5.176207	4.810742	2.406327
H	−3.633785	6.584687	2.870224
H	−3.861214	5.731561	0.609974
Si	−0.335830	2.675740	5.681347
H	−1.259996	3.358928	6.628265
H	−0.311612	1.221846	5.997392
H	1.034521	3.217231	5.882274
Si	0.877049	7.141569	−1.096509
H	0.731953	7.508693	−2.533894
H	−0.470277	7.198912	−0.467697
H	1.761381	8.156206	−0.461463
Si	5.347752	3.627553	−1.216794
H	6.038753	4.866527	−0.760867
H	5.846210	2.466732	−0.442765
H	5.692319	3.437752	−2.653205
Si	−1.533573	−7.182841	0.451048
H	−0.426040	−7.401625	−0.518140
H	−1.514673	−8.267454	1.467959
H	−2.816348	−7.248477	−0.302008
Si	−0.916327	−4.169842	5.276278
H	−0.125807	−5.333578	5.758201
H	−0.248527	−2.902826	5.670687
H	−2.253579	−4.221453	5.931059
Si	−0.453808	−1.965518	−5.389512
H	−1.337500	−2.184766	−6.565769
H	0.118597	−0.594803	−5.454330
H	0.669461	−2.939065	−5.448510
Si	−5.315225	−3.580079	−2.845589
H	−6.155847	−2.711687	−3.718013
H	−5.338558	−4.950885	−3.424676
H	−5.909615	−3.612207	−1.484029
C	4.036821	−3.176404	0.970210
C	1.948048	−2.317635	1.777620
C	3.381794	−2.621005	2.251381
H	3.822269	−4.248114	0.856180
H	5.113974	−3.038118	0.893719
H	1.391119	−3.245889	1.625639
H	1.386363	−1.712340	2.502276
H	3.390734	−3.307611	3.110860

H	3.868987	−1.693177	2.560657
Si	2.823914	−2.218247	−0.152569
Rh	0.957873	−0.404262	0.759464
C	1.975155	−3.497637	−1.275492
H	1.276022	−3.087460	−2.005863
H	1.443408	−4.249001	−0.680701
H	2.767334	−4.016830	−1.831723
C	3.621125	−0.955145	−1.362915
C	2.768784	−0.457556	−2.370791
C	5.008542	−0.678670	−1.499869
C	3.228913	0.232478	−3.489460
H	1.701467	−0.612831	−2.264995
C	5.466879	−0.001845	−2.647752
C	4.598826	0.445615	−3.639503
H	2.525554	0.589820	−4.237383
H	6.531513	0.195824	−2.737828
H	4.988359	0.969582	−4.508275
C	6.056362	−1.025699	−0.493223
C	7.151510	−1.824803	−0.860611
C	6.018467	−0.489931	0.803708
C	8.170767	−2.102968	0.050982
H	7.192013	−2.243075	−1.863317
C	7.043639	−0.762088	1.711446
H	5.182986	0.136664	1.101573
C	8.120104	−1.571076	1.341570
H	9.003572	−2.734929	−0.247217
H	6.998561	−0.336713	2.710648
H	8.914936	−1.783837	2.051785
Cl	2.720957	0.790612	1.962875

TS2

C	3.631879	−1.134155	−2.016843
C	1.328993	−1.930509	−2.671103
C	2.378722	−0.988786	−2.873404
H	4.013683	−2.157352	−2.068766
H	4.433103	−0.465761	−2.349409
H	1.548947	−2.822956	−2.094470
H	0.578155	−2.036025	−3.446016
H	2.437371	−0.509380	−3.851993
H	1.872844	0.387593	−2.372122
Si	2.926077	−0.544178	−0.325804
C	3.813572	1.115667	−0.009563
H	3.515518	1.609827	0.919379
H	4.894222	0.939765	0.034805
H	3.620407	1.810870	−0.833513
C	3.308573	−1.696633	1.158965
C	2.324447	−1.845201	2.155372
C	4.540359	−2.375694	1.357620
C	2.522879	−2.615358	3.302270
H	1.365022	−1.353518	2.023548
C	4.725797	−3.164213	2.505401
C	3.732755	−3.284322	3.476894
H	1.734958	−2.696048	4.046574
H	5.674158	−3.678996	2.636730
H	3.905782	−3.895163	4.358995
C	−2.218825	0.685292	1.370815
C	−1.614634	−0.615048	1.371658
C	−1.390380	−1.275555	2.588815
C	−1.748167	−0.737527	3.836467
C	−2.359844	0.495445	3.816404
C	−2.586044	1.171925	2.619897
C	−2.544356	1.549720	0.191337
C	−1.603190	2.223668	−0.649257
C	−2.046856	3.109599	−1.635293
C	−3.405062	3.398577	−1.843014
C	−4.301159	2.757766	−1.017859
C	−3.876607	1.865307	−0.036696
H	−0.937409	−2.259072	2.579948
H	−1.563645	−1.271231	4.762044
H	−1.322737	3.606650	−2.267175
H	−3.728188	4.091323	−2.611750
P	−1.060191	−1.439704	−0.198499
P	0.206625	1.895044	−0.433411
Rh	0.727045	−0.263344	−1.377015
Cl	−0.791635	0.377489	−3.406594
C	5.697805	−2.297229	0.406168
C	5.976132	−3.358244	−0.469768
C	6.578961	−1.205669	0.432954
C	7.085137	−3.315035	−1.316669
H	5.313572	−4.219550	−0.487135
C	7.689405	−1.161036	−0.412940
H	6.401728	−0.396694	1.135868

C	7.943362	−2.213674	−1.293809
H	7.279743	−4.144100	−1.992098
H	8.360540	−0.306887	−0.375632
H	8.807568	−2.179912	−1.951726
C	−0.830709	−3.222259	0.321922
C	−1.932453	−3.982431	0.755243
C	0.412980	−3.853900	0.227723
C	−1.815045	−5.340555	1.079548
H	−2.904157	−3.505607	0.833146
C	0.575766	−5.220045	0.531426
H	1.269538	−3.269233	−0.083299
C	−0.550023	−5.941769	0.949815
H	−0.443169	−7.001759	1.178034
C	−2.638126	−1.680870	−1.151436
C	−3.904840	−1.560385	−0.566423
C	−2.544941	−2.147764	−2.469672
C	−5.071883	−1.913155	−1.268235
H	−3.991714	−1.202476	0.454403
C	−3.685596	−2.497594	−3.208299
H	−1.567452	−2.234682	−2.926914
C	−4.937865	−2.383924	−2.584227
H	−5.830803	−2.678737	−3.134131
C	0.404196	2.463716	1.331405
C	−0.229622	3.653788	1.734620
C	1.164408	1.763633	2.271137
C	−0.096348	4.157326	3.035193
H	−0.837536	4.194216	1.014504
C	1.322517	2.229205	3.591965
H	1.636116	0.834254	1.974752
C	0.692373	3.430623	3.946262
H	0.818048	3.810211	4.959187
C	1.080022	3.254016	−1.368065
C	1.761279	4.297851	−0.727452
C	1.128190	3.185628	−2.772319
C	2.467427	5.274974	−1.452939
H	1.758546	4.351013	0.355652
C	1.810019	4.150058	−3.531388
H	0.617489	2.363092	−3.269421
C	2.474142	5.186732	−2.852963
H	3.014400	5.935830	−3.428419
O	−5.669399	2.859347	−0.994269
O	−4.978571	1.373872	0.631515
O	−3.177070	2.383099	2.894548
O	−2.802286	1.247058	4.871559
C	−6.068754	2.201756	0.209553
H	−6.275453	2.952369	0.986909
H	−6.941676	1.578360	0.012551
C	−3.512314	2.343647	4.284727
H	−4.593428	2.179758	4.395854
H	−3.200823	3.275762	4.760327
Si	−0.967957	5.746721	3.538085
H	−2.067074	5.475824	4.508879
H	−0.021851	6.688730	4.195255
H	−1.552907	6.388513	2.332549
Si	2.337485	1.290333	4.873204
H	1.639552	0.059899	5.333499
H	3.665113	0.903770	4.330174
H	2.529131	2.185088	6.047133
Si	3.380799	6.660321	−0.566817
H	4.064942	7.512192	−1.576202
H	2.444870	7.510888	0.220504
H	4.396977	6.120981	0.378575
Si	1.844004	4.045781	−5.413301
H	2.700975	5.150165	−5.926736
H	2.411476	2.748754	−5.869909
H	0.482601	4.190273	−5.994026
Si	−3.531474	−3.070841	−4.994100
H	−2.207886	−3.716342	−5.203391
H	−4.606331	−4.060173	−5.288689
H	−3.670138	−1.946410	−5.957364
Si	−6.762622	−1.792982	−0.460923
H	−7.485172	−0.539414	−0.821817
H	−7.618502	−2.929029	−0.900326
H	−6.627522	−1.829580	1.020281
Si	−3.318052	−6.332372	1.630324
H	−3.824619	−7.213344	0.542419
H	−2.967961	−7.197621	2.790033
H	−4.402291	−5.395029	2.026512
Si	2.242331	−6.081723	0.372088
H	3.084051	−5.372608	−0.627356
H	2.979281	−6.132004	1.662683
H	2.023880	−7.482307	−0.082517

TS3

C	−1.630423	3.940788	−1.822566
C	−0.517116	5.762860	−0.476714
C	−0.465250	4.634142	−1.194799
H	−2.524583	4.579917	−1.773238
H	−1.403713	3.756280	−2.879928
H	−1.457783	6.271482	−0.273865
H	0.383120	6.229335	−0.085590
H	0.508010	4.180004	−1.385082
H	−0.173606	0.705517	−2.366501
Si	−2.258217	2.203743	−1.193796
C	−3.450372	1.740604	−2.594356
H	−3.985075	0.801779	−2.449134
H	−4.199790	2.531039	−2.722697
H	−2.870516	1.674783	−3.522963
C	−3.146761	2.639169	0.457366
C	−2.297664	3.245750	1.410794
C	−4.532202	2.603181	0.766113
C	−2.767177	3.807128	2.597862
H	−1.235669	3.325854	1.193487
C	−4.999339	3.182933	1.959785
C	−4.134007	3.781791	2.872116
H	−2.072306	4.274188	3.290674
H	−6.064827	3.147265	2.172227
H	−4.524705	4.221855	3.785999
C	1.836450	−1.621710	1.515381
C	2.259588	−0.256304	1.555536
C	2.672709	0.315999	2.764315
C	2.699174	−0.400445	3.974278
C	2.310599	−1.719919	3.915520
C	1.901244	−2.307171	2.718789
C	1.522448	−2.382092	0.265094
C	0.374934	−2.254297	−0.586539
C	0.268954	−3.074501	−1.718859
C	1.229120	−4.037709	−2.071772
C	2.311983	−4.160036	−1.232311
C	2.441548	−3.355073	−0.103404
H	3.010379	1.344814	2.778504
H	3.028561	0.057566	4.900347
H	−0.596829	−2.987524	−2.360244
H	1.115055	−4.654335	−2.956160
P	2.213425	0.704599	−0.026989
P	−0.972538	−0.993532	−0.264215
Rh	−0.190047	1.036282	−0.827056
Cl	0.635415	1.868601	−3.469139
C	−5.576568	1.990416	−0.111817
C	−6.567192	2.798753	−0.692679
C	−5.648186	0.603808	−0.307385
C	−7.587077	2.240168	−1.464329
H	−6.527066	3.874584	−0.542783
C	−6.671189	0.042578	−1.073622
H	−4.901916	−0.037984	0.152547
C	−7.642298	0.858575	−1.657211
H	−8.338297	2.884666	−1.913658
H	−6.709910	−1.033961	−1.214028
H	−8.437640	0.420814	−2.254676
C	−2.374480	−1.673428	−1.285088
C	−2.401511	−1.388031	−2.658244
C	−3.363089	−2.520254	−0.759671
C	−3.359135	−1.957262	−3.515615
H	−1.654288	−0.710433	−3.062991
C	−4.344537	−3.102939	−1.578659
H	−3.370869	−2.738740	0.302176
C	−4.315427	−2.817543	−2.954410
H	−5.057138	−3.275183	−3.607552
C	−1.466079	−1.406783	1.472744
C	−1.490103	−2.748025	1.895202
C	−1.830790	−0.402783	2.376869
C	−1.891355	−3.102091	3.189616
H	−1.184072	−3.525197	1.200735
C	−2.214851	−0.715425	3.696343
H	−1.812008	0.632653	2.047973
C	−2.242875	−2.066348	4.073957
H	−2.541009	−2.318448	5.090587
C	3.598415	−0.036155	−1.001412
C	4.745820	−0.553081	−0.378349
C	3.510113	−0.051999	−2.398864
C	5.803595	−1.085141	−1.130061
H	4.810402	−0.541334	0.706354
C	4.554826	−0.571116	−3.187461
H	2.622447	0.360435	−2.872280
C	5.686517	−1.080581	−2.533334

H	6.501509	−1.484122	−3.132549
C	2.869550	2.372590	0.436413
C	4.056633	2.886383	−0.099979
C	2.117528	3.187107	1.303850
C	4.512473	4.177795	0.222683
H	4.637233	2.270099	−0.779429
C	2.556501	4.463902	1.681949
H	1.182674	2.805876	1.710069
C	3.757348	4.940628	1.124734
H	4.111073	5.933426	1.398529
O	3.385219	−5.000929	−1.336190
O	3.617808	−3.664174	0.538501
O	1.581882	−3.625570	2.950128
O	2.256301	−2.642225	4.928083
C	4.145181	−4.811406	−0.137069
H	4.037856	−5.695554	0.505943
H	5.192007	−4.632790	−0.393551
C	2.045722	−3.898603	4.277756
H	2.996770	−4.447745	4.224258
H	1.286699	−4.465999	4.818059
Si	−1.949878	−4.907023	3.715390
H	−0.965698	−5.194094	4.797210
H	−3.295489	−5.263785	4.241157
H	−1.635659	−5.768091	2.545749
Si	−2.677981	0.600415	4.967273
H	−4.030131	1.162562	4.721700
H	−2.676979	−0.057076	6.303415
H	−1.688016	1.708083	4.975042
Si	−5.635394	−4.266183	−0.851188
H	−7.013228	−3.739190	−1.050899
H	−5.565746	−5.605027	−1.497976
H	−5.382772	−4.416582	0.606397
Si	−3.374120	−1.569480	−5.362570
H	−4.225439	−2.583661	−6.042156
H	−3.932497	−0.219499	−5.634626
H	−1.995500	−1.633306	−5.914212
Si	4.438574	−0.576638	−5.069955
H	5.618317	−1.314604	−5.601083
H	3.198564	−1.257774	−5.526046
H	4.452372	0.803199	−5.622518
Si	7.319002	−1.798075	−0.276755
H	7.296547	−3.290219	−0.272453
H	8.566140	−1.378068	−0.970850
H	7.355328	−1.337167	1.136418
Si	6.096242	4.862484	−0.534528
H	6.485234	6.094720	0.202357
H	7.195528	3.864043	−0.432762
H	5.914621	5.200810	−1.971706
Si	1.596089	5.495244	2.931184
H	2.376446	5.637400	4.192958
H	1.327326	6.861744	2.412167
H	0.315675	4.813337	3.248214

TS4

C	−0.722732	4.737299	−1.337505
C	−1.438661	6.991190	−0.434034
C	−0.498447	6.141076	−0.861533
H	−1.788072	4.555845	−1.526070
H	−0.201682	4.576645	−2.291784
H	−2.494341	6.726323	−0.428753
H	−1.187932	7.988848	−0.082835
H	0.541803	6.469495	−0.846460
Si	−0.033055	3.413190	−0.098597
C	−0.944525	3.702224	1.551498
H	−0.443564	3.207416	2.390545
H	−0.997438	4.775472	1.772656
H	−1.971454	3.322988	1.512922
C	1.807918	3.834152	0.138770
C	2.183440	4.521504	1.307466
C	2.826765	3.475302	−0.785192
C	3.512662	4.830254	1.603552
H	1.415987	4.832167	2.011230
C	4.166310	3.753040	−0.448324
C	4.512144	4.419679	0.725175
H	3.760289	5.367257	2.515625
H	4.960810	3.420153	−1.108579
H	5.558607	4.611709	0.948180
C	−1.012123	−2.365514	−0.912193
C	−1.674182	−1.193763	−1.396373
C	−1.960887	−1.074592	−2.767577
C	−1.684044	−2.087947	−3.698899
C	−1.099931	−3.234170	−3.202509

C	−0.776824	−3.358592	−1.853861
C	−0.597025	−2.625000	0.499819
C	0.487838	−1.982712	1.175650
C	0.804936	−2.356644	2.488326
C	0.111446	−3.360201	3.187599
C	−0.910059	−3.987811	2.509406
C	−1.244489	−3.626382	1.205961
H	−2.428021	−0.166069	−3.130143
H	−1.921984	−1.976821	−4.750978
H	1.630076	−1.869739	2.993022
H	0.376084	−3.632973	4.203301
P	−1.976630	0.297134	−0.329004
P	1.461640	−0.656300	0.301209
Rh	0.111700	1.199546	−0.822477
C	2.558244	2.825903	−2.108384
C	3.449642	3.090998	−3.170004
C	1.481655	1.927773	−2.349259
C	3.341469	2.466589	−4.409986
H	4.241495	3.819443	−3.026072
C	1.391002	1.307791	−3.614797
H	0.153580	2.272323	−2.050236
C	2.312876	1.548332	−4.630009
H	4.046200	2.708617	−5.200965
H	0.557595	0.634787	−3.802429
H	2.213334	1.046801	−5.589323
C	−3.572657	0.989112	−1.013326
C	−4.593740	0.184578	−1.549659
C	−3.806831	2.363720	−0.899939
C	−5.818840	0.724026	−1.968339
H	−4.427146	−0.883102	−1.653946
C	−5.028423	2.946634	−1.286921
H	−3.018863	2.990580	−0.496179
C	−6.019526	2.107614	−1.816260
H	−6.972935	2.540752	−2.114195
C	−2.659547	−0.343387	1.285187
C	−3.718277	−1.263204	1.361566
C	−2.146035	0.184228	2.472892
C	−4.264884	−1.654121	2.591245
H	−4.120866	−1.688896	0.447659
C	−2.667707	−0.174887	3.730901
H	−1.321456	0.889057	2.407875
C	−3.726388	−1.092513	3.764884
H	−4.142733	−1.380366	4.729019
C	2.632868	−0.097173	1.629714
C	2.214761	0.902727	2.522861
C	3.907758	−0.653724	1.796868
C	3.025296	1.324602	3.587391
H	1.237485	1.353984	2.377215
C	4.766178	−0.234279	2.829106
H	4.237375	−1.431742	1.115244
C	4.299539	0.744609	3.718368
H	4.946254	1.064863	4.534301
C	2.595413	−1.663662	−0.776905
C	2.689279	−3.059200	−0.677863
C	3.432985	−0.993285	−1.684298
C	3.600899	−3.792622	−1.455995
H	2.052240	−3.582310	0.027384
C	4.371546	−1.689404	−2.466068
H	3.359600	0.087094	−1.765622
C	4.440569	−3.086554	−2.331987
H	5.176756	−3.635943	−2.917063
O	−0.723693	−4.362337	−3.880598
O	−0.173453	−4.577667	−1.643530
O	−2.319575	−4.379907	0.790240
O	−1.749809	−4.980551	2.945024
C	−0.309009	−5.294885	−2.876106
H	−1.075694	−6.074005	−2.762493
H	0.655506	−5.725215	−3.153545
C	−2.452964	−5.410458	1.774783
H	−1.999459	−6.338083	1.396069
H	−3.507679	−5.548931	2.015954
Si	−5.345372	4.795307	−1.110343
H	−4.984364	5.265974	0.253822
H	−4.555373	5.584241	−2.093403
H	−6.791527	5.049727	−1.349148
Si	−7.146974	−0.375520	−2.723357
H	−8.494813	0.053100	−2.261475
H	−7.132891	−0.312980	−4.211593
H	−6.908757	−1.786484	−2.316312
Si	−5.675934	−2.894063	2.658743
H	−5.228025	−4.219522	3.173488
H	−6.761681	−2.416426	3.557304

H	−6.220030	−3.091290	1.288904
Si	−1.974311	0.550457	5.322904
H	−2.326521	1.988695	5.474302
H	−2.539748	−0.200450	6.476098
H	−0.491472	0.438470	5.350202
Si	6.494125	−0.959592	3.003354
H	7.456273	−0.330935	2.056467
H	6.985369	−0.728906	4.388848
H	6.471898	−2.421807	2.726677
Si	2.435497	2.609884	4.829558
H	2.278379	1.998927	6.179348
H	3.415137	3.722372	4.957278
H	1.121503	3.155218	4.404359
Si	3.696497	−5.663725	−1.314121
H	2.856433	−6.345295	−2.342034
H	5.097282	−6.123589	−1.515869
H	3.216531	−6.101087	0.023606
Si	5.534981	−0.809216	−3.659330
H	4.926751	−0.620208	−5.003600
H	5.934292	0.516954	−3.123595
H	6.749748	−1.655254	−3.827567

TS5

C	−3.729838	0.200457	−2.440502
C	−1.443306	1.175347	−2.825763
C	−2.713517	0.650205	−3.494343
H	−3.954876	1.049287	−1.781741
H	−4.677335	−0.126295	−2.890611
H	−1.648428	2.171972	−2.421921
H	−0.635349	1.282234	−3.567889
H	−3.157508	1.442312	−4.120587
H	−2.481488	−0.180409	−4.169023
Si	−3.026883	−1.224756	−1.385631
C	−3.845436	−2.857525	−1.931948
H	−4.892946	−2.885545	−1.616637
H	−3.805646	−2.961584	−3.020849
H	−3.337940	−3.724583	−1.494449
C	−3.389646	−1.233833	0.517986
C	−2.306118	−1.210333	1.413998
C	−4.685262	−1.454558	1.076003
C	−2.449964	−1.404144	2.789843
H	−1.313867	−1.045170	1.008822
C	−4.817811	−1.638760	2.463966
C	−3.718129	−1.621454	3.319916
H	−1.574785	−1.383428	3.432644
H	−5.813914	−1.783951	2.873899
H	−3.857726	−1.770022	4.387745
C	1.512004	0.838467	2.052306
C	0.257070	1.446910	1.715813
C	−0.646013	1.760479	2.739583
C	−0.401895	1.499998	4.099038
C	0.796723	0.896836	4.401419
C	1.714808	0.583387	3.402215
C	2.688997	0.619580	1.152699
C	2.828233	−0.358456	0.120202
C	4.046790	−0.471391	−0.566206
C	5.163438	0.335446	−0.292117
C	5.016050	1.262485	0.714724
C	3.816869	1.388459	1.411031
H	−1.577937	2.249308	2.495583
H	−1.120723	1.767562	4.865344
H	4.150773	−1.221049	−1.339079
H	6.093838	0.223789	−0.837752
P	−0.206344	1.760230	−0.067863
P	1.389049	−1.429804	−0.369322
Rh	−0.507808	−0.075879	−1.397120
Cl	−1.096041	−2.039590	−2.708153
C	−5.959289	−1.508768	0.294957
C	−6.801268	−2.629542	0.412533
C	−6.391033	−0.442358	−0.507555
C	−8.018636	−2.689546	−0.264970
H	−6.482379	−3.466940	1.027239
C	−7.610964	−0.498672	−1.184886
H	−5.776177	0.446396	−0.590540
C	−8.428365	−1.623467	−1.069383
H	−8.645805	−3.571923	−0.167372
H	−7.924354	0.343861	−1.795768
H	−9.376826	−1.668511	−1.597748
O	5.927399	2.172262	1.184357
O	3.943789	2.394549	2.344091
O	2.826070	0.007348	3.979887
O	1.292484	0.533219	5.625810

C	5.340777	2.704325	2.375676
H	5.800933	2.227767	3.253654
H	5.472593	3.787138	2.393929
C	2.662009	0.190560	5.390261
H	2.898415	−0.741248	5.906767
H	3.307551	1.013572	5.728751
C	1.259187	−2.664441	1.009103
C	2.190700	−2.778281	2.048041
C	0.170589	−3.552063	0.975629
C	2.052284	−3.756392	3.050084
H	3.038658	−2.101080	2.077195
C	0.004264	−4.550301	1.947270
H	−0.552140	−3.463473	0.168345
C	0.957792	−4.632335	2.977114
H	0.845323	−5.400363	3.741696
C	2.146967	−2.474237	−1.709193
C	2.713421	−3.730652	−1.469007
C	2.171423	−1.967983	−3.019794
C	3.296889	−4.487297	−2.503269
H	2.706761	−4.128771	−0.458600
C	2.749050	−2.683349	−4.077823
H	1.721028	−0.998014	−3.211540
C	3.308428	−3.943077	−3.795621
H	3.765782	−4.513113	−4.602821
C	1.181177	2.871165	−0.610060
C	1.668358	3.891605	0.223801
C	1.741626	2.714135	−1.881200
C	2.692751	4.752363	−0.193648
H	1.237770	4.011567	1.214499
C	2.774365	3.554178	−2.340214
H	1.363949	1.916327	−2.515866
C	3.230654	4.564512	−1.481477
H	4.028341	5.222534	−1.823008
C	−1.623903	2.973481	0.047979
C	−1.511264	4.285274	−0.429302
C	−2.867407	2.560782	0.565351
C	−2.584461	5.194580	−0.370999
H	−0.570693	4.615122	−0.856209
C	−3.948011	3.449174	0.684318
H	−2.987747	1.532994	0.896815
C	−3.783112	4.763720	0.210332
H	−4.609656	5.467361	0.298797
Si	3.301792	−3.886339	4.448470
H	2.860318	−3.143246	5.664446
H	3.482099	−5.309347	4.844179
H	4.608878	−3.321337	4.020270
Si	−1.453861	−5.740975	1.868817
H	−1.002258	−7.116017	1.515246
H	−2.132370	−5.819233	3.191296
H	−2.416695	−5.274136	0.839747
Si	4.038817	−6.182017	−2.159661
H	4.756469	−6.651520	−3.375388
H	5.000061	−6.119837	−1.023849
H	2.991594	−7.180587	−1.809264
Si	2.732729	−1.993597	−5.829329
H	4.045352	−2.241595	−6.488169
H	1.679452	−2.632427	−6.664349
H	2.480115	−0.529338	−5.779912
Si	3.517208	3.338491	−4.057668
H	2.531118	3.673017	−5.120868
H	4.686447	4.249548	−4.186156
H	3.964725	1.936239	−4.270981
Si	3.325197	6.108040	0.945540
H	4.728094	5.849375	1.379250
H	3.314106	7.430147	0.262463
H	2.464893	6.171737	2.155909
Si	−2.407028	6.943012	−1.046644
H	−3.550773	7.764639	−0.567384
H	−1.133431	7.557286	−0.581168
H	−2.402245	6.959240	−2.535233
Si	−5.572068	2.946925	1.500393
H	−5.960280	3.983234	2.497236
H	−6.675168	2.848270	0.506374
H	−5.407292	1.641269	2.184720

TS6

C	3.607399	1.051407	0.468932
C	1.461742	2.192569	1.301683
C	2.422902	1.158593	1.416720
H	3.923297	0.012098	0.356510
H	3.320134	1.399631	−0.532573
H	1.547998	2.907976	0.487590

H	0.987115	2.575189	2.203570	C	5.222063	−2.730957	−1.095238
H	2.628140	0.793671	2.421511	H	5.822714	−1.113384	−2.385377
H	1.741928	−0.348571	1.069788	C	5.795625	−2.485420	1.236949
Si	5.109533	2.091063	0.995522	H	6.856555	−0.688765	1.764887
C	4.665052	3.920837	1.039055	C	5.204216	−3.225792	0.211437
H	4.463194	4.302475	0.030607	H	4.769164	−3.301373	−1.901937
H	3.758170	4.056450	1.637312	H	5.798311	−2.867689	2.254223
H	5.455347	4.531721	1.487504	H	4.735434	−4.181887	0.427522
C	6.626157	1.812395	−0.106474	O	−4.709924	−1.120596	−4.370802
C	7.345841	2.968247	−0.472194	O	−4.653596	−2.101799	−2.283441
C	7.046517	0.572321	−0.659068	O	−5.778278	−0.581607	0.202828
C	8.428221	2.927289	−1.350778	O	−6.256718	−1.700362	2.168088
H	7.051611	3.932276	−0.068078	C	−5.372067	−2.060742	−3.519867
C	8.125839	0.547466	−1.556979	H	−6.401729	−1.722032	−3.332403
C	8.815466	1.708231	−1.902549	H	−5.352268	−3.047539	−3.983906
H	8.958021	3.841676	−1.604002	C	−6.841229	−1.101964	1.007619
H	8.436298	−0.408079	−1.971003	H	−7.389502	−1.866703	0.438514
H	9.653137	1.656120	−2.593172	H	−7.499374	−0.285166	1.310928
C	−3.217942	−0.407328	−1.183174	C	0.245446	−3.020062	1.345543
C	−2.519290	0.815266	−1.438202	C	0.218797	−4.370361	0.976253
C	−2.563899	1.384341	−2.718073	C	0.890552	−2.669059	2.541719
C	−3.273134	0.814652	−3.789983	C	0.823042	−5.365490	1.766743
C	−3.949751	−0.353818	−3.524027	H	−0.276861	−4.658444	0.054007
C	−3.916860	−0.936098	−2.259061	C	1.496364	−3.629025	3.367696
C	−3.357393	−1.101415	0.135417	H	0.915137	−1.618247	2.819436
C	−2.330891	−1.792756	0.854339	C	1.448254	−4.973965	2.960713
C	−2.649235	−2.460714	2.044876	H	1.905762	−5.736149	3.590300
C	−3.947251	−2.497025	2.583071	C	−0.509115	−2.401557	−1.361581
C	−4.923794	−1.835712	1.873353	C	−1.435350	−3.348387	−1.822729
C	−4.628987	−1.166130	0.688373	C	0.534921	−2.010051	−2.210012
H	−2.043772	2.315489	−2.902246	C	−1.327569	−3.915462	−3.103855
H	−3.293346	1.278726	−4.769874	H	−2.259037	−3.640234	−1.175797
H	−1.867766	−2.980617	2.584878	C	0.686797	−2.561768	−3.493862
H	−4.166612	−3.022715	3.505820	H	1.228639	−1.252936	−1.848691
P	−1.499287	1.607677	−0.095753	C	−0.255503	−3.512204	−3.919235
P	−0.547376	−1.661760	0.339426	H	−0.155519	−3.945439	−4.913516
Rh	0.363570	0.419381	0.653699	C	−2.788649	2.084093	1.148007
Cl	5.579332	1.599775	3.003748	C	−2.428776	2.095871	2.500616
C	6.397694	−0.735602	−0.341962	C	−4.099592	2.438567	0.792482
C	5.818862	−1.499780	−1.369381	C	−3.341372	2.473585	3.502633
C	6.390569	−1.252206	0.963189	H	−1.417682	1.788123	2.760185

C	−5.044542	2.812115	1.760372
H	−4.385764	2.414123	−0.255867
C	−4.640019	2.830849	3.108367
H	−5.357663	3.127439	3.871876
C	−1.045060	3.241238	−0.864785
C	−1.713222	4.444965	−0.611495
C	0.069493	3.262940	−1.719903
C	−1.295488	5.656942	−1.192923
H	−2.570919	4.443571	0.054700
C	0.503144	4.442708	−2.343844
H	0.605660	2.329398	−1.883807
C	−0.194035	5.631701	−2.062054
H	0.135107	6.559663	−2.526117
Si	2.372134	−3.119430	4.954208
H	1.985688	−4.022333	6.073612
H	3.852499	−3.195107	4.808102
H	1.998527	−1.722372	5.296691
Si	0.805531	−7.168194	1.228091
H	1.880198	−7.462825	0.239088
H	1.018026	−8.040523	2.414700
H	−0.498316	−7.505672	0.594870
Si	−2.840314	2.488509	5.317449
H	−3.998442	2.950666	6.129384
H	−2.439525	1.131568	5.778633
H	−1.692251	3.406874	5.550520
Si	−6.804901	3.241889	1.260777
H	−7.757416	2.146081	1.601646
H	−7.272617	4.466297	1.966017
H	−6.862875	3.463702	−0.208124
Si	−2.179110	7.271669	−0.798509
H	−1.854519	8.276422	−1.846714
H	−3.651645	7.059437	−0.758806
H	−1.761935	7.821141	0.521221
Si	1.970876	4.434762	−3.521934
H	1.603295	3.891314	−4.858945
H	2.461884	5.827467	−3.702084
H	3.069766	3.592563	−2.975902
Si	2.120621	−2.053123	−4.599942
H	1.767931	−2.309708	−6.022748
H	2.427012	−0.608969	−4.418226
H	3.358608	−2.823696	−4.291431
Si	−2.588479	−5.171356	−3.708873
H	−3.606914	−4.557982	−4.608059
H	−1.914886	−6.251153	−4.480717
H	−3.300648	−5.766237	−2.546961

TS7

H	1.982657	−0.373034	−1.590660
Si	2.490680	−2.885773	−0.759325
C	−2.569198	1.531394	0.765340
C	−2.452398	0.173323	1.201117
C	−2.939445	−0.197173	2.460133
C	−3.547972	0.714701	3.342887
C	−3.654755	2.015897	2.905241
C	−3.179947	2.401106	1.652844
C	−2.213162	2.022113	−0.600504
C	−0.902518	2.126257	−1.159578
C	−0.748360	2.508750	−2.502061
C	−1.828732	2.855882	−3.328528
C	−3.082487	2.792626	−2.758644
C	−3.258680	2.387384	−1.439268
H	−2.871754	−1.230976	2.775294
H	−3.923307	0.404260	4.311806
H	0.246633	2.532701	−2.932134
H	−1.683739	3.151359	−4.361687
P	−1.654347	−1.054189	0.052145
P	0.611973	1.535679	−0.262212
Rh	0.588036	−0.646791	−0.848729
Cl	0.525598	−2.785263	−2.039192
O	−4.295945	3.082479	−3.325647
O	−4.599087	2.398951	−1.134460
O	−3.389420	3.750531	1.485619
O	−4.186473	3.101057	3.552903
C	−5.278221	2.682778	−2.362710
H	−5.986552	3.501177	−2.205291
H	−5.788435	1.777306	−2.715225
C	−4.256294	4.129902	2.558812
H	−5.287557	4.207368	2.185369
H	−3.912799	5.072536	2.987388
C	1.939098	2.737614	−0.784050
C	1.648655	4.047941	−1.197714
C	3.282210	2.370053	−0.618341

C	2.661579	4.981915	−1.463965
H	0.612954	4.348915	−1.318414
C	4.327865	3.283948	−0.849875
H	3.508875	1.360152	−0.286536
C	3.993053	4.580870	−1.271408
H	4.791393	5.301506	−1.441657
C	0.419076	2.132345	1.490196
C	0.107705	3.468701	1.783179
C	0.662483	1.249076	2.545499
C	0.021848	3.930598	3.104016
H	−0.079513	4.161998	0.968666
C	0.594135	1.672310	3.886489
H	0.907077	0.217949	2.303224
C	0.269546	3.012932	4.140861
H	0.205155	3.353467	5.173763
C	−2.975088	−1.174844	−1.252688
C	−4.337886	−1.209995	−0.912122
C	−2.617333	−1.207548	−2.605027
C	−5.338171	−1.288668	−1.892075
H	−4.620130	−1.167221	0.136744
C	−3.589004	−1.290262	−3.621171
H	−1.563322	−1.159938	−2.862606
C	−4.938700	−1.331432	−3.242289
H	−5.700578	−1.395397	−4.018203
C	−1.811804	−2.673086	0.944206
C	−2.522846	−3.754279	0.406737
C	−1.102494	−2.872763	2.142154
C	−2.553777	−5.008517	1.041896
H	−3.059646	−3.618948	−0.526791
C	−1.128477	−4.100286	2.823354
H	−0.525634	−2.047427	2.554509
C	−1.860276	−5.157075	2.252062
H	−1.881403	−6.119201	2.759818
Si	−7.155075	−1.308848	−1.405824
H	−7.827804	−0.029824	−1.774265
H	−7.881118	−2.408665	−2.097048
H	−7.266453	−1.490220	0.065357
Si	−3.088361	−1.351369	−5.436265
H	−2.491978	−2.666215	−5.796342
H	−4.303329	−1.140263	−6.270303
H	−2.093389	−0.290446	−5.744734
Si	−0.218268	−4.348814	4.453916
H	−0.926539	−3.683079	5.582392
H	−0.139547	−5.805226	4.741609
H	1.154965	−3.782815	4.381277
Si	−3.491452	−6.453514	0.280202
H	−3.640170	−7.524949	1.301366
H	−4.840794	−6.016915	−0.171674
H	−2.775104	−7.015727	−0.897011
Si	0.924702	0.488002	5.307696
H	2.341943	0.533277	5.763407
H	0.062432	0.838835	6.468520
H	0.627489	−0.904865	4.880805
Si	−0.428147	5.720124	3.462329
H	−1.817100	5.848353	3.988910
H	0.484002	6.302421	4.484034
H	−0.334118	6.510794	2.206968
Si	2.242868	6.714037	−2.066898
H	3.244327	7.687218	−1.553295
H	2.244837	6.797511	−3.554453
H	0.887329	7.098286	−1.588403
Si	6.147211	2.853802	−0.601127
H	6.738710	2.185008	−1.788590
H	6.885508	4.127758	−0.375585
H	6.325581	1.976846	0.583202
C	3.533602	−1.882986	0.494205
C	3.009069	−1.835072	1.803282
C	4.845644	−1.373700	0.296233
C	3.729580	−1.340999	2.887631
H	2.007335	−2.216401	1.980859
C	5.565597	−0.884356	1.404956
C	5.024828	−0.863295	2.686399
H	3.290771	−1.344478	3.881760
H	6.567824	−0.499198	1.240967
H	5.608147	−0.475927	3.517419
C	5.552984	−1.319727	−1.019549
C	5.008043	−0.652404	−2.128142
C	6.834858	−1.883589	−1.147026
C	5.719592	−0.556938	−3.325459
H	4.020284	−0.207957	−2.052097
C	7.542335	−1.795883	−2.346129
H	7.269065	−2.409265	−0.300611

C	6.987454	−1.129494	−3.440918
H	5.279699	−0.030513	−4.168595
H	8.526806	−2.249921	−2.424856
H	7.538677	−1.057223	−4.374677
C	3.508274	−3.498312	−2.224492
H	3.559882	−2.770266	−3.036254
H	4.530086	−3.742981	−1.918726
H	3.029375	−4.404974	−2.610005
C	1.887248	−4.416326	0.227629
H	1.386938	−5.069984	−0.495387
H	1.126439	−4.116110	0.957582
C	3.018981	−5.143496	0.896723
H	3.445060	−4.664798	1.778229
C	3.545082	−6.300000	0.479882
H	3.161486	−6.822661	−0.394418
H	4.375707	−6.768936	1.000818

TS8

C	−2.626856	1.449490	0.326011
C	−2.580128	0.188491	1.001546
C	−3.337975	0.000338	2.163589
C	−4.159754	0.999691	2.716220
C	−4.201085	2.201051	2.046278
C	−3.456362	2.407379	0.887566
C	−1.970693	1.754858	−0.980530
C	−0.566480	1.832423	−1.232654
C	−0.108572	2.059873	−2.539455
C	−0.970667	2.265030	−3.629394
C	−2.321404	2.235089	−3.357781
C	−2.796001	1.988666	−2.073411
H	−3.326396	−0.961758	2.658544
H	−4.740154	0.824665	3.615364
H	0.958303	2.084775	−2.728092
H	−0.591983	2.439552	−4.630423
P	−1.512793	−1.177569	0.298478
P	0.691656	1.435705	0.072146
O	−3.371837	2.380781	−4.226481
O	−4.171143	1.960423	−2.094891
O	−3.663026	3.695551	0.443804
O	−4.903856	3.338025	2.355741
C	−4.550861	2.366028	−3.413880
H	−4.981628	3.376120	−3.376534
H	−5.265904	1.647225	−3.822423
C	−4.781840	4.171035	1.198710
H	−5.693937	4.086810	0.589802
H	−4.599018	5.200193	1.509591
C	−2.046673	−2.670686	1.271756
C	−1.696697	−2.747699	2.632962
C	−2.677350	−3.778283	0.690965
C	−2.006186	−3.867089	3.419034
H	−1.163378	−1.912603	3.081706
C	−2.982473	−4.933577	1.435571
H	−2.933741	−3.746713	−0.363413
C	−2.649104	−4.953150	2.797626
H	−2.883214	−5.837809	3.386912
C	−2.396341	−1.433964	−1.321269
C	−3.798764	−1.481489	−1.399515
C	−1.655272	−1.547810	−2.500023
C	−4.460025	−1.656562	−2.623261
H	−4.380206	−1.369109	−0.487971
C	−2.275260	−1.733090	−3.750900
H	−0.575117	−1.461124	−2.432087
C	−3.676157	−1.787018	−3.786050
H	−4.172278	−1.923850	−4.746017
C	2.159829	2.461639	−0.469813
C	3.461939	1.975212	−0.324035
C	1.987176	3.786650	−0.911948
C	4.587232	2.786429	−0.578544
H	3.587866	0.949635	0.008476
C	3.075481	4.618274	−1.204054
H	0.982434	4.178234	−1.035015
C	4.370035	4.099982	−1.015420
H	5.229488	4.740679	−1.206082
C	0.208049	2.452503	1.558971
C	−0.392090	3.718398	1.475850
C	0.557053	1.957393	2.820726
C	−0.632531	4.492503	2.620823
H	−0.692269	4.104621	0.506172
C	0.336349	2.701681	3.994422
H	1.010602	0.969007	2.869206
C	−0.252531	3.968319	3.870315
H	−0.420439	4.562120	4.767559

Si	−1.432389	6.187306	2.485267
H	−2.854248	6.176239	2.934840
H	−0.714038	7.176293	3.334766
H	−1.401649	6.642727	1.069886
Si	0.816067	2.015799	5.679132
H	0.502040	3.031560	6.720544
H	0.063385	0.768643	5.989693
H	2.267940	1.693981	5.742528
Si	2.807046	6.371324	−1.829100
H	2.962806	6.462230	−3.308439
H	1.429544	6.814436	−1.482722
H	3.793741	7.300044	−1.213619
Si	6.350455	2.181434	−0.302388
H	7.258135	3.351969	−0.459327
H	6.518359	1.625743	1.065992
H	6.754575	1.142296	−1.283864
Si	−3.811193	−6.415984	0.622377
H	−2.911995	−7.067867	−0.368932
H	−4.162813	−7.407813	1.673523
H	−5.050630	−6.004520	−0.092471
Si	−1.576657	−3.915329	5.252160
H	−2.660752	−3.318448	6.081778
H	−1.393606	−5.327885	5.681017
H	−0.328308	−3.148498	5.503778
Si	−1.269632	−1.908401	−5.333066
H	−2.177956	−1.741802	−6.499293
H	−0.199120	−0.877492	−5.393413
H	−0.622879	−3.245721	−5.426351
Si	−6.339048	−1.667555	−2.704228
H	−6.854207	−0.449254	−3.393080
H	−6.836985	−2.848348	−3.461111
H	−6.889808	−1.696030	−1.324098
C	3.230149	−4.307536	0.660666
C	1.398897	−2.931411	1.411666
C	2.680968	−3.622116	1.939122
H	2.832405	−5.325509	0.554573
H	4.317420	−4.361621	0.593306
H	0.566247	−3.639467	1.364256
H	1.072486	−2.101855	2.076763
H	2.480214	−4.303225	2.778053
H	3.387572	−2.865474	2.291838
Si	2.208974	−3.117648	−0.437626
Rh	0.874052	−0.761456	0.535005
H	2.378660	−0.381025	0.941471
C	3.210844	−2.027781	−1.652538
C	2.499222	−1.564628	−2.779279
C	4.613280	−1.802858	−1.640111
C	3.109316	−0.919913	−3.852454
H	1.428131	−1.727353	−2.825487
C	5.224284	−1.171323	−2.740559
C	4.490124	−0.727852	−3.836633
H	2.511489	−0.584652	−4.696286
H	6.298337	−1.009806	−2.713616
H	4.992340	−0.236073	−4.665694
C	5.524714	−2.185031	−0.519976
C	6.634274	−3.011623	−0.766881
C	5.353456	−1.670403	0.774427
C	7.532841	−3.329146	0.251812
H	6.779509	−3.418788	−1.764089
C	6.258626	−1.979213	1.792259
H	4.505603	−1.024050	0.982761
C	7.349010	−2.812257	1.536549
H	8.377197	−3.980816	0.041842
H	6.111039	−1.563461	2.785728
H	8.051179	−3.054828	2.329740
C	1.014594	−4.140644	−1.507750
H	0.508217	−4.883496	−0.880148
H	0.239717	−3.562271	−2.018563
H	1.584879	−4.683021	−2.272677

TS9

Rh	−0.153670	1.019440	−1.140801
P	−1.117864	−1.000436	−0.307968
P	2.060110	0.623917	−0.035607
Si	−2.139388	1.906255	−2.204340
Si	−1.520021	−2.847578	−5.624521
Si	−5.927612	−3.597394	−2.056979
Si	−3.426281	−4.188700	3.808450
Si	−4.280111	1.452925	3.775977
Si	7.206014	2.947506	−0.972970
Si	2.911837	6.187406	0.894453
Si	6.438450	−2.947654	0.768861

Si	3.802040	−2.648443	−4.299144	C	3.138659	−4.779047	2.488133
O	2.790845	−3.392216	2.448254	C	−0.074466	−1.895748	5.355720
O	2.740272	−5.355441	1.239866	C	−3.742699	2.118608	−1.150409
O	0.257846	−2.292943	4.021342	C	−4.790125	1.207986	−1.406063
O	0.598668	−0.660191	5.622245	C	−6.042171	1.297861	−0.798049
C	0.114106	−2.357837	0.092862	C	−6.296309	2.334772	0.097613
C	0.119104	−3.556240	−0.634937	C	−5.284585	3.250416	0.379189
C	0.968295	−4.638323	−0.341763	C	−4.011149	3.152953	−0.213282
C	1.811647	−4.481868	0.733849	C	−3.015430	4.180777	0.217016
C	1.828044	−3.297699	1.466324	C	−3.328073	5.547058	0.109511
C	1.019577	−2.204777	1.188564	C	−2.459650	6.526896	0.590493
C	1.158023	−1.025405	2.097525	C	−1.264407	6.160182	1.212128
C	0.810254	−1.181698	3.430294	C	−0.941291	4.807080	1.329503
C	1.024930	−0.205252	4.402328	C	−1.800822	3.828740	0.827014
C	1.641288	0.986555	4.095211	C	−2.743670	1.073864	−3.821237
C	2.011859	1.175164	2.751155	C	−1.519467	3.610381	−2.837646
C	1.780390	0.218322	1.755485	C	−0.097308	3.393190	−3.371012
C	−2.152199	−1.845175	−1.603953	C	0.747798	2.677587	−2.315620
C	−1.608267	−1.980505	−2.893811	H	−0.577146	−3.685803	−1.451850
C	−2.295742	−2.640834	−3.921441	H	0.944451	−5.552179	−0.925113
C	−3.586004	−3.130620	−3.644401	H	1.839201	1.739068	4.850532
C	−4.180879	−2.977673	−2.384032	H	2.506946	2.102859	2.493661
C	−3.438040	−2.342478	−1.368776	H	−0.630276	−1.547244	−3.090016
C	−2.188213	−1.145646	1.215509	H	−4.143098	−3.633640	−4.433282
C	−2.409152	−2.389515	1.830031	H	−3.875692	−2.232585	−0.381646
C	−3.177380	−2.510223	2.997359	H	−1.961826	−3.278473	1.395119
C	−3.722236	−1.338040	3.550860	H	−4.308411	−1.409562	4.467124
C	−3.531922	−0.076636	2.965455	H	−2.602585	0.955424	1.308913
C	−2.761051	−0.004297	1.789443	H	4.952325	1.030067	−0.715699
C	3.222211	2.083539	0.005243	H	5.545964	5.216125	0.004067
C	4.560833	1.991793	−0.403362	H	1.691460	3.443723	0.670004
C	5.413835	3.109015	−0.418319	H	4.281729	−0.942477	1.207048
C	4.894970	4.344304	−0.004745	H	5.662300	−3.334667	−2.089123
C	3.554866	4.488852	0.394411	H	2.296647	−0.696748	−2.578623
C	2.734804	3.348898	0.380718	H	2.592541	−5.269116	3.307504
C	3.194299	−0.710501	−0.634914	H	4.217803	−4.880626	2.607107
C	4.200965	−1.264698	0.171992	H	−1.159725	−1.746906	5.432133
C	5.098883	−2.217378	−0.331083	H	0.272912	−2.657517	6.058177
C	4.965642	−2.605656	−1.678023	H	−4.629495	0.408161	−2.121831
C	3.965524	−2.081936	−2.510799	H	−6.814729	0.569887	−1.034007
C	3.085082	−1.128570	−1.965332	H	−7.267019	2.430882	0.577134

H	−5.469610	4.052405	1.089308
H	−4.260233	5.837682	−0.367466
H	−2.720599	7.576860	0.485825
H	−0.594442	6.918931	1.606780
H	−0.028073	4.510106	1.838528
H	−1.535091	2.780032	0.928087
H	−3.534021	1.685260	−4.276864
H	−3.130024	0.059666	−3.701261
H	−1.911635	1.019992	−4.534746
H	−1.493505	4.347095	−2.027891
H	−2.188375	4.006532	−3.614232
H	0.380385	4.351796	−3.629711
H	−0.123751	2.805829	−4.299396
H	0.779130	3.287042	−1.402642
H	1.781116	2.515055	−2.637018
H	0.344399	1.090964	−2.629662
H	−0.391382	−1.892082	−5.772867
H	−2.530710	−2.598354	−6.687447
H	−0.993729	−4.228464	−5.816627
H	−5.995767	−4.297857	−0.745426
H	−6.320946	−4.540377	−3.138344
H	−6.913377	−2.481352	−2.026142
H	−2.807431	−5.239830	2.959249
H	−4.871958	−4.493356	3.990685
H	−2.791018	−4.231882	5.156916
H	−5.725460	1.600985	3.458447
H	−3.554048	2.671790	3.344121
H	−4.161037	1.306973	5.254536
H	7.890305	4.253528	−0.777427
H	7.297573	2.566964	−2.409221
H	7.916650	1.904822	−0.182589
H	4.080762	7.080005	1.118204
H	2.121944	6.106364	2.153521
H	2.048838	6.789708	−0.155547
H	6.554232	−2.135376	2.008506
H	7.747950	−2.962480	0.062097
H	6.129977	−4.352264	1.159498
H	2.592568	−3.494429	−4.493089
H	5.002375	−3.449948	−4.659275
H	3.696092	−1.481291	−5.215311

TS10

C	1.574888	−4.829484	−0.192682
H	0.853577	−5.126710	−0.967253
H	1.509625	−5.612212	0.581430
Si	0.922027	−3.252207	0.688779
C	2.171774	−2.925536	2.091846
H	1.755843	−2.310934	2.896279
H	2.508121	−3.873352	2.532999
H	3.058264	−2.411053	1.704122
C	−0.739164	−3.834334	1.418078
C	−0.782619	−4.184878	2.778567
C	−1.923361	−3.987112	0.645436
C	−1.943167	−4.662318	3.392079
H	0.118142	−4.094816	3.380889
C	−3.095943	−4.423133	1.289941
C	−3.112410	−4.762846	2.641547
H	−1.933609	−4.939444	4.443183
H	−4.022529	−4.483003	0.727699
H	−4.037464	−5.100282	3.102109
C	0.576474	2.464029	−1.095628
C	1.529980	1.449958	−1.438317
C	2.071827	1.427552	−2.729952
C	1.716416	2.346402	−3.733115
C	0.781681	3.297400	−3.392549
C	0.244451	3.351820	−2.108638
C	0.009065	2.741139	0.261340
C	−1.003909	1.984354	0.925855
C	−1.504560	2.423390	2.158611
C	−1.056334	3.595720	2.793179
C	−0.091570	4.321593	2.130961
C	0.415476	3.901580	0.902816
H	2.810036	0.679206	−2.984400
H	2.162188	2.309324	−4.720998
H	−2.287395	1.856556	2.645697
H	−1.462441	3.917779	3.745754
P	1.914698	0.077991	−0.226357
P	−1.642140	0.443573	0.104403
Rh	0.077926	−1.341782	−0.423131
C	−1.973403	−3.741493	−0.831857
C	−2.864894	−4.514464	−1.605372
C	−1.170879	−2.776621	−1.498477

C	−2.997868	−4.345750	−2.980868
H	−3.453391	−5.287128	−1.120277
C	−1.299813	−2.644272	−2.896359
H	0.263435	−2.710565	−1.281179
C	−2.210094	−3.398606	−3.636143
H	−3.691550	−4.969559	−3.538241
H	−0.654305	−1.936981	−3.413140
H	−2.283231	−3.264865	−4.712522
C	2.993141	−4.830869	−0.781727
H	3.047363	−4.107358	−1.602610
H	3.715684	−4.486160	−0.028830
C	3.426458	−6.209834	−1.297112
H	4.438092	−6.183556	−1.721508
H	3.423216	−6.952086	−0.488869
H	2.744594	−6.570777	−2.077315
O	0.517546	5.489582	2.510635
O	1.369475	4.798581	0.478867
O	−0.607467	4.429068	−2.020758
O	0.282647	4.321757	−4.153066
C	1.241519	5.923372	1.353964
H	0.676413	6.718430	0.846255
H	2.233127	6.266079	1.653103
C	−0.742598	4.925912	−3.356653
H	−0.609658	6.010960	−3.355435
H	−1.727744	4.646917	−3.752773
C	−2.726595	1.179901	−1.215238
C	−3.265030	2.471872	−1.098086
C	−3.040511	0.419551	−2.349035
C	−4.098561	3.012834	−2.088466
H	−3.028582	3.063429	−0.219076
C	−3.879611	0.921843	−3.362361
H	−2.629508	−0.581394	−2.436697
C	−4.394075	2.218889	−3.211725
H	−5.045867	2.618827	−3.987063
C	−2.887664	−0.172078	1.333188
C	−4.265292	−0.153944	1.089251
C	−2.429664	−0.671621	2.565605
C	−5.188913	−0.609799	2.049101
H	−4.629646	0.227172	0.140172
C	−3.318138	−1.079407	3.569713
H	−1.358617	−0.720371	2.745434
C	−4.696127	−1.046561	3.286415
H	−5.401496	−1.371276	4.049906
C	2.525725	1.044198	1.241530
C	3.413103	2.124262	1.094095
C	2.100213	0.696747	2.526093
C	3.894174	2.836079	2.201731
H	3.727878	2.411677	0.094159
C	2.552505	1.386627	3.667222
H	1.393074	−0.121515	2.630807
C	3.452921	2.445422	3.480672
H	3.816026	2.985375	4.353854
C	3.507399	−0.640894	−0.886932
C	4.753457	−0.487056	−0.265968
C	3.446071	−1.413679	−2.060551
C	5.924375	−1.059010	−0.799651
H	4.821558	0.082794	0.654601
C	4.594843	−1.954709	−2.656613
H	2.469832	−1.597967	−2.504085
C	5.827253	−1.767821	−2.005234
H	6.728261	−2.195917	−2.441348
Si	−2.700998	−1.576823	5.276636
H	−2.927317	−0.468304	6.248749
H	−3.434884	−2.765306	5.787124
H	−1.243823	−1.857796	5.232714
Si	−7.033966	−0.625390	1.682321
H	−7.417084	−1.773540	0.814520
H	−7.785589	−0.736415	2.961833
H	−7.437945	0.625442	0.983652
Si	−4.782182	4.755914	−1.910433
H	−4.047591	5.723144	−2.776729
H	−6.214896	4.803413	−2.309898
H	−4.642827	5.201115	−0.499175
Si	−4.317918	−0.100414	−4.883409
H	−5.111567	−1.306547	−4.528401
H	−5.130411	0.753657	−5.792804
H	−3.098044	−0.543619	−5.610383
Si	4.493607	−2.889580	−4.288294
H	4.730102	−1.979672	−5.444817
H	5.530663	−3.955146	−4.328219
H	3.143501	−3.490917	−4.443220
Si	7.574674	−0.880576	0.088197

H	8.675024	−1.211745	−0.856544
H	7.752489	0.512848	0.580846
H	7.671369	−1.792353	1.261552
Si	5.084049	4.274070	1.972295
H	4.451234	5.572773	2.341004
H	6.288464	4.113237	2.831754
H	5.500568	4.342512	0.547380
Si	1.970694	0.911093	5.393331
H	2.542913	1.875512	6.370725
H	0.486512	0.948236	5.487364
H	2.414856	−0.462058	5.757849

TS11

Rh	−0.056427	−1.530694	0.377755
P	1.932923	−0.513626	−0.026654
P	−1.288556	0.576050	0.354614
Si	−1.251525	−3.586529	−0.879423
Si	4.918459	−5.277508	0.706088
Si	7.237241	−0.896951	−2.147201
Si	5.606445	3.342718	2.052134
Si	2.295345	0.277556	5.559315
Si	−6.808970	1.430355	1.657720
Si	−3.029413	−0.031663	5.686463
Si	−3.719742	4.776187	−2.615546
Si	−2.602150	−0.218465	−5.139983
O	0.465946	3.919392	−2.605448
O	1.081278	3.124864	−4.691756
O	2.446794	4.347920	−0.240458
O	1.852280	5.547692	1.638111
C	1.799483	0.660836	−1.449071
C	2.139506	0.190885	−2.726540
C	1.938315	0.942265	−3.896258
C	1.367910	2.186710	−3.735393
C	1.002984	2.660872	−2.478369
C	1.175879	1.937892	−1.305111
C	0.742375	2.566582	−0.021637
C	1.372898	3.737201	0.369778
C	1.027636	4.458786	1.509715
C	0.011894	4.038225	2.337059
C	−0.657464	2.859395	1.960371
C	−0.328285	2.120371	0.817209
C	3.476137	−1.503899	−0.403334
C	3.599572	−2.796240	0.118840
C	4.788760	−3.538360	−0.003163
C	5.868892	−2.949548	−0.675906
C	5.785843	−1.655563	−1.220414
C	4.585909	−0.945728	−1.061217
C	2.650747	0.460419	1.390216
C	3.657985	1.421357	1.217183
C	4.267823	2.049190	2.312452
C	3.850486	1.679377	3.604927
C	2.843203	0.726773	3.816707
C	2.253111	0.126076	2.688451
C	−2.700843	0.636533	1.560573
C	−4.012387	0.974278	1.209065
C	−5.046456	1.010926	2.164087
C	−4.727358	0.722086	3.498404
C	−3.425523	0.359931	3.888932
C	−2.433700	0.300129	2.899554
C	−2.056080	1.195949	−1.224941
C	−2.547120	2.508699	−1.321329
C	−3.081916	3.009853	−2.517270
C	−3.093411	2.160451	−3.638504
C	−2.606433	0.845563	−3.585240
C	−2.096795	0.377248	−2.359083
C	0.381476	4.173378	−4.012233
C	2.552643	5.626507	0.392130
C	−3.016091	−3.138200	−1.438843
C	−3.574135	−3.164585	−2.722828
C	−4.893720	−2.755930	−2.943465
C	−5.668020	−2.295827	−1.874732
C	−5.136105	−2.265910	−0.585705
C	−3.820068	−2.695174	−0.363999
C	−3.180297	−2.801761	0.965744
C	−3.920623	−2.920395	2.146930
C	−3.286552	−3.198787	3.359420
C	−1.908253	−3.404962	3.397043
C	−1.163434	−3.327555	2.213740
C	−1.763088	−2.976837	0.986074
C	−1.105435	−5.454560	−0.531856
C	−0.160523	−3.289949	−2.442171
C	1.176470	−4.041330	−2.538050

C	1.845463	−3.887264	−3.910796
H	2.578509	−0.794929	−2.828212
H	2.217970	0.562877	−4.872858
H	−0.267674	4.589278	3.228227
H	−1.479084	2.535313	2.585176
H	2.742201	−3.224069	0.631838
H	6.799246	−3.506937	−0.772289
H	4.515026	0.060746	−1.462274
H	3.967726	1.689914	0.211060
H	4.327315	2.142190	4.467627
H	1.472851	−0.624599	2.806037
H	−4.239262	1.212814	0.175167
H	−5.512951	0.772033	4.251401
H	−1.427237	−0.010650	3.169152
H	−2.495446	3.155009	−0.449463
H	−3.483224	2.539622	−4.583353
H	−1.708266	−0.633137	−2.283632
H	0.856890	5.132843	−4.237207
H	−0.671354	4.170754	−4.320530
H	3.602941	5.853025	0.580083
H	2.081131	6.389172	−0.244715
H	−2.986082	−3.516202	−3.567628
H	−5.315706	−2.794061	−3.944370
H	−6.688355	−1.962181	−2.045863
H	−5.744894	−1.903250	0.238165
H	−5.003357	−2.838642	2.118175
H	−3.878746	−3.298632	4.265768
H	−1.417142	−3.663015	4.331826
H	−0.107596	−3.574269	2.244466
H	−1.123267	−6.029459	−1.465846
H	−1.924241	−5.804065	0.104894
H	−0.161498	−5.678100	−0.019799
H	0.006007	−2.218866	−2.603149
H	−0.806191	−3.626412	−3.271294
H	1.023622	−5.110260	−2.339524
H	1.857198	−3.679463	−1.760531
H	2.805951	−4.415492	−3.950709
H	2.034184	−2.831687	−4.144516
H	1.209330	−4.288644	−4.709929
H	0.812103	−2.883364	0.400410
H	6.345094	−5.700028	0.690341
H	4.128884	−6.255447	−0.092061
H	4.411445	−5.316187	2.104579
H	7.126202	0.586212	−2.116930
H	7.269004	−1.329159	−3.572609
H	8.520155	−1.311364	−1.517460
H	6.123425	3.247126	0.661018
H	6.726998	3.137355	3.009948
H	5.095936	4.727663	2.259833
H	0.967326	0.866798	5.885980
H	3.291472	0.804863	6.530825
H	2.188287	−1.198047	5.718030
H	−7.530487	0.238977	1.127785
H	−6.807966	2.470351	0.593601
H	−7.558461	1.932954	2.840799
H	−3.990319	−1.027853	6.235355
H	−3.125086	1.190731	6.533243
H	−1.649399	−0.570600	5.786453
H	−5.163933	4.818809	−2.974491
H	−2.982100	5.548700	−3.655974
H	−3.525855	5.441081	−1.300476
H	−1.662352	−1.355651	−4.980251
H	−2.168216	0.614653	−6.296334
H	−3.954684	−0.749304	−5.461761

TS12

C	−3.016040	2.628840	−2.352645
C	−0.514297	2.393194	−2.337317
C	−1.756514	2.536958	−3.223832
H	−2.967250	3.550277	−1.756028
H	−3.938039	2.679553	−2.946072
H	−0.405260	3.301728	−1.732130
H	0.391763	2.319225	−2.959586
H	−1.672273	3.430938	−3.865768
H	−1.836409	1.679266	−3.906974
Si	−3.029300	1.128204	−1.175633
C	−4.333985	−0.150276	−1.726646
H	−4.240843	−1.081256	−1.153248
H	−5.357298	0.217677	−1.608690
H	−4.179606	−0.402236	−2.783392
C	−3.425402	1.567195	0.662132
C	−2.414690	1.432132	1.633779

C	−4.709296	1.975969	1.119217
C	−2.629757	1.678550	2.991591
H	−1.432664	1.103750	1.300205
C	−4.919119	2.213500	2.489162
C	−3.895014	2.071451	3.423973
H	−1.813873	1.555452	3.699412
H	−5.905847	2.531859	2.815802
H	−4.086604	2.269253	4.475581
C	2.014943	−0.660080	1.770246
C	1.691882	0.729518	1.637795
C	1.462622	1.502116	2.783143
C	1.525442	0.978254	4.087014
C	1.824715	−0.360650	4.196405
C	2.067820	−1.144212	3.069352
C	2.421903	−1.584060	0.664555
C	1.569344	−2.138365	−0.340917
C	2.094345	−3.031188	−1.284216
C	3.442328	−3.432344	−1.292175
C	4.242650	−2.911916	−0.300321
C	3.739334	−2.017616	0.643044
H	1.231294	2.554324	2.675615
H	1.356583	1.600251	4.959152
H	1.438498	−3.454233	−2.034934
H	3.825122	−4.127648	−2.031146
P	1.427307	1.476770	−0.044057
P	−0.224620	−1.651431	−0.388731
Rh	−0.494034	0.653559	−1.121357
C	−5.894439	2.182571	0.228942
C	−7.040224	1.385059	0.390399
C	−5.927677	3.208752	−0.727089
C	−8.172844	1.589305	−0.398235
H	−7.030667	0.589963	1.131371
C	−7.061605	3.416012	−1.515429
H	−5.067572	3.860543	−0.839113
C	−8.186119	2.604601	−1.357490
H	−9.044638	0.953983	−0.264265
H	−7.067225	4.219242	−2.247720
H	−9.067763	2.764970	−1.972306
H	−1.882593	0.122906	−1.865886
O	1.982109	−1.110845	5.331235
O	2.393710	−2.419592	3.467818
O	4.758101	−1.636108	1.488188
O	5.577469	−3.127490	−0.069616
C	2.170239	−2.456984	4.882305
H	3.046079	−2.886454	5.376451
H	1.267806	−3.043828	5.094551
C	5.825139	−2.549890	1.216090
H	5.829161	−3.342573	1.978564
H	6.771560	−2.008529	1.195004
C	1.439266	3.307883	0.300461
C	2.560602	4.126674	0.113940
C	0.244583	3.904053	0.738189
C	2.515916	5.509388	0.367836
H	3.486890	3.687721	−0.241920
C	0.163433	5.274984	1.030068
H	−0.638374	3.280215	0.847361
C	1.312884	6.060085	0.836011
H	1.265632	7.126846	1.047419
C	3.056989	1.216085	−0.885292
C	4.280005	1.298421	−0.200208
C	3.070503	0.953081	−2.259956
C	5.504784	1.140408	−0.866304
H	4.272122	1.481028	0.871290
C	4.275545	0.788028	−2.966924
H	2.118662	0.867697	−2.778033
C	5.477651	0.888626	−2.250659
H	6.419110	0.760966	−2.783214
C	−0.878720	−2.528660	1.119351
C	−0.241559	−3.649939	1.673226
C	−2.088336	−2.097964	1.681581
C	−0.792289	−4.346920	2.761744
H	0.693128	−3.992875	1.239476
C	−2.674698	−2.765786	2.771488
H	−2.580745	−1.225614	1.262108
C	−2.013098	−3.891228	3.289017
H	−2.465885	−4.433902	4.118238
C	−0.896097	−2.734057	−1.749037
C	−0.800264	−2.260605	−3.069406
C	−1.508681	−3.973648	−1.529656
C	−1.281257	−3.002464	−4.158758
H	−0.349264	−1.283749	−3.233528
C	−2.027540	−4.739472	−2.590755

H	−1.591090	−4.351114	−0.515066
C	−1.898409	−4.238757	−3.894680
H	−2.292673	−4.821859	−4.725417
Si	−1.098015	−2.364944	−5.920901
H	0.140238	−2.886883	−6.564983
H	−2.257382	−2.810148	−6.740805
H	−1.029242	−0.880368	−5.916384
Si	−2.890080	−6.379489	−2.262651
H	−2.987186	−7.145008	−3.534755
H	−2.125129	−7.179218	−1.266862
H	−4.265612	−6.184235	−1.726403
Si	0.078982	−5.854444	3.472977
H	0.839332	−5.520886	4.712311
H	−0.910900	−6.905992	3.831243
H	1.041773	−6.392312	2.476287
Si	−4.298367	−2.179810	3.528177
H	−5.086688	−1.423700	2.523105
H	−5.077121	−3.367623	3.977375
H	−4.072820	−1.315547	4.718378
Si	−1.438020	6.044143	1.657914
H	−1.327743	7.524427	1.549069
H	−2.598673	5.575776	0.856785
H	−1.687797	5.700064	3.084661
Si	4.023318	6.594150	0.063015
H	3.913007	7.833700	0.878577
H	5.264894	5.865289	0.441005
H	4.143699	6.988081	−1.368131
Si	4.274106	0.453524	−4.820107
H	4.039309	1.698053	−5.602847
H	5.596229	−0.104390	−5.213198
H	3.203554	−0.518022	−5.169617
Si	7.128832	1.254007	0.074670
H	7.794352	−0.074775	0.190937
H	8.080687	2.162083	−0.621138
H	6.868581	1.767441	1.444992

TS13

C	−4.291539	−1.418973	−2.456059
C	−2.345383	−1.871179	−0.721675
C	−2.962571	−2.127789	−2.113492
H	−4.141189	−0.338212	−2.546212
H	−4.617149	−1.758243	−3.452600
H	−1.727822	−2.744170	−0.481765
H	−3.123893	−1.851620	0.041218
H	−2.233442	−1.891598	−2.901793
H	−3.135353	−3.213023	−2.206454
Si	−5.765264	−1.745273	−1.303337
C	−7.337923	−0.970933	−2.030258
H	−7.217551	0.105016	−2.195281
H	−7.579348	−1.433933	−2.995225
H	−8.197591	−1.118164	−1.365900
C	−5.477083	−1.228527	0.504573
C	−5.936381	−2.080625	1.524498
C	−4.741908	−0.076529	0.880942
C	−5.691948	−1.816990	2.874090
H	−6.484713	−2.981813	1.257576
C	−4.488138	0.174094	2.235669
C	−4.958075	−0.686449	3.230389
H	−6.065832	−2.492956	3.639019
H	−3.932672	1.064267	2.518250
H	−4.757439	−0.466638	4.275895
C	2.987416	−0.104346	0.442282
C	2.461353	−1.021076	−0.518628
C	3.272588	−1.459299	−1.575168
C	4.605543	−1.046077	−1.743783
C	5.101864	−0.177199	−0.798608
C	4.309300	0.273165	0.254585
C	2.298404	0.413443	1.664470
C	1.240719	1.378078	1.707917
C	0.817014	1.878837	2.945501
C	1.365362	1.467099	4.172524
C	2.361584	0.519376	4.113245
C	2.813900	0.024246	2.892952
H	2.876487	−2.165845	−2.292429
H	5.211761	−1.404810	−2.568232
H	0.034460	2.625384	2.976874
H	1.022364	1.879538	5.114911
P	0.705722	−1.621553	−0.360044
P	0.285916	1.810158	0.167497
Rh	−1.165019	−0.110768	−0.460383
C	−4.297742	0.914488	−0.154643
C	−5.306451	1.747939	−0.675297

C	−2.965210	1.049929	−0.617204
C	−5.044821	2.690262	−1.666596
H	−6.315124	1.643662	−0.283990
C	−2.723523	2.038201	−1.595694
H	−2.175174	0.415211	0.634715
C	−3.740282	2.824717	−2.138729
H	−5.844229	3.317597	−2.052202
H	−1.714476	2.193671	−1.965012
H	−3.504340	3.552030	−2.912050
H	−6.002929	−3.222162	−1.228657
O	6.347672	0.389865	−0.718948
O	5.039635	1.157431	1.018354
O	3.847789	−0.855403	3.116803
O	3.083110	−0.032686	5.139315
C	6.390606	0.996859	0.577227
H	6.925843	0.334406	1.272994
H	6.868155	1.974493	0.504463
C	3.895201	−1.044961	4.535525
H	3.493172	−2.035562	4.784864
H	4.926783	−0.938257	4.881667
C	0.622785	−2.894368	−1.710200
C	0.692304	−4.273728	−1.492489
C	0.437586	−2.432899	−3.025418
C	0.594043	−5.193942	−2.554058
H	0.815935	−4.643142	−0.478903
C	0.359618	−3.311514	−4.114843
H	0.351700	−1.361708	−3.197899
C	0.436964	−4.692177	−3.853754
H	0.361658	−5.393251	−4.683309
C	0.799571	−2.623605	1.196850
C	1.943696	−3.373679	1.515388
C	−0.284221	−2.627157	2.082538
C	2.016572	−4.134512	2.691707
H	2.792767	−3.354846	0.837389
C	−0.252593	−3.379015	3.272463
H	−1.152170	−2.021805	1.832320
C	0.903201	−4.123904	3.553190
H	0.938343	−4.710035	4.470559
C	−0.567825	3.408332	0.615702
C	−0.176468	4.653250	0.104560
C	−1.701577	3.365014	1.446928
C	−0.866298	5.837368	0.421789
H	0.684473	4.710330	−0.552428
C	−2.407801	4.523437	1.805233
H	−2.033751	2.402992	1.824735
C	−1.967419	5.752824	1.285483
H	−2.495686	6.664150	1.560634
C	1.595452	2.418918	−0.996014
C	2.704065	3.167783	−0.567995
C	1.441826	2.167089	−2.363261
C	3.643311	3.673082	−1.478604
H	2.829246	3.358286	0.494894
C	2.359936	2.653670	−3.313010
H	0.585081	1.578503	−2.687946
C	3.446699	3.408666	−2.847599
H	4.159078	3.804042	−3.569998
Si	0.662677	−7.048749	−2.235551
H	0.683604	−7.759739	−3.541867
H	1.887115	−7.408205	−1.468153
H	−0.515216	−7.512460	−1.453262
Si	0.147519	−2.662019	−5.869600
H	1.435944	−2.687861	−6.617241
H	−0.827737	−3.501335	−6.615956
H	−0.336285	−1.257498	−5.816928
Si	−1.711904	−3.395062	4.465305
H	−2.907429	−4.037310	3.859403
H	−1.310607	−4.172827	5.670178
H	−2.077260	−2.016233	4.884153
Si	3.569465	−5.112916	3.102159
H	4.287296	−4.524335	4.269322
H	3.240478	−6.522210	3.448640
H	4.484608	−5.092090	1.930943
Si	−3.918004	4.450809	2.928299
H	−4.025700	5.732334	3.677965
H	−5.178531	4.251539	2.165707
H	−3.773126	3.331129	3.897176
Si	−0.327612	7.488879	−0.301516
H	−0.898543	8.592791	0.516259
H	1.157155	7.595843	−0.304512
H	−0.796689	7.656430	−1.705268
Si	2.145865	2.296777	−5.149316
H	3.113121	3.126535	−5.916043

H	2.402502	0.862855	−5.457058
H	0.762144	2.617465	−5.591606
Si	5.117373	4.676554	−0.878764
H	6.382738	3.891583	−0.936398
H	5.307372	5.884017	−1.727467
H	4.889829	5.091303	0.530226

TS14-sp^2

C	0.109597	4.946975	1.309578
H	−0.965806	4.978508	1.528098
H	0.336862	5.889346	0.785434
Si	0.436610	3.547741	0.035443
C	2.179430	3.925305	−0.639445
H	2.515942	3.229116	−1.413906
H	2.189997	4.937974	−1.065177
H	2.918962	3.904496	0.167006
C	−0.827422	3.778134	−1.363768
C	−0.394462	4.098375	−2.662918
C	−2.213943	3.552915	−1.150401
C	−1.276054	4.184773	−3.743539
H	0.660717	4.291876	−2.839693
C	−3.082974	3.618198	−2.252063
C	−2.629273	3.930265	−3.535204
H	−0.906026	4.441262	−4.733048
H	−4.137120	3.410695	−2.105632
H	−3.334766	3.973021	−4.361045
C	1.291842	−2.547370	0.208971
C	1.947315	−1.438404	0.832090
C	2.665989	−1.643915	2.018063
C	2.789853	−2.898129	2.640848
C	2.163498	−3.954857	2.020258
C	1.444083	−3.773782	0.842298
C	0.527457	−2.549563	−1.077146
C	−0.761828	−1.968023	−1.301240
C	−1.410804	−2.178461	−2.524116
C	−0.855639	−2.935754	−3.570575
C	0.383352	−3.487395	−3.338361
C	1.040415	−3.301469	−2.124374
H	3.173012	−0.809254	2.482980
H	3.359118	−3.024685	3.555157
H	−2.399084	−1.767686	−2.679981
H	−1.384553	−3.086304	−4.505160
P	1.803345	0.288145	0.127470
P	−1.502809	−0.862796	0.005371
Rh	−0.311050	1.277371	0.382493
C	−2.783435	3.219048	0.200745
C	−3.985316	3.836429	0.639238
C	−2.146504	2.262124	1.043277
C	−4.575756	3.421496	1.841894
C	−2.770725	1.892175	2.244228
H	−0.697135	2.409750	1.459128
C	−3.994021	2.437526	2.631140
H	−5.495999	3.902469	2.166402
H	−2.277743	1.182076	2.901483
H	−4.464824	2.127040	3.560972
C	−4.662914	4.985151	−0.088222
H	−3.959630	5.576803	−0.679085
H	−5.453857	4.645829	−0.769539
H	−5.138726	5.650514	0.641000
C	0.892101	4.906213	2.632373
H	1.971333	4.867491	2.428648
H	0.648478	3.979349	3.170861
C	0.598332	6.104829	3.544246
H	1.163265	6.046597	4.482967
H	0.864326	7.048856	3.052204
H	−0.468213	6.153289	3.796601
O	1.150072	−4.261571	−4.171042
O	2.248722	−3.961381	−2.161480
O	0.903744	−4.980237	0.455417
O	2.108374	−5.269025	2.405943
C	−3.282148	−0.701907	−0.506420
C	−4.333233	−1.231036	0.253332
C	−3.601529	0.013710	−1.675286
C	−5.675644	−1.102564	−0.145984
H	−4.107929	−1.761336	1.172224
C	−4.923182	0.116387	−2.138224
H	−2.802941	0.483411	−2.243988
C	−5.945113	−0.454784	−1.359132
H	−6.974711	−0.393895	−1.708332
C	−1.600447	−2.011386	1.456811
C	−2.061542	−3.331009	1.329982
C	−1.190468	−1.555469	2.714517

C	−2.131363	−4.190767	2.436596
H	−2.361643	−3.692265	0.349500
C	−1.248074	−2.382151	3.851196
H	−0.796417	−0.544330	2.787412
C	−1.723293	−3.692507	3.687758
H	−1.767811	−4.348689	4.556285
C	2.470614	0.033058	−1.586353
C	3.561403	−0.811772	−1.852717
C	1.842647	0.680352	−2.656962
C	4.046528	−0.995648	−3.155377
H	4.028537	−1.345431	−1.029177
C	2.289837	0.515196	−3.982052
H	0.979535	1.308533	−2.446019
C	3.394647	−0.320371	−4.204212
H	3.750882	−0.457543	−5.224173
C	3.195257	1.151043	1.019785
C	4.482503	1.313205	0.498173
C	2.923370	1.662462	2.301028
C	5.498230	1.963417	1.225068
H	4.704287	0.940473	−0.496509
C	3.914889	2.283512	3.075295
H	1.911624	1.568225	2.689449
C	5.198096	2.423955	2.514701
H	5.982104	2.905671	3.097516
C	1.509706	−5.959444	1.304219
H	2.288081	−6.497836	0.744368
H	0.742807	−6.641766	1.675767
C	2.206263	−4.762735	−3.346677
H	3.155485	−4.675645	−3.878035
H	1.993253	−5.806503	−3.073570
Si	3.552179	2.900879	4.818106
H	4.514302	2.300583	5.783996
H	3.686673	4.379686	4.913116
H	2.172399	2.508338	5.204385
Si	7.207880	2.215980	0.478949
H	8.179042	2.505193	1.568189
H	7.638874	0.993558	−0.252890
H	7.228336	3.352822	−0.482375
Si	5.511349	−2.128851	−3.479058
H	5.124058	−3.293134	−4.326215
H	6.601269	−1.410826	−4.194712
H	6.031260	−2.639758	−2.183808
Si	1.436846	1.367282	−5.430095
H	1.648076	2.840098	−5.404334
H	2.022221	0.832105	−6.689833
H	−0.025570	1.104669	−5.422922
Si	−5.346833	0.934315	−3.781082
H	−6.449259	0.168518	−4.425889
H	−5.816733	2.337886	−3.620389
H	−4.161077	0.930169	−4.676074
Si	−7.067921	−1.793776	0.914105
H	−8.284553	−1.963902	0.074322
H	−6.678374	−3.112222	1.485428
H	−7.405263	−0.889062	2.047482
Si	−2.721981	−5.964360	2.232451
H	−1.592322	−6.933293	2.328504
H	−3.701591	−6.323014	3.293569
H	−3.355111	−6.121298	0.896965
Si	−0.709399	−1.748543	5.540303
H	−1.848097	−1.148719	6.290203
H	−0.173002	−2.877254	6.348115
H	0.339594	−0.707577	5.380893

TS14-sp^3

C	4.340370	1.643970	−1.111537
H	3.839621	2.438518	−1.684390
H	4.452597	0.798789	−1.799874
Si	3.149863	1.184107	0.322499
C	2.960647	2.834007	1.283034
H	2.219662	2.808235	2.088093
H	3.922307	3.117809	1.729379
H	2.667195	3.636391	0.598374
C	4.026329	−0.002637	1.557804
C	3.919068	0.260313	2.937607
C	4.786482	−1.138442	1.169988
C	4.528753	−0.541495	3.905291
H	3.360736	1.131266	3.271240
C	5.402753	−1.936015	2.147848
C	5.278316	−1.647160	3.507637
H	4.424323	−0.297420	4.959815
H	5.982851	−2.799289	1.830964
H	5.764931	−2.280543	4.245139

C	−2.874070	0.556024	−0.625434	O	−4.856369	1.311096	1.415231
C	−1.836733	1.401103	−1.136561	O	−5.077907	−0.410863	−1.206038
C	−1.974186	1.949615	−2.419648	O	−5.258750	0.526959	−3.310665
C	−3.088104	1.721463	−3.245787	C	−5.806736	1.152101	2.474081
C	−4.081148	0.920677	−2.729889	H	−6.713818	0.671197	2.080056
C	−3.967692	0.364500	−1.459150	H	−6.029890	2.126438	2.911717
C	−2.938165	−0.092940	0.719766	C	−5.992523	−0.125190	−2.269238
C	−2.132134	−1.192307	1.150706	H	−6.410947	−1.059325	−2.648975
C	−2.368704	−1.785486	2.397239	H	−6.781381	0.546992	−1.902019
C	−3.384146	−1.352140	3.268063	C	−1.581795	−2.347105	−1.453532
C	−4.162992	−0.304309	2.830628	C	−2.814177	−3.019519	−1.417612
C	−3.943756	0.295780	1.591953	C	−0.963957	−2.129465	−2.689949
H	−1.200501	2.599556	−2.805062	C	−3.427615	−3.482608	−2.590846
H	−3.162255	2.163776	−4.233076	H	−3.300439	−3.176745	−0.458192
H	−1.764431	−2.627846	2.709423	C	−1.541942	−2.582578	−3.890388
H	−3.553861	−1.830105	4.226531	H	−0.022258	−1.584727	−2.705279
P	−0.275498	1.740405	−0.156576	C	−2.769280	−3.258110	−3.815181
P	−0.726451	−1.747139	0.072967	H	−3.227362	−3.617459	−4.735392
Rh	1.174939	−0.085481	−0.130950	C	−0.162101	−3.316935	0.885839
C	5.005751	−1.504272	−0.262565	C	−0.414809	−4.591305	0.366399
C	3.936468	−1.806564	−1.139903	C	0.612476	−3.214790	2.057986
C	6.324701	−1.578935	−0.740112	C	0.067316	−5.755255	0.995593
C	4.243383	−2.150185	−2.468545	H	−0.998435	−4.685750	−0.544032
C	6.608284	−1.916952	−2.062312	C	1.085547	−4.348753	2.733343
C	5.555018	−2.202200	−2.933493	H	0.844034	−2.227467	2.452863
H	3.425819	−2.390375	−3.145878	C	0.799050	−5.611780	2.182010
H	7.638215	−1.958255	−2.406450	H	1.158256	−6.505408	2.690258
H	5.753676	−2.471411	−3.967866	C	0.377501	3.255835	−1.025108
C	2.513345	−1.825848	−0.691330	C	0.175397	4.566860	−0.580728
H	1.932850	−2.517248	−1.304872	C	1.125660	3.056188	−2.199037
H	2.436585	−2.138522	0.354224	C	0.689475	5.673060	−1.284220
H	1.989242	−0.422801	−1.440559	H	−0.380546	4.738779	0.335045
H	7.137653	−1.349298	−0.056005	C	1.629914	4.130496	−2.947441
C	5.733072	2.145960	−0.683296	H	1.315659	2.035235	−2.521692
H	5.629224	3.036382	−0.048411	C	1.396810	5.433439	−2.470978
H	6.224696	1.385134	−0.063637	H	1.779236	6.281728	−3.037201
C	6.639115	2.480018	−1.875776	C	−0.978007	2.413721	1.425170
H	6.188642	3.253240	−2.511451	C	−2.070261	3.296744	1.460683
H	7.620208	2.846863	−1.547982	C	−0.409993	2.001028	2.635048
H	6.802975	1.592031	−2.498356	C	−2.575519	3.790452	2.672326
O	−5.212943	0.308092	3.465247	H	−2.540338	3.592194	0.526171

C	−0.889221	2.463832	3.874594
H	0.415896	1.293048	2.599155
C	−1.966230	3.362526	3.867117
H	−2.347858	3.731781	4.817920
Si	2.596558	3.838031	−4.538630
H	1.983606	4.604609	−5.659468
H	4.008787	4.287209	−4.406906
H	2.569659	2.390327	−4.870775
Si	0.444554	7.424536	−0.639458
H	0.582455	8.387037	−1.765487
H	−0.908827	7.563795	−0.035610
H	1.447843	7.777492	0.402457
Si	−4.035885	4.975196	2.685917
H	−5.214394	4.377109	3.376177
H	−3.701384	6.235859	3.402820
H	−4.419777	5.294447	1.286175
Si	−0.114719	1.893877	5.493737
H	1.287035	2.376847	5.625133
H	−0.916034	2.438103	6.622782
H	−0.096028	0.408858	5.580320
Si	−0.699926	−2.282446	−5.548408
H	0.664170	−2.877173	−5.570225
H	−1.519329	−2.911010	−6.619141
H	−0.568998	−0.827721	−5.832088
Si	−5.089992	−4.358949	−2.517895
H	−6.187544	−3.494576	−3.039310
H	−5.074139	−5.598034	−3.341484
H	−5.400991	−4.704499	−1.106138
Si	−0.264414	−7.456699	0.260292
H	0.058033	−8.495337	1.274950
H	−1.694184	−7.584218	−0.134584
H	0.564963	−7.702277	−0.951285
Si	2.059735	−4.197989	4.340357
H	1.398848	−5.008896	5.401882
H	3.447915	−4.707679	4.186512
H	2.089406	−2.776187	4.763526

TS15-*S*

C	0.472958	−2.732186	1.110120
C	−0.496323	−2.626291	0.064639
C	−0.771216	−3.741863	−0.736610
C	−0.136380	−4.986353	−0.570101
C	0.780253	−5.074538	0.452120
C	1.063168	−3.978152	1.261500
C	0.815188	−1.686453	2.122836
C	1.538764	−0.473197	1.893511
C	1.870687	0.345859	2.982843
C	1.518362	0.045962	4.309979
C	0.808054	−1.116192	4.507838
C	0.481647	−1.952998	3.444345
H	−1.524406	−3.667472	−1.509821
H	−0.372445	−5.833923	−1.204273
H	2.422027	1.260520	2.807365
H	1.797004	0.694650	5.133380
P	−1.381314	−0.999520	−0.184472
P	1.871544	0.166709	0.172858
O	0.358984	−1.656206	5.686856
O	−0.179824	−3.060169	3.930037
O	2.013728	−4.343231	2.193466
O	1.540092	−6.152276	0.848391
C	−0.443706	−2.778392	5.306631
H	−0.167218	−3.644597	5.914117
H	−1.505174	−2.525002	5.430589
C	2.059038	−5.769100	2.125627
H	1.425359	−6.192478	2.919297
H	3.092752	−6.104459	2.214121
C	−2.712489	−1.417459	−1.418131
C	−2.353952	−1.755314	−2.734901
C	−4.078166	−1.301593	−1.113668
C	−3.314314	−2.026755	−3.726200
H	−1.296831	−1.809667	−2.988536
C	−5.079107	−1.539437	−2.071961
H	−4.367208	−1.013380	−0.108855
C	−4.667731	−1.911772	−3.363996
H	−5.426581	−2.108644	−4.118989
C	−2.332484	−0.922413	1.411184
C	−2.988622	−2.048665	1.930578
C	−2.371733	0.276087	2.133793
C	−3.699307	−2.001128	3.141458
H	−2.933410	−2.982848	1.377022
C	−3.049526	0.375226	3.363281
H	−1.838906	1.132982	1.729594

C	−3.706629	−0.775556	3.835083
H	−4.234002	−0.720593	4.786825
C	3.123924	1.508250	0.507271
C	2.681311	2.828669	0.695725
C	4.493317	1.240381	0.617480
C	3.570067	3.868290	1.016197
H	1.619482	3.031564	0.584515
C	5.430596	2.250165	0.907918
H	4.843837	0.224702	0.463138
C	4.938884	3.548191	1.109705
H	5.646333	4.341465	1.347083
C	2.930644	−1.119351	−0.640265
C	3.753108	−2.012723	0.064882
C	2.971349	−1.122535	−2.040172
C	4.620800	−2.894355	−0.602524
H	3.717160	−2.016172	1.151157
C	3.833179	−1.973664	−2.756017
H	2.306397	−0.436323	−2.561828
C	4.642151	−2.846158	−2.010013
H	5.313672	−3.517770	−2.543708
Si	5.744941	−4.110473	0.318372
Si	3.905660	−1.891919	−4.647497
Si	7.272659	1.824561	1.032498
Si	2.995118	5.649070	1.328740
Si	−6.920963	−1.387784	−1.641912
Si	−2.788098	−2.511311	−5.484439
Si	−3.056473	1.979611	4.373926
Si	−4.600054	−3.538203	3.791424
C	−3.354694	2.695367	−1.889436
C	−1.377601	1.703218	−2.950140
C	−2.927136	1.862716	−3.140845
H	−3.877643	2.084584	−1.144896
H	−3.973841	3.569313	−2.105408
H	−1.054794	0.649354	−2.863397
H	−0.781805	2.130847	−3.760207
H	−3.441086	0.900022	−3.209788
H	−3.132735	2.412332	−4.066557
Si	−1.516591	2.955564	−1.464487
Rh	0.027409	0.798064	−0.934241
H	1.098877	1.802400	−1.598180
C	−0.793885	4.635058	−1.984591
C	0.412796	4.631633	−2.710673
C	−1.443252	5.881004	−1.784840
C	0.964375	5.800103	−3.237532
H	0.928598	3.687448	−2.867452
C	−0.887103	7.049404	−2.333695
C	0.304846	7.016016	−3.054264
H	1.896633	5.757751	−3.795123
H	−1.391051	7.998107	−2.167506
H	0.717991	7.934819	−3.462656
C	−2.704662	6.016009	−0.999918
C	−2.798069	5.539886	0.317975
C	−3.820779	6.666347	−1.553019
C	−3.973339	5.698036	1.054317
H	−1.932233	5.072126	0.778269
C	−4.997247	6.821251	−0.819238
H	−3.766130	7.035694	−2.573754
C	−5.078478	6.335988	0.487843
H	−4.019770	5.333435	2.077072
H	−5.851983	7.318871	−1.270320
H	−5.993586	6.457899	1.061220
H	−1.100422	2.590336	−0.057750
C	−7.130624	−0.353363	−0.070420
H	−8.194957	−0.232760	0.167226
H	−6.652790	−0.817557	0.800362
H	−6.703245	0.649426	−0.189284
C	−7.831154	−0.545425	−3.075089
H	−8.901381	−0.451819	−2.852346
H	−7.439273	0.462160	−3.257062
H	−7.740925	−1.110022	−4.010810
C	−7.654055	−3.116256	−1.369588
H	−7.535614	−3.745876	−2.259649
H	−7.165160	−3.631320	−0.533848
H	−8.726198	−3.059262	−1.143119
C	−1.820784	−1.087291	−6.273923
H	−0.918385	−0.847319	−5.699812
H	−1.504781	−1.343329	−7.293022
H	−2.429168	−0.176962	−6.329967
C	−1.693322	−4.057063	−5.402182
H	−0.796913	−3.886968	−4.793643
H	−2.235032	−4.905646	−4.967248
H	−1.358096	−4.354088	−6.403750

C	−4.322928	−2.887041	−6.529493
H	−4.978477	−2.013406	−6.626645
H	−4.025460	−3.185028	−7.542481
H	−4.916787	−3.707012	−6.108209
C	−6.349849	−3.620774	3.065811
H	−6.942694	−2.742661	3.348531
H	−6.322139	−3.662423	1.970193
H	−6.884462	−4.511735	3.418548
C	−3.630293	−5.084379	3.282568
H	−3.661870	−5.245644	2.198412
H	−2.575040	−5.006069	3.568994
H	−4.046588	−5.981279	3.757699
C	−4.724198	−3.457972	5.682696
H	−5.243031	−4.344507	6.068046
H	−3.736833	−3.422860	6.158712
H	−5.286663	−2.580290	6.022873
C	−1.663651	3.111831	3.775445
H	−0.688565	2.616892	3.854783
H	−1.798996	3.406099	2.728067
H	−1.624947	4.029928	4.374796
C	−4.726995	2.855290	4.172718
H	−5.557017	2.218865	4.502627
H	−4.764148	3.780440	4.762094
H	−4.910508	3.117790	3.123862
C	−2.783326	1.552870	6.201464
H	−2.755300	2.462396	6.814395
H	−3.582738	0.916263	6.599893
H	−1.834419	1.022577	6.346547
C	7.810587	0.910681	−0.538168
H	8.864441	0.610648	−0.479449
H	7.215758	0.003795	−0.701373
H	7.692347	1.544095	−1.425355
C	7.563857	0.705441	2.536546
H	7.287014	1.211563	3.469052
H	6.969614	−0.214298	2.472439
H	8.618734	0.413696	2.615315
C	8.291656	3.410176	1.227542
H	9.360353	3.171056	1.291911
H	8.156704	4.087724	0.376059
H	8.024922	3.959958	2.138127
C	3.784307	6.262306	2.942640
H	4.879899	6.241117	2.898729
H	3.484766	7.296896	3.152272
H	3.476130	5.647445	3.796728
C	3.553864	6.768043	−0.095100
H	3.297359	7.815882	0.106278
H	4.638625	6.714737	−0.248095
H	3.066942	6.481151	−1.034147
C	1.112930	5.709425	1.492610
H	0.753393	5.047636	2.289910
H	0.782723	6.727860	1.731946
H	0.619744	5.416597	0.558943
C	7.546101	−3.809334	−0.195895
H	7.685751	−3.926791	−1.277358
H	7.870611	−2.796238	0.070239
H	8.221292	−4.516892	0.301818
C	5.266772	−5.884545	−0.156623
H	5.852650	−6.619536	0.410049
H	4.203537	−6.086073	0.018254
H	5.457657	−6.066958	−1.221429
C	5.583735	−3.855431	2.187432
H	5.959175	−2.869829	2.489655
H	4.543068	−3.927291	2.522618
H	6.169435	−4.606854	2.731685
C	4.964792	−3.314082	−5.316319
H	4.984627	−3.290681	−6.412938
H	6.003542	−3.249642	−4.970681
H	4.571641	−4.292435	−5.015099
C	2.150262	−2.024945	−5.346663
H	1.695353	−2.990654	−5.095950
H	1.503158	−1.236893	−4.942968
H	2.149237	−1.927192	−6.439302
C	4.665069	−0.236711	−5.173481
H	5.688205	−0.130646	−4.793638
H	4.702578	−0.144951	−6.266317
H	4.081532	0.608000	−4.787923

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C	1.489103	4.246530	−2.325358
C	0.944374	1.981068	−2.878906
C	2.165834	2.926549	−2.781506
H	2.056761	4.825610	−1.590966

H	1.274267	4.899500	−3.179964
H	1.164271	0.900049	−2.802027
H	0.420559	2.101968	−3.834482
H	2.854607	2.566052	−2.013395
H	2.729398	3.004493	−3.721480
Si	−0.088108	3.286719	−1.762724
C	0.775989	−1.833230	2.087205
C	1.517759	−0.625397	1.894989
C	1.978030	0.086691	3.010420
C	1.756482	−0.327089	4.335984
C	1.065398	−1.505175	4.501460
C	0.599333	−2.226725	3.406366
C	0.289787	−2.764952	1.023664
C	−0.736536	−2.514548	0.057801
C	−1.115464	−3.540311	−0.821743
C	−0.543569	−4.823405	−0.807525
C	0.431344	−5.048790	0.137483
C	0.825226	−4.047055	1.018816
H	2.556941	0.988567	2.860411
H	2.130128	0.242920	5.179562
H	−1.895530	−3.350575	−1.547226
H	−0.864649	−5.597070	−1.496468
P	1.848831	−0.008405	0.163965
P	−1.507796	−0.826348	−0.167211
Rh	−0.105065	0.690438	−1.077961
H	−1.452469	1.126056	−1.826253
O	1.153493	−6.193189	0.373622
O	1.821101	−4.538906	1.838337
O	−0.055767	−3.354239	3.862234
O	0.718574	−2.153182	5.666262
C	1.841395	−5.947692	1.602166
H	1.320982	−6.464050	2.422757
H	2.875816	−6.286117	1.515389
C	0.320112	−3.457196	5.236085
H	1.171487	−4.148375	5.330318
H	−0.535996	−3.789693	5.823258
C	3.135648	1.310287	0.436460
C	2.730563	2.543390	0.981782
C	4.476627	1.159891	0.057517
C	3.637958	3.591579	1.205209
H	1.682260	2.679950	1.235927
C	5.419352	2.192620	0.224297
H	4.795313	0.224027	−0.388074
C	4.973888	3.387334	0.810401
H	5.689582	4.195601	0.958422
C	2.854723	−1.401893	−0.534696
C	3.815489	−2.094177	0.220994
C	2.668285	−1.760371	−1.874419
C	4.601456	−3.114361	−0.337874
H	3.942127	−1.831745	1.268332
C	3.430045	−2.773898	−2.486860
H	1.891348	−1.246253	−2.436394
C	4.387844	−3.427946	−1.695418
H	4.981065	−4.221466	−2.146891
C	−2.996973	−1.244928	−1.214408
C	−2.892451	−1.160421	−2.613012
C	−4.207221	−1.680410	−0.662789
C	−3.953144	−1.518798	−3.459621
H	−1.957629	−0.796741	−3.030464
C	−5.310904	−2.030727	−1.465157
H	−4.301470	−1.740824	0.417128
C	−5.152084	−1.947076	−2.856197
H	−5.991427	−2.219336	−3.495148
C	−2.317386	−0.457729	1.459824
C	−2.702998	−1.454749	2.371205
C	−2.659863	0.874098	1.727182
C	−3.430627	−1.147587	3.533003
H	−2.435854	−2.487292	2.163639
C	−3.404372	1.232125	2.867413
H	−2.340717	1.634102	1.016056
C	−3.772003	0.201535	3.747018
H	−4.349177	0.457492	4.634416
Si	−3.959747	−2.459662	4.793225
Si	−3.917424	3.031876	3.171507
Si	−6.928631	−2.585199	−0.649467
Si	−3.815154	−1.436171	−5.347065
Si	7.230522	1.956176	−0.288290
Si	3.136991	5.228750	2.026037
Si	3.149309	−3.208270	−4.311001
Si	5.897596	−4.032504	0.696287
C	−1.686745	3.907611	−2.596177
C	−2.260931	3.130355	−3.619429

C	−2.356900	5.104812	−2.232660
C	−3.441073	3.495190	−4.266053
H	−1.786332	2.194144	−3.898954
C	−3.559547	5.452274	−2.873446
C	−4.100756	4.662270	−3.884632
H	−3.844511	2.867291	−5.056594
H	−4.059893	6.371605	−2.580202
H	−5.025947	4.959907	−4.371563
C	−1.858598	6.053581	−1.189171
C	−2.665632	6.373791	−0.084169
C	−0.631363	6.721455	−1.328818
C	−2.254266	7.318502	0.856693
H	−3.621266	5.871428	0.034887
C	−0.220154	7.669676	−0.389949
H	−0.011270	6.519409	−2.195376
C	−1.028734	7.971006	0.707448
H	−2.894103	7.546918	1.705297
H	0.727917	8.183562	−0.525596
H	−0.710100	8.712006	1.435872
H	−0.241835	3.300361	−0.275794
C	3.516606	6.664011	0.846336
H	2.906032	6.598828	−0.061575
H	3.303693	7.628867	1.323609
H	4.569619	6.671681	0.539831
C	4.162462	5.449091	3.607798
H	5.238699	5.458443	3.397044
H	3.915280	6.395863	4.104307
H	3.972869	4.639485	4.322609
C	1.298976	5.203965	2.457273
H	0.673976	5.087853	1.564926
H	1.052663	4.389872	3.149259
H	1.003244	6.143979	2.938469
C	7.332078	0.718535	−1.718192
H	6.946547	−0.269984	−1.441832
H	6.761190	1.064943	−2.587877
H	8.373753	0.585650	−2.036152
C	7.955609	3.616076	−0.845208
H	8.998740	3.491269	−1.161374
H	7.398721	4.031027	−1.693575
H	7.946755	4.364484	−0.043813
C	8.227797	1.301398	1.187101
H	8.188275	1.994837	2.035759
H	7.839621	0.335637	1.533028
H	9.282832	1.159928	0.920797
C	5.462748	−3.875326	2.532759
H	5.593907	−2.848513	2.895131
H	4.420504	−4.156644	2.722026
H	6.108357	−4.519522	3.142408
C	7.618975	−3.297570	0.388778
H	8.384973	−3.825215	0.971002
H	7.901578	−3.363398	−0.668802
H	7.655378	−2.239366	0.674607
C	5.919554	−5.861790	0.192036
H	6.624157	−6.427774	0.814004
H	4.932501	−6.327698	0.297073
H	6.230533	−5.991947	−0.851475
C	4.081968	−4.800243	−4.743223
H	3.901197	−5.074738	−5.789860
H	5.165893	−4.688672	−4.619562
H	3.758559	−5.643497	−4.121409
C	1.294715	−3.452197	−4.609822
H	0.896662	−4.266879	−3.993826
H	0.728693	−2.546586	−4.359812
H	1.091478	−3.691795	−5.661064
C	3.781357	−1.790726	−5.399763
H	4.856380	−1.627750	−5.257646
H	3.613162	−2.002126	−6.463239
H	3.271040	−0.849007	−5.163920
C	−4.047071	−3.175810	−6.067429
H	−3.260827	−3.855845	−5.718408
H	−5.011638	−3.609946	−5.777315
H	−4.009605	−3.157502	−7.163926
C	−2.116229	−0.774224	−5.855939
H	−1.305730	−1.425908	−5.508334
H	−2.042292	−0.713307	−6.948865
H	−1.929893	0.229999	−5.457280
C	−5.173382	−0.297921	−6.022101
H	−5.127549	−0.230470	−7.116246
H	−6.173377	−0.660870	−5.755474
H	−5.074898	0.716623	−5.617929
C	−8.205202	−3.032577	−1.976440
H	−9.144379	−3.353774	−1.509248

H	−8.437761	−2.179418	−2.624871
H	−7.859681	−3.854349	−2.615043
C	−6.591508	−4.103871	0.435901
H	−6.234957	−4.950819	−0.162350
H	−5.827705	−3.891140	1.194068
H	−7.499769	−4.424738	0.961222
C	−7.598344	−1.181794	0.433663
H	−8.521442	−1.481298	0.945823
H	−6.872256	−0.887996	1.201325
H	−7.821822	−0.291072	−0.165395
C	−3.525189	−4.192080	4.164926
H	−3.782171	−4.948206	4.917488
H	−4.084715	−4.437636	3.253752
H	−2.458799	−4.291380	3.934715
C	−5.835007	−2.352997	5.059391
H	−6.163998	−3.067016	5.824979
H	−6.143667	−1.353326	5.387850
H	−6.381293	−2.580360	4.136191
C	−3.093173	−2.109511	6.445482
H	−3.290477	−2.902879	7.177875
H	−2.007844	−2.013764	6.326924
H	−3.450465	−1.168155	6.881115
C	−4.945744	3.633621	1.698137
H	−4.383950	3.559529	0.759668
H	−5.858459	3.036839	1.582985
H	−5.246727	4.681107	1.827251
C	−2.373665	4.108165	3.373471
H	−1.767963	3.769692	4.222747
H	−1.740814	4.076746	2.479664
H	−2.638939	5.158149	3.548815
C	−4.967735	3.140546	4.746553
H	−5.281906	4.177618	4.918340
H	−5.876721	2.531166	4.676815
H	−4.413482	2.816280	5.635507

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C	−0.874710	−5.347051	−0.340247
C	0.578762	−5.889861	−2.327104
C	0.429828	−5.590437	−1.031193
H	−1.711249	−5.548318	−1.019314
H	−0.974177	−6.037704	0.511806
H	−0.276755	−5.986103	−2.992909
H	1.558281	−6.067633	−2.762930
H	1.323818	−5.521449	−0.408932
Si	−1.117645	−3.593633	0.432325
C	−0.049304	−3.645813	2.029006
H	−0.218782	−2.769447	2.661967
H	−0.334677	−4.535345	2.609916
H	1.019084	−3.710243	1.805437
C	−2.900222	−3.524456	1.101995
C	−3.377959	−4.006651	2.326240
C	−3.810296	−2.906317	0.215077
C	−4.731384	−3.901018	2.662957
H	−2.696916	−4.486894	3.025553
C	−5.161790	−2.773820	0.563724
C	−5.618595	−3.275518	1.781894
H	−5.093823	−4.305309	3.604870
H	−5.862132	−2.282011	−0.105921
H	−6.669174	−3.179790	2.044623
C	1.482888	2.268660	−0.791535
C	2.146558	1.056232	−1.163203
C	2.802407	0.976265	−2.398253
C	2.834990	2.037230	−3.320058
C	2.175259	3.188919	−2.955010
C	1.531735	3.294938	−1.724049
C	0.862123	2.570119	0.535220
C	−0.353300	2.027083	1.056758
C	−0.835737	2.480443	2.291806
C	−0.182357	3.457738	3.063708
C	0.978617	3.978265	2.539634
C	1.474716	3.541502	1.313729
H	3.317506	0.063812	−2.669023
H	3.357822	1.952533	−4.266307
H	−1.766569	2.086356	2.676764
H	−0.582800	3.790871	4.014861
P	1.987645	−0.463047	−0.098228
P	−1.279198	0.735270	0.072739
Rh	−0.115110	−1.345629	−0.344359
C	−3.238396	−2.537645	−1.100279
C	−4.030698	−2.342580	−2.239127
C	−1.818645	−2.596531	−1.227095
C	−3.450900	−2.244335	−3.505816

H	−5.113221	−2.322737	−2.150087
C	−1.270912	−2.598594	−2.526306
H	0.699869	−2.727179	−0.533346
C	−2.073120	−2.400536	−3.657632
H	−4.084081	−2.102301	−4.377887
H	−0.211189	−2.785434	−2.660028
H	−1.625000	−2.391896	−4.647819
O	2.073126	4.370702	−3.640424
O	1.005922	4.559282	−1.595684
O	2.655327	4.200872	1.047357
O	1.815814	4.926877	3.069633
C	1.190224	5.190804	−2.867271
H	1.643327	6.175441	−2.721418
H	0.222562	5.271854	−3.378882
C	2.708338	5.264159	2.002778
H	2.373762	6.198044	1.527820
H	3.723174	5.352670	2.392364
C	3.352668	−1.564095	−0.735561
C	3.125889	−2.291822	−1.917505
C	4.590969	−1.705107	−0.099896
C	4.115219	−3.103167	−2.490526
H	2.152536	−2.214963	−2.393405
C	5.599375	−2.540933	−0.618843
H	4.782216	−1.161642	0.819192
C	5.348311	−3.214059	−1.821689
H	6.129645	−3.841282	−2.248975
C	2.668564	0.085363	1.534420
C	3.744533	0.982431	1.633310
C	2.121179	−0.446146	2.705356
C	4.283075	1.343013	2.877418
H	4.161063	1.408885	0.724308
C	2.631948	−0.113883	3.973824
H	1.278426	−1.125661	2.612026
C	3.711637	0.779854	4.034162
H	4.116940	1.049031	5.008479
C	−2.838898	0.566425	1.063626
C	−4.068851	1.106692	0.673871
C	−2.766615	−0.122502	2.287647
C	−5.212212	0.996377	1.487433
H	−4.141029	1.625972	−0.276694
C	−3.866675	−0.208327	3.152185
H	−1.820949	−0.577748	2.573326
C	−5.083061	0.356543	2.728521
H	−5.952810	0.287685	3.379692
C	−1.811213	1.766753	−1.379042
C	−2.179635	3.114743	−1.230897
C	−1.816651	1.202289	−2.659126
C	−2.556137	3.899074	−2.330764
H	−2.161245	3.559314	−0.239498
C	−2.184530	1.955106	−3.791528
H	−1.517391	0.163949	−2.769783
C	−2.548007	3.297108	−3.603370
H	−2.827693	3.892129	−4.472096
Si	1.898347	−0.853617	5.542175
H	2.392727	−0.082674	6.714738
H	0.412741	−0.792324	5.504520
H	2.294014	−2.278396	5.714298
Si	5.721412	2.549661	2.984312
H	5.297115	3.872530	3.523942
H	6.782147	2.026360	3.887644
H	6.289117	2.758854	1.626718
Si	3.807767	−4.006360	−4.113639
H	2.487029	−3.600906	−4.660001
H	4.866671	−3.661248	−5.103291
H	3.831477	−5.483625	−3.934395
Si	7.235832	−2.752150	0.286267
H	7.660811	−1.459585	0.889520
H	7.137461	−3.756064	1.381918
H	8.274252	−3.212601	−0.674635
Si	−3.707103	−0.987978	4.858245
H	−4.983715	−1.638925	5.254756
H	−2.599573	−1.976576	4.876725
H	−3.403424	0.056190	5.879579
Si	−6.868153	1.688150	0.925711
H	−7.494571	0.837517	−0.125040
H	−7.792650	1.749102	2.089861
H	−6.704911	3.054966	0.358609
Si	−3.026765	5.705233	−2.100146
H	−2.038359	6.608202	−2.757459
H	−4.357604	5.996797	−2.699617
H	−3.060939	6.020444	−0.648228
Si	−2.190375	1.205936	−5.519065

H	−3.404427	0.381451	−5.768886
H	−2.176029	2.314255	−6.513184
H	−0.996452	0.345957	−5.731250

TS17

C	3.569659	1.428209	0.860506
C	2.264760	−0.673838	1.529259
C	2.560033	0.698415	1.729281
H	3.459679	1.127618	−0.188013
H	3.401144	2.512897	0.895642
H	2.737198	−1.197056	0.699844
H	2.032825	−1.293452	2.391691
H	2.517176	1.053472	2.758109
Si	5.387326	1.117130	1.368557
C	5.628184	1.478972	3.209985
H	6.680981	1.367338	3.491023
H	5.319020	2.501346	3.460104
H	5.040862	0.792316	3.831259
C	6.576960	2.044567	0.239203
C	6.756371	3.410128	0.004074
C	7.383260	1.106863	−0.456951
C	7.719701	3.856279	−0.906866
H	6.145663	4.141545	0.529893
C	8.345054	1.559303	−1.368355
C	8.509461	2.928063	−1.589201
H	7.854519	4.920402	−1.082519
H	8.970043	0.854294	−1.909910
H	9.258790	3.270874	−2.298289
C	−2.702258	−0.033296	−1.667675
C	−1.935898	1.168381	−1.537333
C	−1.583653	1.891616	−2.685192
C	−1.950442	1.499971	−3.984369
C	−2.692972	0.345810	−4.090182
C	−3.053984	−0.387506	−2.962904
C	−3.241997	−0.876234	−0.555586
C	−2.489491	−1.706873	0.333504
C	−3.161074	−2.502127	1.272065
C	−4.561530	−2.536790	1.390990
C	−5.269929	−1.741976	0.518955
C	−4.621385	−0.942543	−0.419089
H	−1.004079	2.800158	−2.581035
H	−1.666442	2.080113	−4.855424
H	−2.588344	−3.137127	1.935353
H	−5.054906	−3.164330	2.124969
P	−1.238884	1.686872	0.109900
P	−0.626088	−1.678322	0.291690
Rh	0.435002	0.314154	0.872889
C	7.116441	−0.321840	−0.132506
C	7.797105	−1.411391	−0.689215
C	6.090020	−0.544795	0.823150
C	7.468714	−2.712223	−0.303162
H	8.584298	−1.256266	−1.422141
C	5.780650	−1.854510	1.200887
H	1.200707	1.650732	1.435813
C	6.464550	−2.938552	0.640766
H	8.001664	−3.552710	−0.740612
H	4.999878	−2.040291	1.934633
H	6.216020	−3.953659	0.939344
O	−3.172071	−0.266626	−5.220323
O	−3.772450	−1.495411	−3.356499
O	−5.565343	−0.234011	−1.132828
O	−6.627816	−1.573302	0.416260
C	−4.036540	−1.305031	−4.750294
H	−5.083884	−0.998187	−4.885182
H	−3.821732	−2.230015	−5.289377
C	−6.815482	−0.845126	−0.800821
H	−7.105569	−1.541036	−1.601896
H	−7.569236	−0.071529	−0.649078
C	−2.735971	1.924585	1.178300
C	−2.576690	1.761531	2.559519
C	−3.997622	2.286097	0.680973
C	−3.640959	1.973268	3.454416
H	−1.598163	1.453196	2.924399
C	−5.088975	2.499696	1.538059
H	−4.130758	2.392039	−0.392815
C	−4.885343	2.344095	2.921584
H	−5.719559	2.511167	3.601348
C	−0.734760	3.452527	−0.228599
C	0.594508	3.698364	−0.600473
C	−1.616778	4.539350	−0.153583
C	1.051666	4.990248	−0.911948
H	1.275609	2.851584	−0.646429

C	−1.198573	5.851230	−0.436319
H	−2.648976	4.365521	0.134120
C	0.136191	6.052316	−0.824741
H	0.470542	7.059185	−1.069438
C	−0.261222	−2.386465	−1.382261
C	0.903763	−1.968791	−2.038623
C	−1.096322	−3.319553	−2.014776
C	1.262041	−2.477761	−3.299365
H	1.522903	−1.218568	−1.551283
C	−0.784695	−3.841463	−3.280736
H	−2.009364	−3.633601	−1.515885
C	0.401654	−3.410326	−3.900856
H	0.657522	−3.805471	−4.883385
C	−0.196991	−3.081943	1.436630
C	0.105822	−4.380498	1.010414
C	−0.146016	−2.801383	2.812655
C	0.452646	−5.394465	1.923084
H	0.077761	−4.609172	−0.050865
C	0.167289	−3.788470	3.759780
H	−0.349902	−1.781894	3.136094
C	0.468174	−5.080053	3.290601
H	0.726638	−5.856152	4.008970
Si	0.902736	−7.120641	1.322617
H	0.737864	−8.088902	2.440241
H	0.022088	−7.519257	0.191085
H	2.313198	−7.192434	0.849329
Si	0.177338	−3.397840	5.601366
H	−1.191277	−3.461818	6.185845
H	1.029701	−4.389827	6.310826
H	0.711430	−2.029132	5.833386
Si	2.850995	−1.930960	−4.149176
H	2.672881	−1.998834	−5.625493
H	3.184446	−0.538097	−3.751240
H	3.997423	−2.808941	−3.785858
Si	−1.946506	−5.052481	−4.127417
H	−2.701725	−4.406835	−5.239622
H	−1.189101	−6.191415	−4.714494
H	−2.929394	−5.569777	−3.139403
Si	−6.774511	2.967605	0.850393
H	−7.732749	1.826475	0.895985
H	−7.375837	4.075745	1.641855
H	−6.633147	3.396807	−0.566142
Si	−3.401875	1.768757	5.309718
H	−4.728684	1.839713	5.979704
H	−2.768645	0.458301	5.621450
H	−2.530906	2.837925	5.871712
Si	2.839755	5.298083	−1.411948
H	3.307161	4.258264	−2.365970
H	2.938768	6.637387	−2.053218
H	3.748223	5.283258	−0.231700
Si	−2.392101	7.297762	−0.283271
H	−2.414905	7.856261	1.097468
H	−1.981092	8.385512	−1.212082
H	−3.772268	6.855749	−0.621167

TS18

C	4.011837	2.590578	−0.079790
C	2.233985	0.718606	−0.274486
C	2.592339	2.088063	0.298283
H	4.104298	2.616933	−1.173366
H	4.120027	3.634484	0.254805
H	2.578733	0.624150	−1.308677
H	2.658890	−0.094023	0.321007
H	2.481277	2.083802	1.391966
Si	5.504599	1.653328	0.637146
C	5.243006	1.312607	2.482631
H	6.143484	0.877784	2.929738
H	5.006470	2.235451	3.026900
H	4.415917	0.609698	2.638364
C	7.112195	2.570640	0.273553
C	7.535599	3.857934	0.612840
C	7.970024	1.735759	−0.487546
C	8.791946	4.324738	0.212985
H	6.887587	4.512358	1.193435
C	9.226102	2.207998	−0.887241
C	9.631608	3.496934	−0.535838
H	9.114010	5.327535	0.481750
H	9.893766	1.581440	−1.472629
H	10.608081	3.856926	−0.850255
C	−3.000951	−1.246694	−1.118092
C	−2.945516	0.125860	−1.519808
C	−3.174372	0.475518	−2.856242

C	−3.484270	−0.472428	−3.846974
C	−3.539219	−1.788050	−3.444522
C	−3.309899	−2.154822	−2.119212
C	−2.871514	−1.758613	0.281473
C	−1.680799	−1.831080	1.072791
C	−1.735771	−2.384246	2.360823
C	−2.914899	−2.896633	2.928495
C	−4.045497	−2.841431	2.145026
C	−4.012673	−2.284773	0.867949
H	−3.085767	1.512751	−3.155770
H	−3.659521	−0.181165	−4.876456
H	−0.831385	−2.446114	2.951523
H	−2.927925	−3.320789	3.926265
P	−2.250740	1.394612	−0.376612
P	−0.047841	−1.254141	0.394832
Rh	0.143625	0.875941	−0.278142
C	7.424710	0.385112	−0.795363
C	8.105815	−0.609184	−1.508733
C	6.118435	0.130498	−0.299652
C	7.504782	−1.849406	−1.728913
H	9.105458	−0.426490	−1.893882
C	5.536949	−1.119765	−0.528160
H	1.878967	2.844038	−0.081046
C	6.222934	−2.109831	−1.239457
H	8.040741	−2.615396	−2.283855
H	4.537437	−1.332401	−0.156531
H	5.759895	−3.078294	−1.411553
Cl	0.476512	1.970414	−2.871169
H	0.133955	0.587965	−1.833598
O	−5.317790	−3.250296	2.442238
O	−5.282569	−2.309019	0.336442
O	−3.469187	−3.515312	−1.990535
O	−3.842822	−2.899775	−4.187563
C	−6.034215	−3.162178	1.204132
H	−6.112813	−4.163128	0.756537
H	−7.016261	−2.723469	1.384385
C	−3.587671	−4.014274	−3.328372
H	−4.425078	−4.714465	−3.381211
H	−2.645751	−4.496912	−3.621907
C	1.133466	−1.670675	1.765005
C	1.211072	−0.788633	2.854808
C	1.990791	−2.777162	1.734341
C	2.098914	−1.006119	3.919367
H	0.567456	0.089509	2.862100
C	2.912942	−3.020787	2.768748
H	1.953870	−3.452504	0.885133
C	2.947906	−2.125668	3.849057
H	3.666076	−2.291926	4.650418
C	0.297773	−2.534111	−0.901168
C	−0.168195	−3.850585	−0.752987
C	1.044652	−2.204507	−2.039437
C	0.104260	−4.836162	−1.714755
H	−0.754821	−4.109084	0.123965
C	1.342664	−3.162455	−3.024821
H	1.391374	−1.183097	−2.158487
C	0.868499	−4.470283	−2.837753
H	1.103658	−5.226339	−3.586044
C	−3.307540	1.362488	1.146179
C	−4.664743	1.008078	1.141851
C	−2.732559	1.808535	2.341758
C	−5.451069	1.108589	2.299840
H	−5.111168	0.639303	0.222013
C	−3.482537	1.925320	3.525496
H	−1.677403	2.079218	2.341587
C	−4.841685	1.578900	3.477488
H	−5.442505	1.680481	4.379837
C	−2.774586	3.028321	−1.079552
C	−4.118952	3.334049	−1.348357
C	−1.805914	4.018230	−1.277012
C	−4.505475	4.600900	−1.808524
H	−4.878194	2.572836	−1.192568
C	−2.150196	5.304311	−1.732581
H	−0.764931	3.774170	−1.091453
C	−3.502631	5.573230	−1.984542
H	−3.787332	6.568900	−2.322681
Si	−6.310599	4.981782	−2.177958
H	−6.704180	6.289075	−1.585098
H	−6.570600	5.052236	−3.642755
H	−7.161832	3.906009	−1.601727
Si	−0.824717	6.610718	−2.025495
H	−0.254286	6.524962	−3.396187
H	−1.431088	7.960778	−1.859979

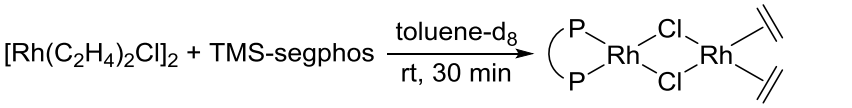
H	0.277864	6.443913	−1.041789
Si	−7.270279	0.630731	2.272316
H	−7.496780	−0.728675	2.839637
H	−8.069309	1.590533	3.080605
H	−7.762937	0.630734	0.869419
Si	−2.687753	2.514402	5.127018
H	−1.820539	3.696873	4.876701
H	−3.755572	2.877319	6.096348
H	−1.841445	1.450691	5.736339
Si	2.149160	0.161440	5.398557
H	1.170164	−0.252069	6.441722
H	3.507152	0.142776	6.002068
H	1.805872	1.540302	4.961242
Si	4.063705	−4.512440	2.702684
H	4.251864	−4.929052	1.288294
H	5.375882	−4.166651	3.309081
H	3.495179	−5.665268	3.455871
Si	−0.564939	−6.582140	−1.507453
H	−1.713345	−6.835360	−2.423878
H	0.484612	−7.590537	−1.816162
H	−1.035797	−6.764685	−0.109159
Si	2.327843	−2.694267	−4.565563
H	2.997172	−3.918742	−5.085299
H	1.439072	−2.163583	−5.633886
H	3.346716	−1.669162	−4.230504

TS19

C	4.209223	−1.006555	−1.232898
C	2.535524	−0.322055	0.576056
C	2.734904	−1.064433	−0.753009
H	4.265881	−1.493457	−2.218881
H	4.511791	0.036737	−1.400863
H	3.045490	−0.858949	1.378811
H	2.943060	0.688213	0.504931
H	2.097389	−0.634294	−1.535884
Si	5.539942	−1.848344	−0.154600
C	4.906089	−3.489190	0.534410
H	5.667041	−3.971136	1.157923
H	4.001083	−3.351677	1.138248
H	4.653646	−4.179615	−0.280302
C	6.380322	−0.738566	1.128238
C	5.903768	−0.137418	2.296704
C	7.740306	−0.550828	0.763202
C	6.744079	0.646582	3.094722
H	4.869473	−0.278397	2.601466
C	8.576568	0.236371	1.564525
C	8.077476	0.832807	2.723393
H	6.361527	1.104240	4.003446
H	9.618422	0.387296	1.294688
H	8.733830	1.441173	3.340738
C	−3.239533	0.799947	−1.018498
C	−3.316438	−0.069719	0.116466
C	−4.413211	0.020232	0.983651
C	−5.472921	0.923797	0.789852
C	−5.393749	1.734144	−0.320153
C	−4.306875	1.667001	−1.189852
C	−2.153809	0.808786	−2.043741
C	−0.794150	1.191265	−1.825241
C	0.133125	1.106613	−2.875809
C	−0.221117	0.719191	−4.177928
C	−1.547866	0.408665	−4.385077
C	−2.474825	0.448634	−3.345793
H	−4.464472	−0.636858	1.842224
H	−6.309520	0.974375	1.477739
H	1.172096	1.350771	−2.686895
H	0.510598	0.666261	−4.976192
P	−1.960807	−1.289680	0.478851
P	−0.144023	1.536816	−0.132203
Rh	0.353319	−0.492888	0.769905
C	8.165731	−1.242970	−0.484020
C	9.452236	−1.193410	−1.034963
C	7.151853	−1.998436	−1.125985
C	9.734470	−1.887253	−2.213170
H	10.239556	−0.618259	−0.554895
C	7.454137	−2.684004	−2.305158
H	2.426498	−2.107051	−0.635072
C	8.740745	−2.633085	−2.851457
H	10.735794	−1.844803	−2.634603
H	6.686745	−3.267850	−2.810817
H	8.967767	−3.171518	−3.768119
Cl	0.873169	−2.678657	1.735936
H	1.461055	0.149504	1.686572

O	−6.260936	2.710003	−0.735285
O	−4.453801	2.622418	−2.169504
O	−3.701060	0.044279	−3.818778
O	−2.157317	−0.004210	−5.538796
C	−5.798472	3.094439	−2.034693
H	−6.430410	2.623429	−2.801125
H	−5.811278	4.182356	−2.117013
C	−3.557908	−0.027550	−5.242902
H	−4.043110	0.845167	−5.702069
H	−3.991588	−0.961665	−5.604078
C	−2.580344	−2.188233	1.968661
C	−3.556770	−3.189385	1.886296
C	−2.058269	−1.847170	3.223582
C	−4.032291	−3.842206	3.036280
H	−3.954254	−3.464754	0.913276
C	−2.510573	−2.470171	4.397318
H	−1.269154	−1.102479	3.271727
C	−3.503563	−3.456702	4.279715
H	−3.874649	−3.941446	5.181967
C	−2.141213	−2.534344	−0.883352
C	−3.313828	−2.638024	−1.646951
C	−1.089228	−3.429802	−1.125158
C	−3.452422	−3.617635	−2.643574
H	−4.130009	−1.945824	−1.463717
C	−1.193833	−4.426870	−2.111004
H	−0.193312	−3.356040	−0.513630
C	−2.380839	−4.502312	−2.856614
H	−2.473983	−5.273120	−3.620221
C	−1.377232	2.620888	0.730733
C	−1.656183	2.392459	2.080533
C	−1.929990	3.746437	0.100480
C	−2.480762	3.264550	2.816812
H	−1.212393	1.520148	2.556136
C	−2.764721	4.633566	0.792843
H	−1.704757	3.933045	−0.946595
C	−3.019714	4.376536	2.154106
H	−3.650414	5.066287	2.712530
C	1.175809	2.834152	−0.340324
C	2.039509	3.053612	0.746165
C	1.258526	3.698032	−1.440118
C	2.987509	4.087589	0.743012
H	1.959485	2.410266	1.618358
C	2.204898	4.737824	−1.492210
H	0.572838	3.567772	−2.271617
C	3.058737	4.912405	−0.393182
H	3.791651	5.717532	−0.418654
Si	2.324647	5.854044	−3.004458
H	2.977230	7.134643	−2.623404
H	3.125340	5.223522	−4.090236
H	0.963971	6.127886	−3.541122
Si	4.119625	4.368901	2.225031
H	5.544280	4.390267	1.801777
H	3.816010	5.675173	2.873082
H	3.901807	3.281123	3.212567
Si	−2.855603	2.947633	4.635375
H	−3.582587	4.124651	5.182246
H	−3.707562	1.739602	4.809882
H	−1.601380	2.741199	5.407263
Si	−3.520528	6.115550	−0.083600
H	−4.937828	5.865427	−0.471070
H	−3.502527	7.311951	0.799975
H	−2.750433	6.398902	−1.323836
Si	−1.764690	−2.032116	6.069980
H	−2.829951	−2.048240	7.111095
H	−0.712658	−3.001242	6.477598
H	−1.163735	−0.673707	6.006717
Si	−5.320871	−5.207547	2.908361
H	−4.698684	−6.559081	2.857753
H	−6.224719	−5.162350	4.090006
H	−6.123551	−5.019876	1.669116
Si	0.216702	−5.641226	−2.410307
H	0.413637	−6.548456	−1.248990
H	−0.118906	−6.461377	−3.606761
H	1.493680	−4.921160	−2.662614
Si	−5.027601	−3.726748	−3.662180
H	−4.862492	−3.112066	−5.011591
H	−5.419116	−5.146607	−3.872537
H	−6.125216	−3.006627	−2.963891

S8. Synthesis and Characterization of [Rh]−Cl



CAT4, quantitative conversion

In a N_2-flushed glovebox, $[Rh(C_2H_4)_2Cl]_2$ (7.8 mg, 0.02 mmol, 1.0 equiv), TMS-segphos (23.7 mg, 0.02 mmol, 1.0 equiv), and toluene-d_8 (2.0 mL) were added into a sealed tube. The reaction mixture was stirred at room temperature for 30 minutes. ^{1}H NMR (500 MHz, toluene-d_8, δ): 8.42−8.40 (m, 4H), 7.89 (s, 2H), 7.79 (s, 2H), 6.91−6.87 (m, 2H), 6.04 (d, J = 10.0 Hz, 2H), 5.24 (br s, 4H), 5.15 (d, J = 5.0 Hz, 4H), 2.59 (br s, 8H), 0.36 (s, 36H), 0.32 (br s, 36H). ^{31}P NMR (162 MHz, toluene-d_8, δ): 49.3 (d, J_{Rh-P} = 199 Hz).

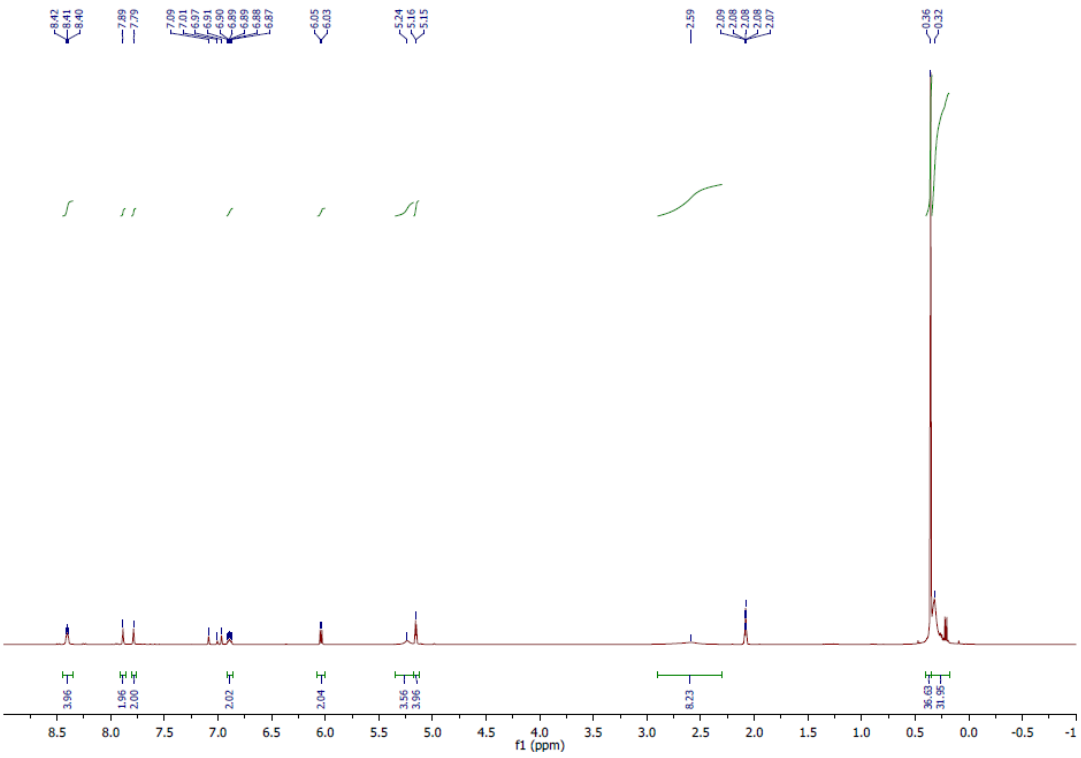


Figure S5. ^{1}H NMR (500 MHz, toluene-d_8) spectrum of **CAT4**.

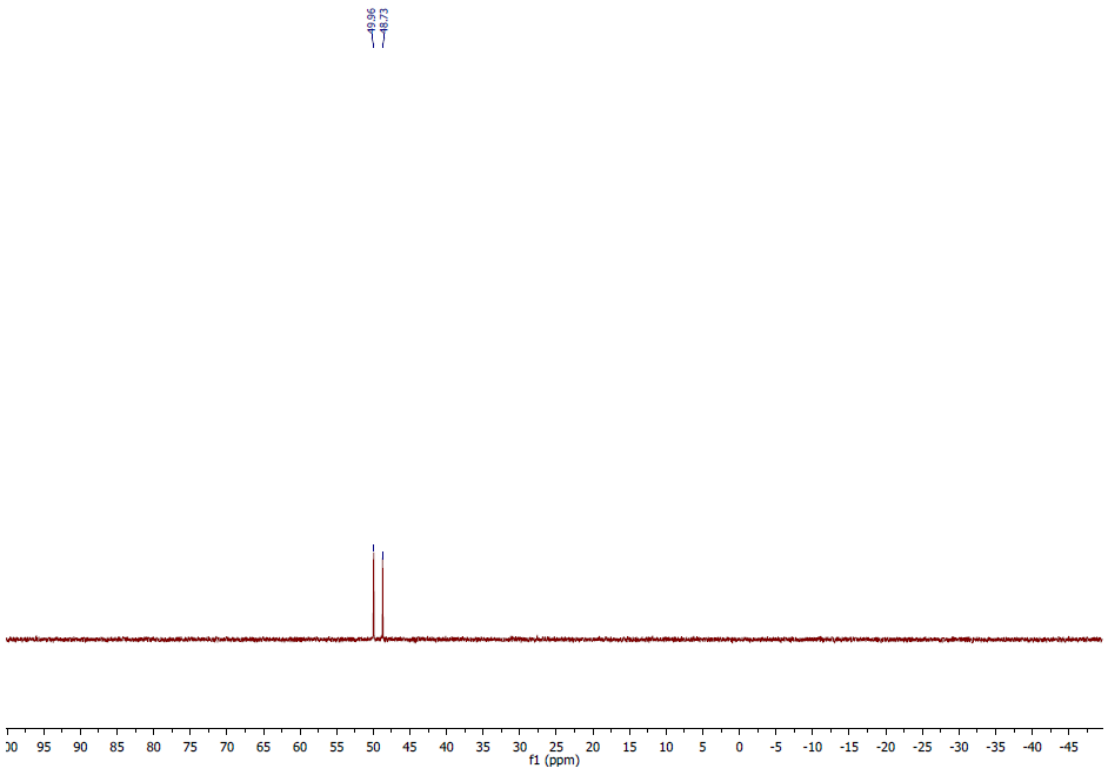


Figure S6. ^{31}P NMR (162 MHz, toluene-d_8) spectrum of **CAT4**.

The addition of 2 equivalents of TMS-segphos did not result in the formation of $[Rh(TMS\text{-}segphos)Cl]_2$ (Figure S7).[7]

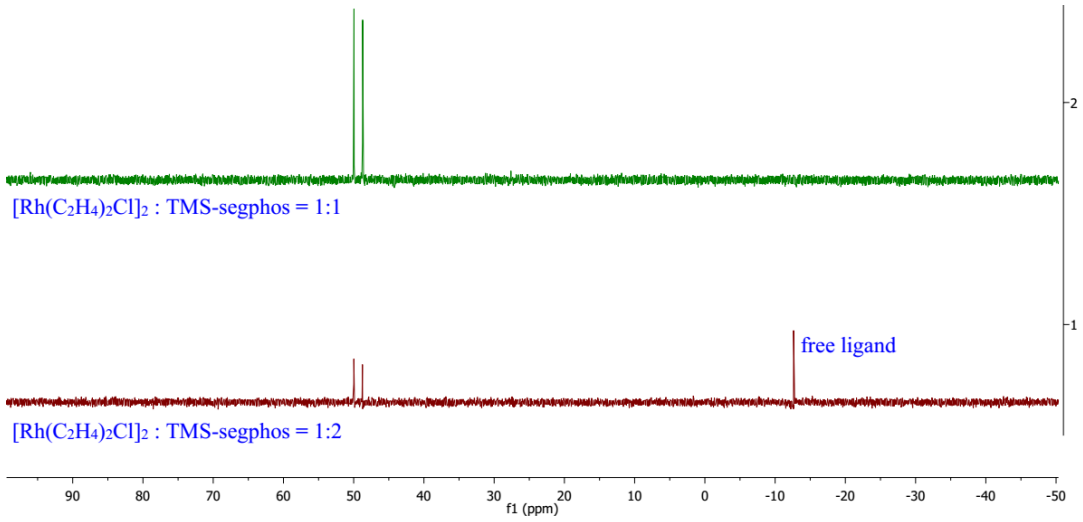
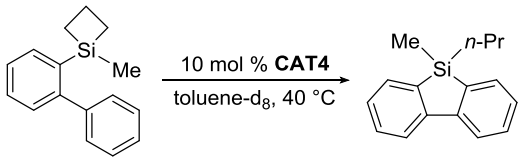


Figure S7. ^{31}P NMR (162 MHz) spectra of 1:1 and 1:2 mixture of $[Rh(C_2H_4)_2Cl]_2$ and TMS-segphos in toluene-d_8.

S9. Kinetic Study on [Rh]−Cl-Catalyzed C−H Silylation



1a **2a**

In a N_2-flushed glovebox, $[Rh(C_2H_4)_2Cl]_2$ (1.9 mg, 0.005 mmol, 10 mol %), TMS-segphos (5.9 mg, 0.005 mmol, 10 mol %), and toluene-d_8 (0.5 mL) were added into an NMR tube with J. Young valve. The reaction mixture was maintained at room temperature for 30 minutes. Then, SCB **1a** (11.9 mg, 0.05 mmol, 1.0 equiv) was added. Subsequently, the reaction was heated to 40 °C and monitored by ^{1}H NMR spectroscopy with 1,2-dimethoxyethane as the internal standard. As depicted in Figure S8, the C−H silylation reaction took place in two stages: an induction period (~1 h) and an active period with a more rapid consumption of substrate **1a**.

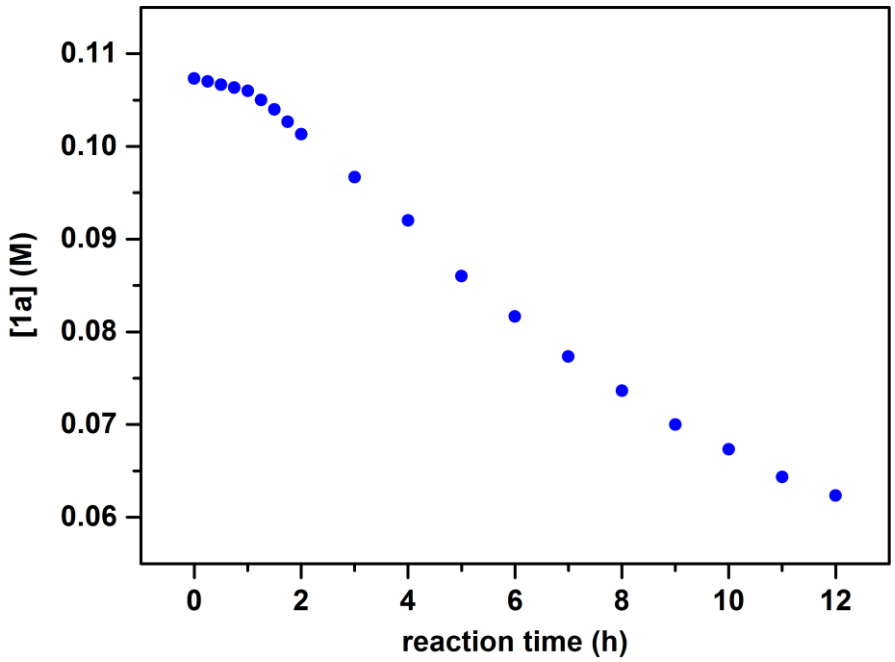
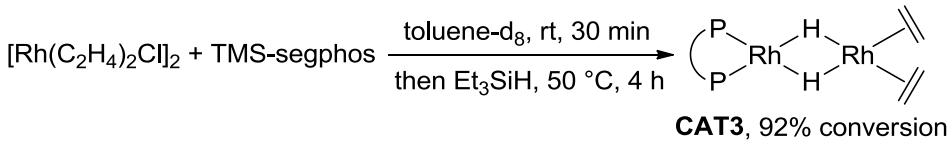


Figure S8. Kinetic profile with [Rh]−Cl as the catalyst.

S10. Synthesis and Characterization of [Rh]−H



CAT3, 92% conversion

In a N_2-flushed glovebox, $[Rh(C_2H_4)_2Cl]_2$ (7.8 mg, 0.02 mmol, 1.0 equiv), TMS-segphos (23.7 mg, 0.02 mmol, 1.0 equiv), and toluene-d_8 (2.0 mL) were added into a sealed tube. The reaction mixture was stirred at room temperature for 30 minutes. Then, Et_3SiH (32 µL, 0.2 mmol, 10 equiv) was added in one portion and the stirring continued for 4 hours at 50 °C. To our disappointment, we were unable to isolate the [Rh]−H complex **CAT3** in its pure form due to its high solubility. ^{1}H NMR (400 MHz, toluene-d_8, δ): 8.39−8.37 (m, 4H), 8.10 (br s, 4H), 7.86 (s, 2H), 7.67 (s, 2H), 7.46 (d, J = 8.0 Hz, 2H), 6.15 (d, J = 8.0 Hz, 2H), 5.15 (d, J = 8.0 Hz, 4H), 0.30 (s, 36H), 0.22 (s, 36H), (−7.22)−(−7.50) (m, J_{H-Rh} = 20.0 Hz, 2H; the coupling constant was determined by a selective ^{31}P-decoupled ^{1}H NMR spectrum). ^{31}P NMR (162 MHz, toluene-d_8, δ): 35.9−34.6 (m, J_{Rh-P} = 135 Hz). HRMS (ESI−IT−TOF, m/z): $[M+Na]^+$ calcd for $C_{66}H_{102}NaO_4P_2Rh_2Si_8^+$: 1473.3410, found: 1473.4149; $[M-Rh(C_2H_4)_2H_2]^+$ calcd for $C_{62}H_{92}O_4P_2RhSi_8^+$: 1289.3675, found: 1289.3659. HRMS (MALDI−TOF, m/z): $[M-Rh(C_2H_4)_2H_2]^+$ calcd for $C_{62}H_{92}O_4P_2RhSi_8^+$: 1289.3675, found: 1289.3619.

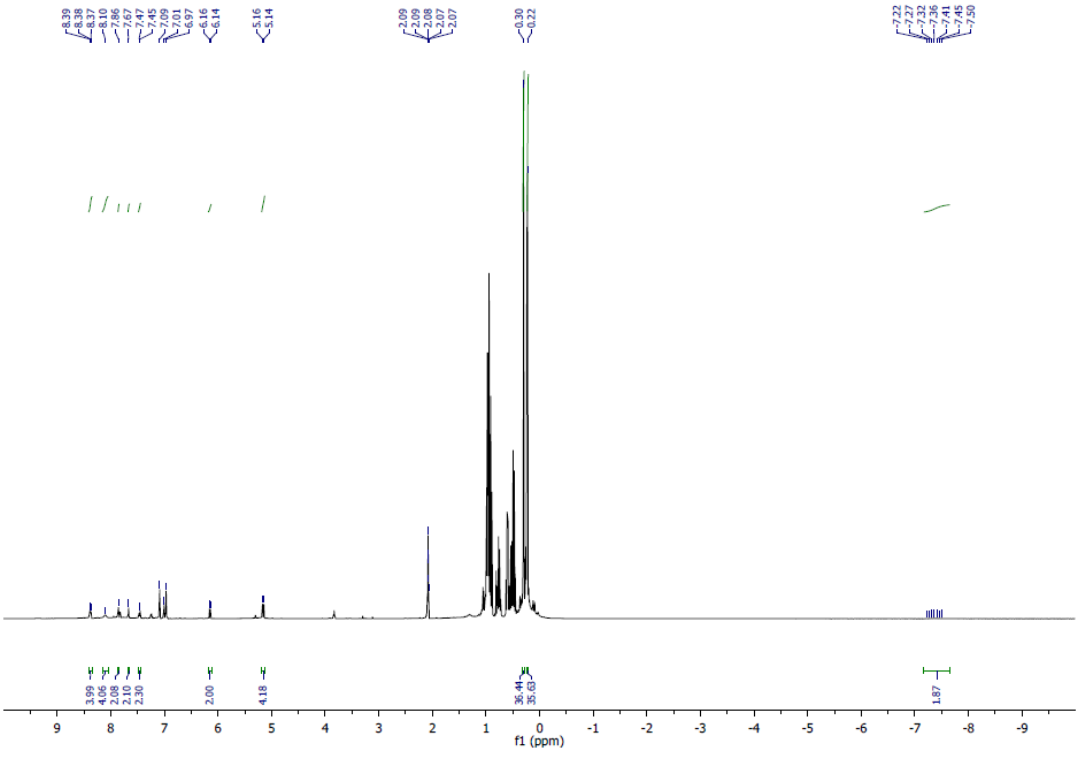


Figure S9. ^{1}H NMR (400 MHz, toluene-d_8) spectrum of **CAT3**.

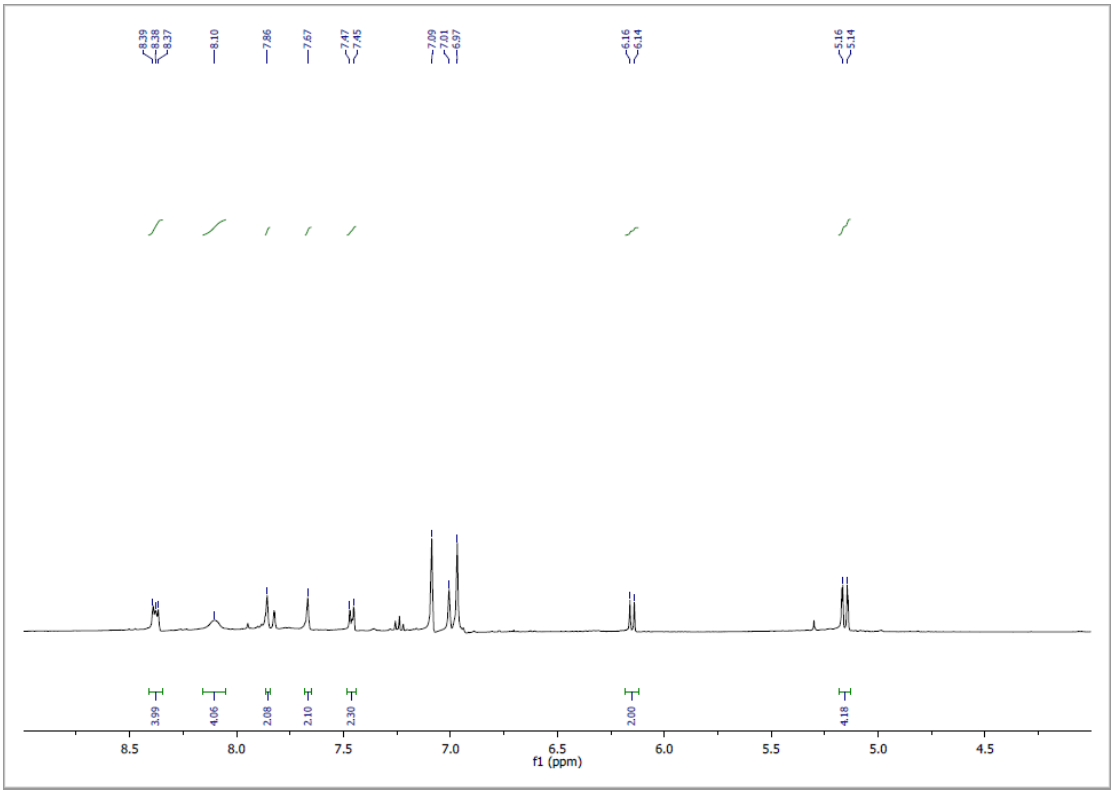


Figure S10. Zoom-in ^{1}H NMR (400 MHz, toluene-d_8) spectrum of **CAT3** (aryl region).

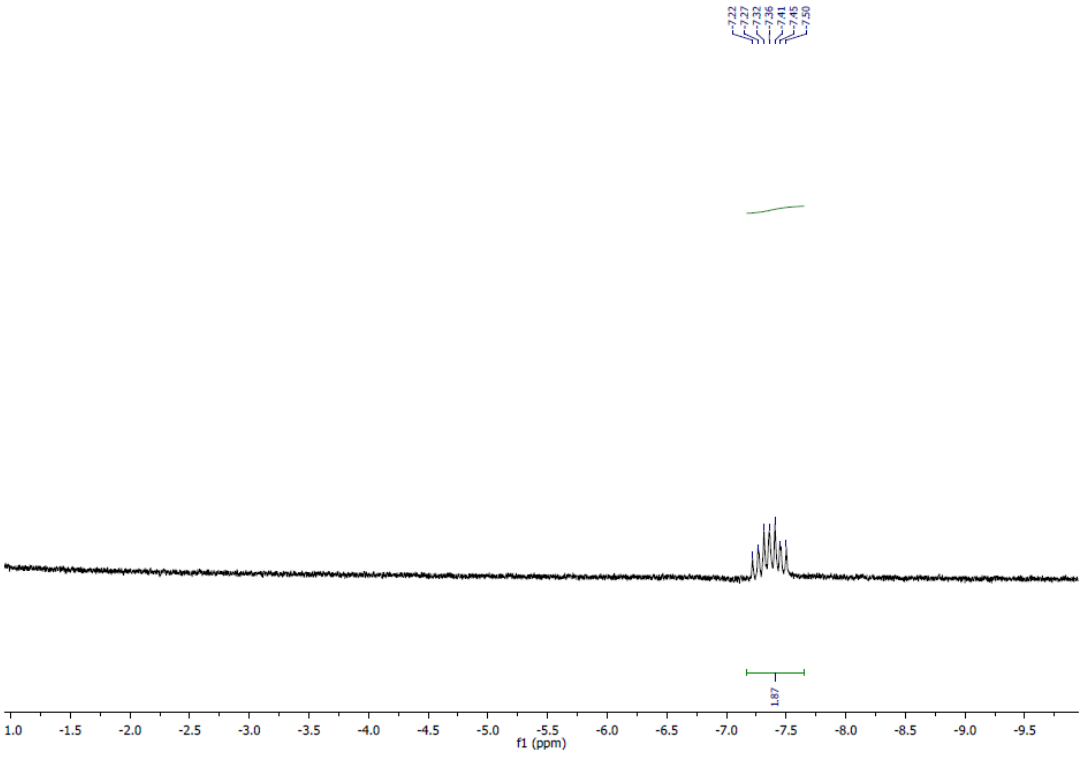


Figure S11. Zoom-in ^{1}H NMR (400 MHz, toluene-d_8) spectrum of **CAT3** (hydride region).

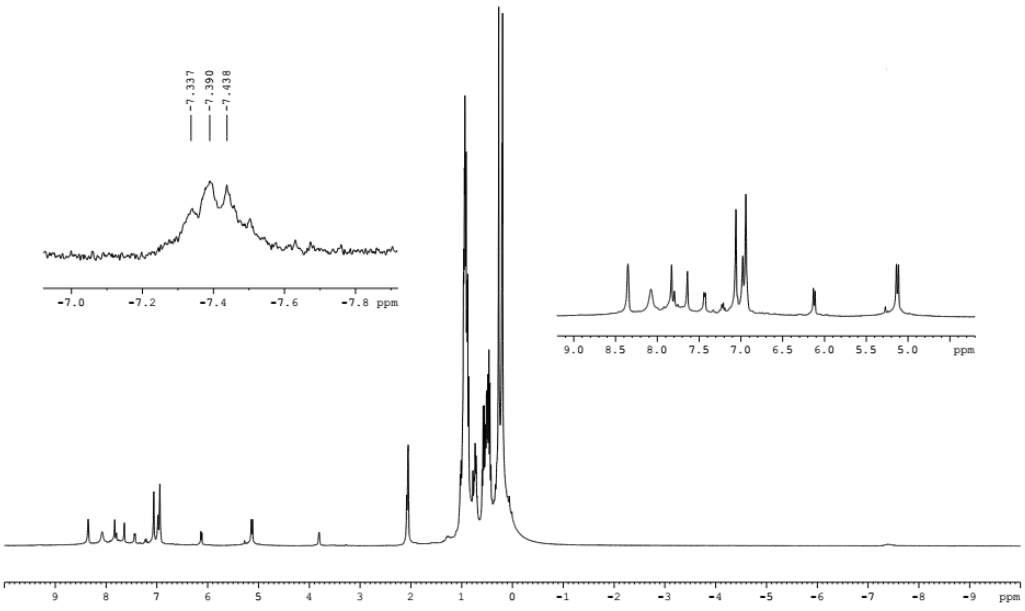


Figure S12. $^{1}H\{^{31}P\}$ NMR (400 MHz, toluene-d_8) spectrum of **CAT3**.

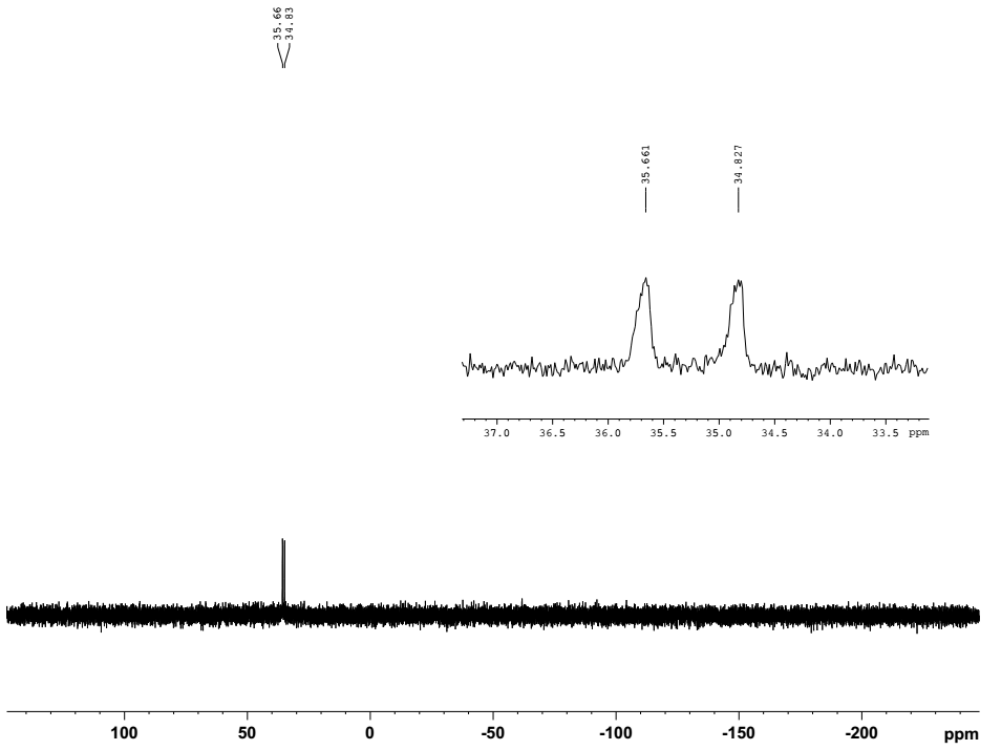


Figure S13. ^{31}P NMR (162 MHz, toluene-d_8) spectrum of **CAT3**.

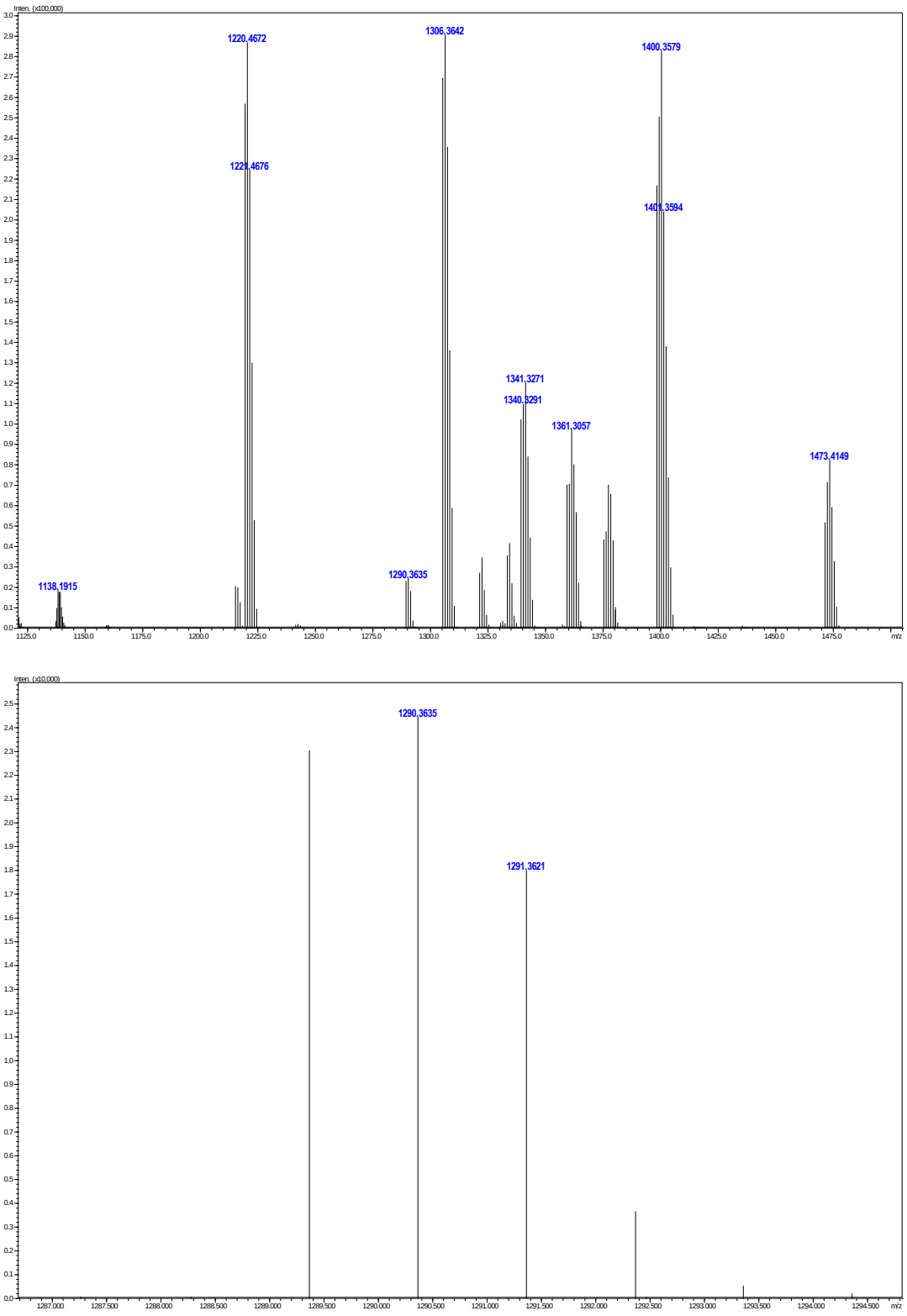
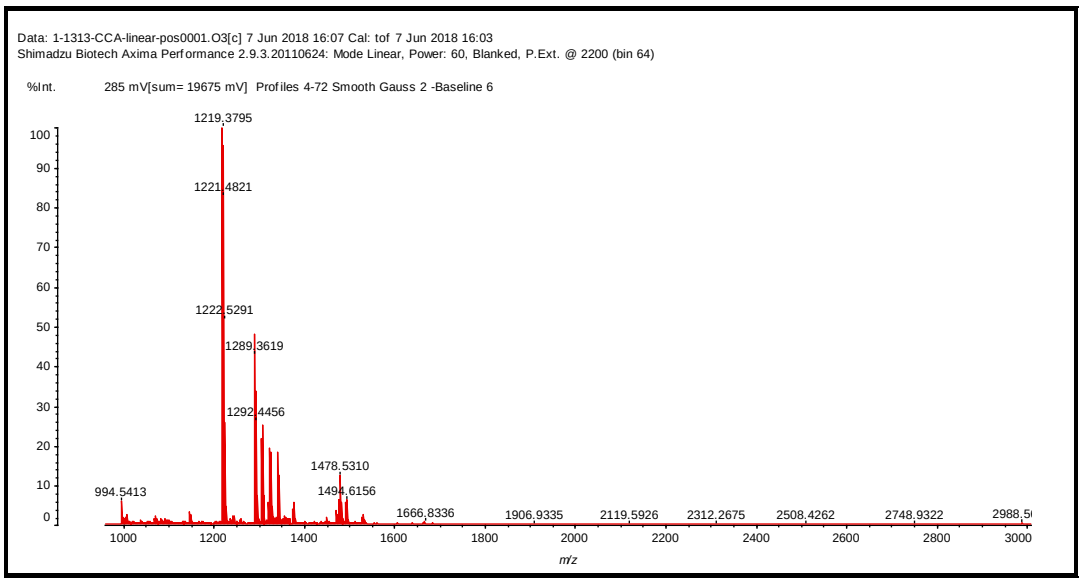


Figure S14. HRMS (ESI−IT−TOF) spectra of **CAT3**.



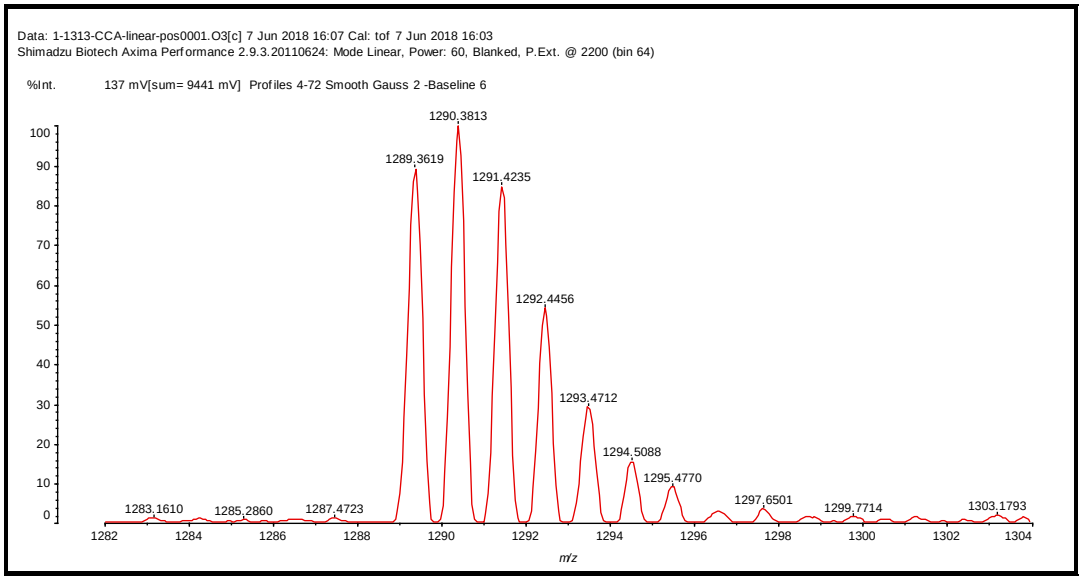
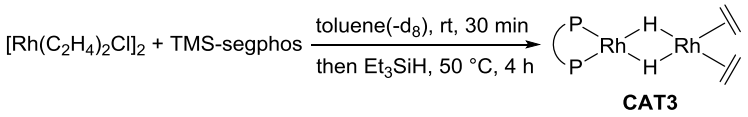


Figure S15. HRMS (MALDI−TOF) spectra of **CAT3**.

S11. Preparation of Stock Solutions



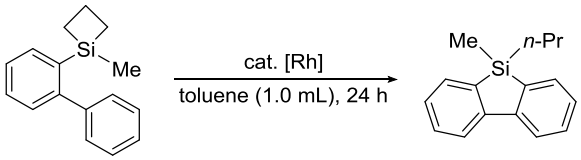
CAT3

Preparation of stock solution I (CAT3 in toluene). In a N_2-flushed glovebox, $[Rh(C_2H_4)_2Cl]_2$ (7.8 mg, 0.02 mmol, 1.0 equiv), TMS-segphos (23.7 mg, 0.02 mmol, 1.0 equiv), and toluene (2.0 mL) were added into a sealed tube. The reaction mixture was stirred at room temperature for 30 minutes. Then, Et_3SiH (32 µL, 0.2 mmol, 10 equiv) was added in one portion and the stirring continued for 4 hours at 50 °C. The stock solution was used directly without any further purification.

Preparation of stock solution II (CAT3 in toluene-d_8). In a N_2-flushed glove box, $[Rh(C_2H_4)_2Cl]_2$ (3.9 mg, 0.01 mmol, 1.0 equiv), TMS-segphos (11.9 mg, 0.01 mmol, 1.0 equiv), and toluene-d_8 (1.0 mL) were added into a sealed tube. The reaction mixture was stirred at room temperature for 30 minutes. Then, Et_3SiH (16 µL, 0.1 mmol, 10 equiv) was added in one portion and the stirring continued for 4 hours at 50 °C. The stock solution was used directly without any further purification.

S12. Evaluation of Catalytic Efficiency

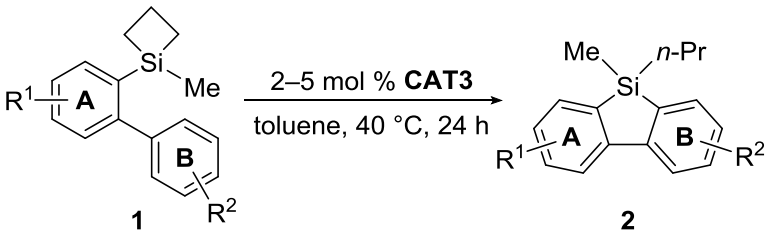
Table S4. Evaluation of Catalytic Efficiency

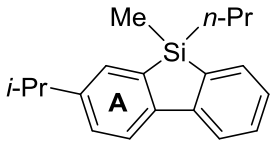


1a **2a**

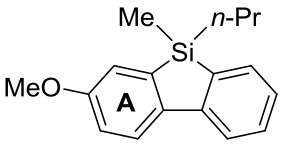
entry	reaction conditions	conversion
1	2 mol % **CAT3**, 40 °C	97%
2	10 mol % **CAT3**, 0 °C	26%
3	5 mol % $[Rh(C_2H_4)_2Cl]_2$, 1 equiv Et_3SiH, 40 °C	not detected
4	5 mol % $[Rh(C_2H_4)_2Cl]_2$, 10 mol % TMS-segphos, 40 °C	24%

For entry 1: in a N_2-flushed glovebox, substrate **1a** (23.8 mg, 0.1 mmol) and 0.2 mL of **stock solution I** were added into a sealed tube and the final volume of the solution was adjusted to 1.0 mL. The sealed tube was then removed from the glovebox and stirred at 40 °C for 24 hours. For entry 2: in a N_2-flushed glovebox, substrate **1a** (23.8 mg, 0.1 mmol) and 1.0 mL of **stock solution I** were added into a sealed tube, which was then removed from the glovebox and stirred at 0 °C for 24 hours. For entry 3: no TMS-segphos was added. For entry 4: no Et_3SiH was added.

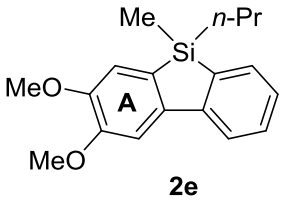




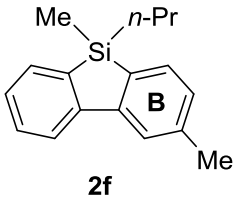
2c
82% yield
(5 mol %)



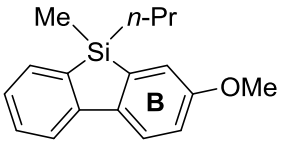
2d
96% yield
(5 mol %)



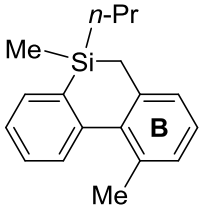
2e
95% yield
(5 mol %)



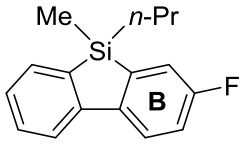
2f
96% yield
(2 mol %)



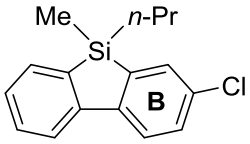
2g
97% yield
(2 mol %)



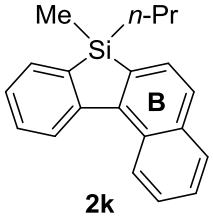
7h
94% yield
(2 mol %)



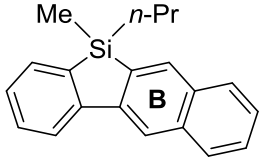
2i
97% yield
(2 mol %)



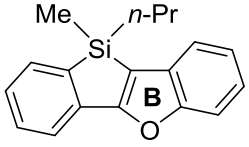
2j
92% yield
(2 mol %)



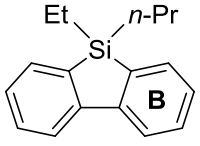
2k
91% yield
(2 mol %)



2l
95% yield
(2 mol %)



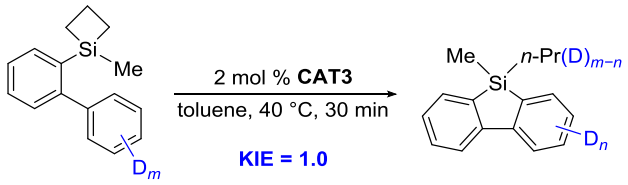
2m
93% yield
(2 mol %)



2n
90% yield
(2 mol %)

In a N_2-flushed glovebox, substrate **1** (0.1 mmol) and 0.2/0.5 mL of **stock solution I** were added into a sealed tube and the final volume of the solution was adjusted to 1.0 mL. The sealed tube was then removed from the glovebox and stirred at 40 °C for 24 hours. The reaction with an embedded ketone functionality (**1g** in ref 1) suffered competitive hydrosilylation due to the presence of excess Et_3SiH.

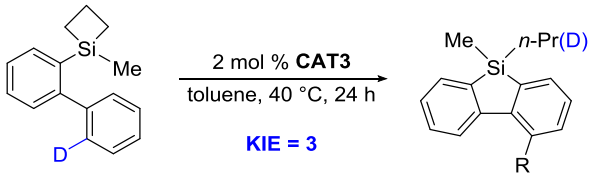
S13. Deuterium-Labeling Experiments



1a, *m* = 0
1a-d$_5$, *m* = 5

2a, *n* = 0, 12% conversion
2a-d$_5$, *n* = 4, 12% conversion

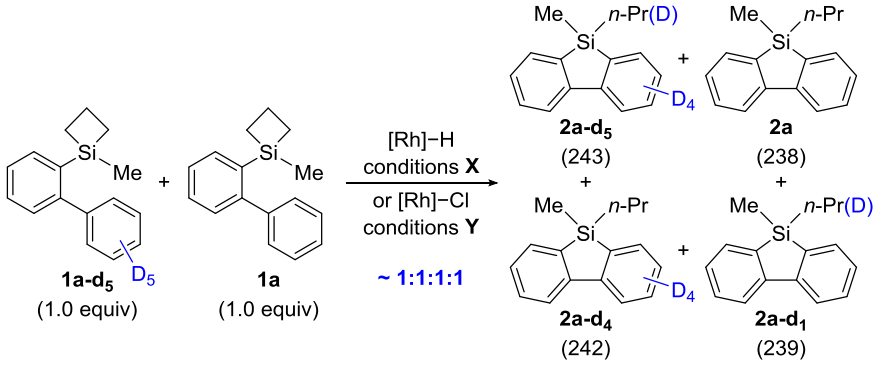
Parallel reactions. In a N_2-flushed glovebox, **1a**/**1a-d$_5$** (0.1 mmol each) and **stock solution I** (0.2 mL each) were added into two separate sealed tubes and the final volumes were adjusted to 1.0 mL. The sealed tubes were then removed from the glovebox and stirred at 40 °C for 30 minutes. Subsequently, the reactions were quenched and the conversions were determined by ^{1}H NMR analysis. The kinetic isotope effect (KIE) was determined to be 1.0, suggesting that the C−H bond activation step should not be rate-limiting.



1a-d$_1$

2a-d$_1$, R = D/H (3:1)

Intramolecular competition. In a N_2-flushed glovebox, substrate **1a-d$_1$** (0.1 mmol) and 0.2 mL of **stock solution I** were added into a sealed tube and the final volume of the solution was adjusted to 1.0 mL. The sealed tube was then removed from the glovebox and stirred at 40 °C for 24 hours. The KIE was determined to be 3 by ^{1}H NMR analysis.



1a-d$_5$ (1.0 equiv)
1a (1.0 equiv)

2a-d$_5$ (243)
2a (238)
2a-d$_4$ (242)
2a-d$_1$ (239)

Crossover experiments. Substrates **1a-d$_5$** and **1a** (0.1 mmol each) were added into two separate sealed tubes, the reactions were performed under conditions **X** and **Y**, respectively. Conditions **X**: **1a-d$_5$** (0.1 mmol, 1.0 equiv), **1a** (0.1 mmol, 1.0 equiv), 2 mol % **CAT3**, 40 °C. Conditions **Y**: **1a-d$_5$** (0.1 mmol, 1.0 equiv), **1a** (0.1 mmol, 1.0 equiv), 5 mol % $[Rh(cod)Cl]_2$, 10 mol % TMS-segphos, 80 °C. Both reactions were monitored by ^{1}H NMR spectroscopy and quenched at low conversions. Then, the products were isolated by preparative thin-layer chromatography and analyzed by EI−MS (Figure S16).

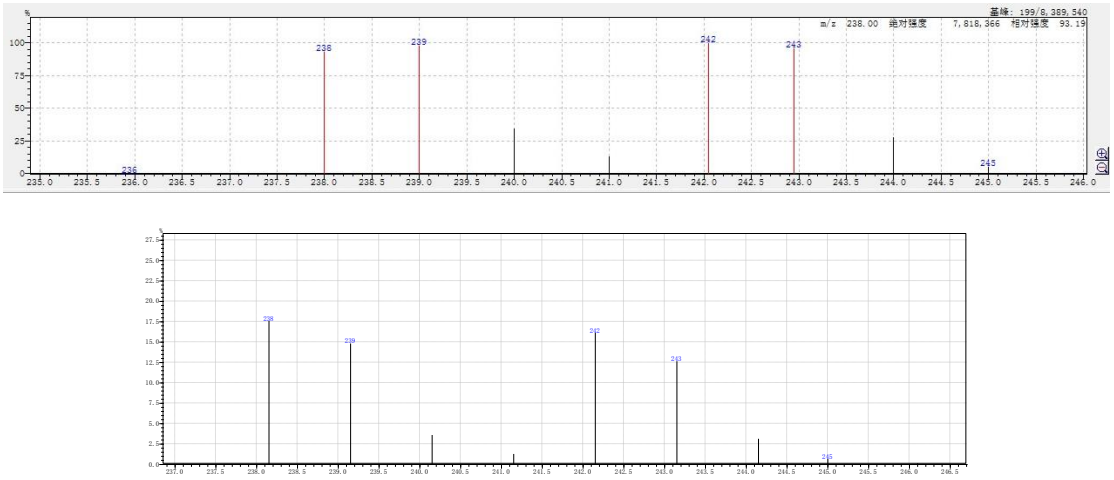
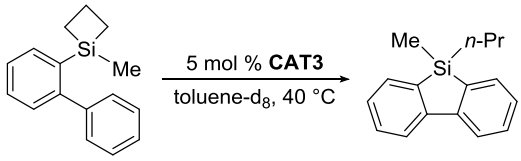


Figure S16. Molecular weight distribution of the products obtained under conditions **X** (up) and **Y** (down).

S14. Kinetic Study on [Rh]−H-Catalyzed C−H Silylation



1a **2a**

In a N_2-flushed glovebox, $[Rh(C_2H_4)_2Cl]_2$ (4.3 mg, 0.011 mmol), TMS-segphos (13.2 mg, 0.011 mmol), and toluene-d_8 (1.0 mL) were added into a sealed tube. The reaction mixture was stirred at room temperature for 30 minutes. Then, Et_3SiH (18 µL, 0.11 mmol) was added in one portion and the stirring continued for 4 hours at 50 °C. To an NMR tube with J. Young valve were added 0.45 mL of the [Rh]−H solution (0.005 mmol **CAT3**, 5 mol %) and substrate **1a** (23.8 mg, 0.1 mmol, 1.0 equiv). The reaction was then heated to 40 °C and monitored by ^1H NMR spectroscopy with 1,2-dimethoxyethane as the internal standard (the time interval between successive data points was set to 2 minutes). As shown in Figure S17, there was no induction period.

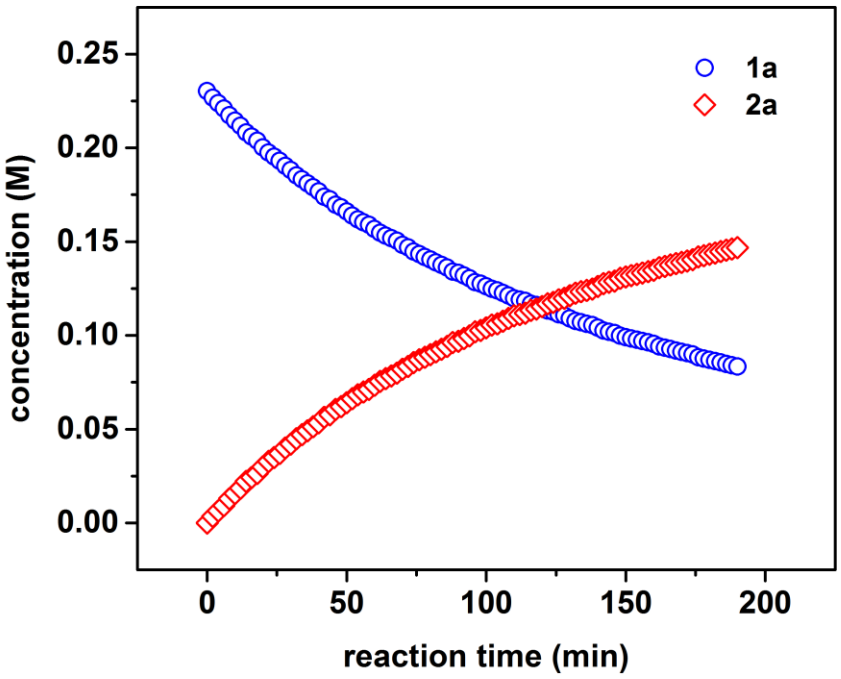


Figure S17. Kinetic profile with [Rh]−H as the catalyst.

Determination of the reaction order in substrate 1a. In a N_2-flushed glove box, substrate **1a** (0.05 - 0.1 mmol each) and 0.25 mL of **stock solution II** were added into separate NMR tubes with J. Young valve and the final volumes were adjusted to 0.4 mL. The reaction was then heated to 40 °C and the rates of starting material consumption were determined by the method of initial rates (Table S5; up to 10% conversion; monitored by ^{1}H NMR spectroscopy with 1,2-dimethoxyethane as the internal standard; the time interval between successive data points was set to 2 minutes). As depicted in Figure S18, a linear correlation was found between ln(rate) and ln[**1a**] and the slope was determined to be 0.93, indicating that the reaction order in substrate **1a** is 1.

Table S5. Rate versus [1a]

Concentration of Substrate 1a/M	**Reaction Rate**/M·min^{-1}	**ln(1a)**	**ln(rate)**
0.1363	0.000588	-1.993	-7.439
0.1611	0.000748	-1.826	-7.198
0.1932	0.000855	-1.644	-7.064
0.2470	0.00104	-1.398	-6.868

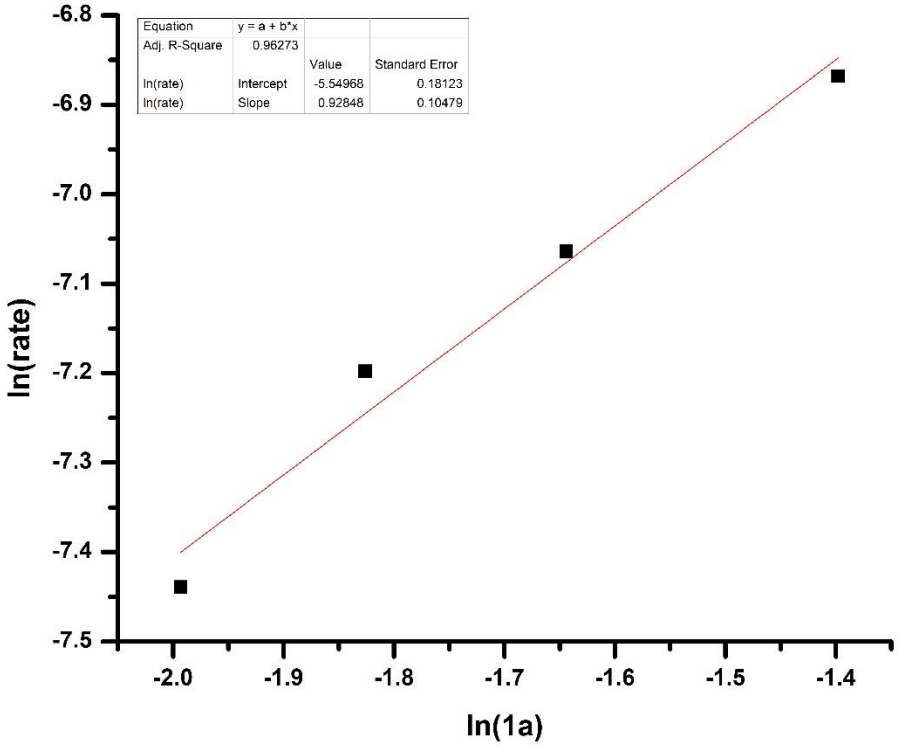
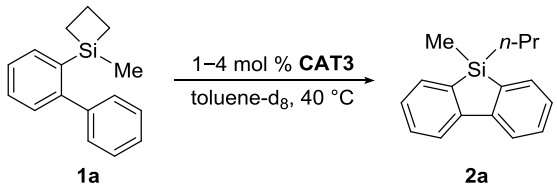


Figure S18. Plot of ln(rate) versus ln[**1a**]. ln(rate) = 0.93 × ln[**1a**] – 5.55. R^2 = 0.963.



1a **2a**

Determination of the reaction order in [Rh]–H catalyst CAT3. In a N_2-flushed glove box, substrate **1a** (0.1 mmol each) and 0.1–0.4 mL of **stock solution II** were added into separate NMR tubes with J. Young valve and the final volumes were adjusted to 0.45 mL. The reaction was then heated to 40 °C and the rates of starting material consumption were determined by the method of initial rates (Table S6; up to 10% conversion; monitored by ^{1}H NMR spectroscopy with 1,2-dimethoxyethane as the internal standard; the time interval between successive data points was set to 2 minutes). As depicted in Figure S19, a linear correlation was found between ln(rate) and ln[**CAT3**] and the slope was determined to be 0.89, indicating that the reaction order in **CAT3** is 1.

Table S6. Rate versus [CAT3]

Concentration of [CAT3]/M	Reaction Rate/M·min^{-1}	ln[CAT3]	ln(rate)
0.00222	0.000365	-6.110	-7.916
0.00444	0.000695	-5.417	-7.272
0.00888	0.00127	-4.724	-6.669
0.0111	0.00153	-4.501	-6.482

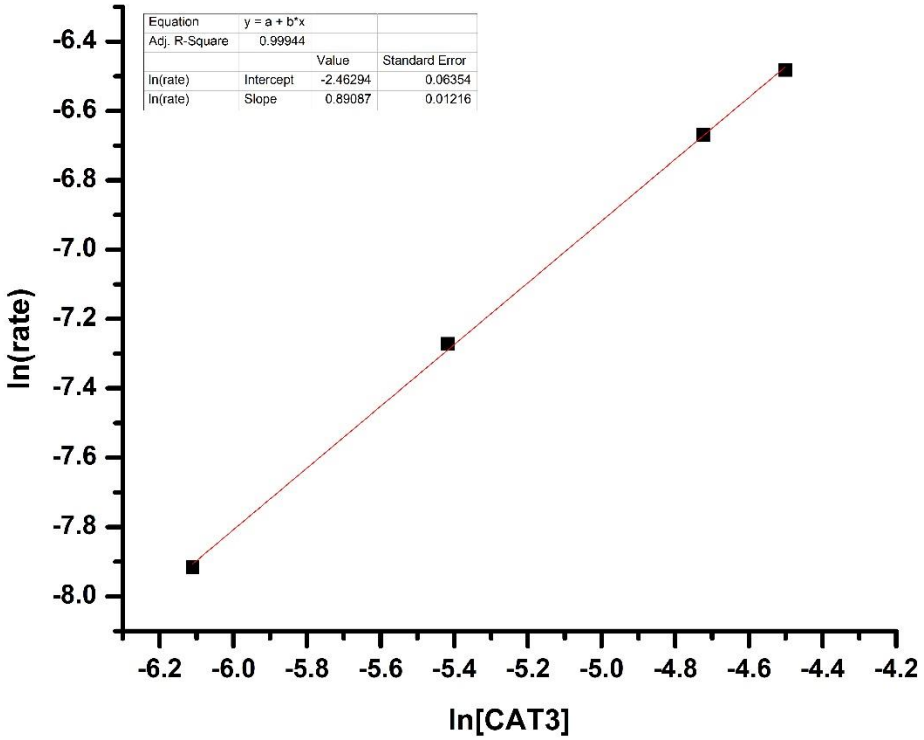
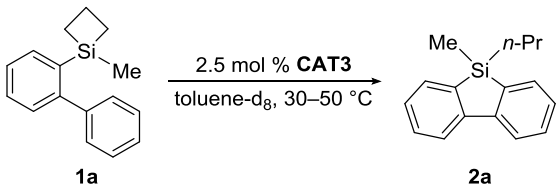


Figure S19. Plot of ln(rate) versus ln[**CAT3**]. ln(rate) = 0.89 × ln[**CAT3**] − 2.46. R^2 = 0.999.



Determination of the activation parameters. In a N_2-flushed glove box, substrate **1a** (0.1 mmol each) and **stock solution II** (0.25 mL each) were added into separate NMR tubes with J. Young valve and the final volumes of the solutions were adjusted to 0.4 mL. The reactions were then heated to 30−50 °C and the rate

constants were determined by the method of initial rates (Table S7; up to 10% conversion; monitored by ^{1}H NMR spectroscopy with 1,2-dimethoxyethane as the internal standard; the time interval between successive data points was set to 2 minutes). The activation energy (E_a) was determined to be 23.4 kcal/mol according to $E_a = -2.303Rd(\lg k)/d(1/T)$ (Figure S20). The activation enthalpy ($\Delta H^‡$) was determined to be 22.8 kcal/mol according to $\Delta H^‡ = Rd[\ln(k/T)]/d(1/T)$ (Figure S21). The activation entropy ($\Delta S^‡$) was determined to be 13.5 cal/(mol·K) according to $\Delta S^‡ = R \times \text{intercept} - R\ln(k_B/h)$.

Table S7. Rate Constant (*k*) versus Temperature (*T*)

T(K)	**1/*T*** (1/K)	***k*** ($M^{-1}\cdot min^{-1}$)	**lg*k***	**ln(*k*/*T*)**
303	0.0033	0.187	-0.728	-7.39
308	0.003247	0.397	-0.401	-6.65
313	0.003195	0.709	-0.149	-6.09
318	0.003145	1.271	0.104	-5.52
323	0.003096	2.108	0.324	-5.03

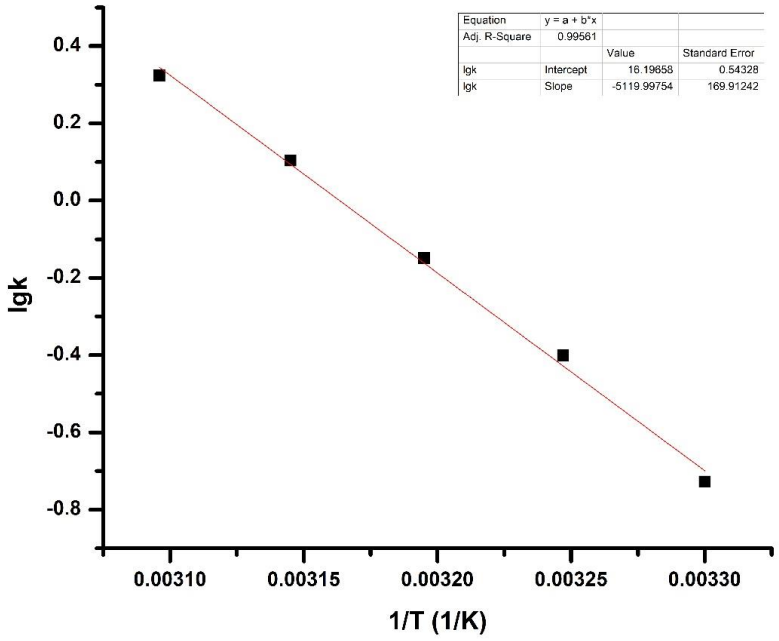


Figure S20. Determination of activation energy (E_a). $\lg k = 16.2 - (5.12\times10^3\ K)/T$. $R^2 = 0.996$.

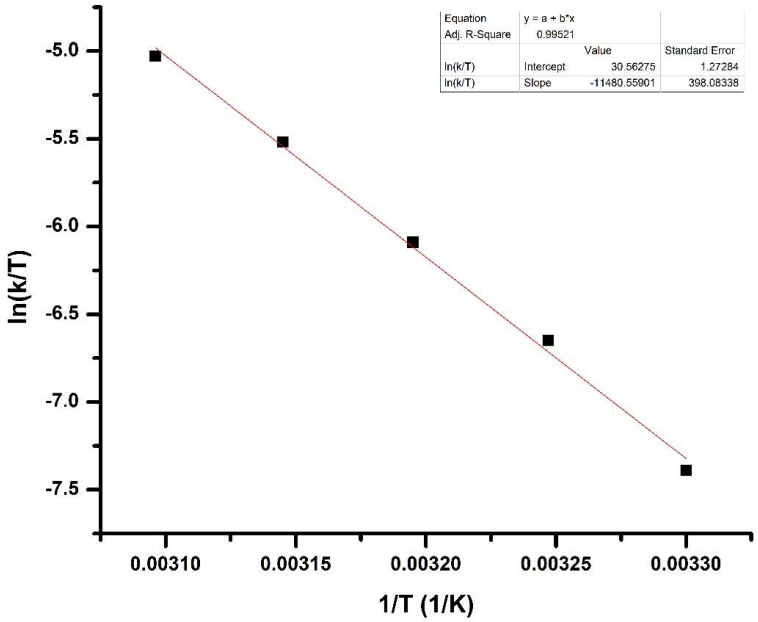
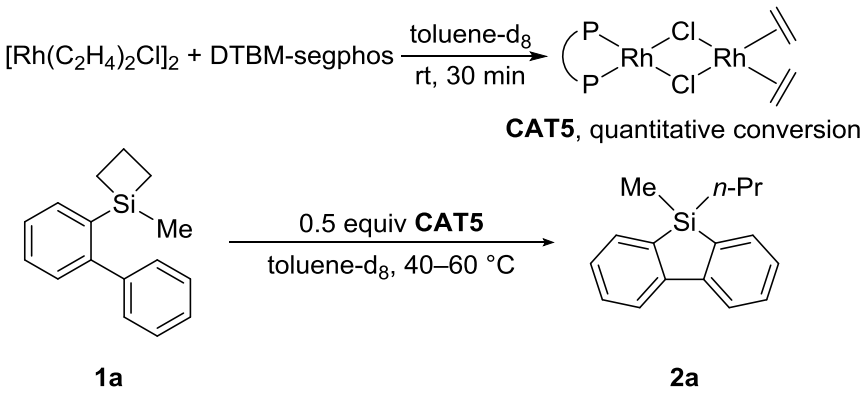


Figure S21. Determination of $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$. $\ln(k/T) = 30.6 - (1.15\times10^4\ \mathrm{K})/T$. $R^2 = 0.995$.

S15. Attempts to Detect Chlorosilane 6a or Its Derivatives

As depicted in the main text, the active rhodium hydride catalyst was generated during the induction period along with the release of chlorosilane **6a**, therefore we employed time-course ^{1}H NMR monitoring on the reaction of substrate **1a** with $[Rh(C_2H_4)_2Cl]_2$ precatalyst and different diphosphine ligands (e.g., DTBM-MeO-biphep, DTBM-segphos, and TMS-segphos in ref 1). To exclude the potential broadening and overlapping of ^{1}H NMR peaks between the optimal ligand TMS-segphos and **1a**, **2a**, or any reaction intermediates (e.g., the distinctive Si−Me peaks of TMS-segphos and **1a**/**2a**/intermediates), and improve the chance to observe any transient species, we identified the less reactive ligand DTBM-segphos was more suitable for NMR study. Subsequently, we carried out variable temperature NMR monitoring on the reaction of substrate **1a** in the presence of stoichiometric DTBM-segphos in an NMR tube. The results clearly suggested the formation of chlorosilane **6a** or its derivatives and the detailed procedure was described as follows.



1a **2a**

$[Rh(C_2H_4)_2Cl]_2$ (9.7 mg, 0.025 mmol, 1.0 equiv), DTBM-segphos (29.5 mg, 0.025 mmol, 1.0 equiv), and toluene-d_8 (0.5 mL) were added into an NMR tube with J-Young valve in a N_2-flushed glove box. The reaction mixture was maintained at room temperature for 30 minutes to generate **CAT5**, then **1a** (11.9 mg, 0.05 mmol, 2.0 equiv) was added. The NMR tube was removed from the glove box and subjected to NMR monitoring as described.

As shown in Figure S22, equal equivalent of precatalyst $[Rh(C_2H_4)_2Cl]_2$ reacted smoothly with DTBM-segphos to generate **CAT5** (line 1), followed by mixing with substrate **1a** and the ^{1}H NMR spectra was collected instantly (line 2). After the mixture was heated under 40 °C for 1 h, the ^{1}H NMR signal remained unchanged (line 3). Further heating the mixture at the same temperature for 3 h, two sets of new apparent Si−Me peaks that can be assigned to product **2a** and byproduct **6a** or its derivatives started to appear (line 4, for zoom-in details see Figure S23). When the mixture was heated at 60 °C for 1 h to 3 h, the two new signals increased with the decrease of starting material. Meanwhile, from 40 °C for 3 h (line 4), a set of new peaks with their chemical shifts ranging from 5.5 to 6.0 ppm started to emerge (for zoom-in details see Figure S24). These characteristic chemical shifts and integral areas [^{1}H NMR (400 MHz, toluene-d_8, δ): 5.90−5.87 (m, 1H), 5.62−5.60 (m, 1H), 5.56−5.36 (m, 1H), 0.06 (s, 3H), see Figure S25 for details] were assigned to be allyl and Si−Me groups possibly belonging to chlorosilane **6a** or its derivatives. When the temperature was increased to 60 °C for 3 h, the new species remained. After that, the reaction mixture was quenched and passed through a short pad of silica gel using ether as eluent. The volatiles were removed by vacuum and the residue was dissolved in hexanes and characterized by GC−MS.

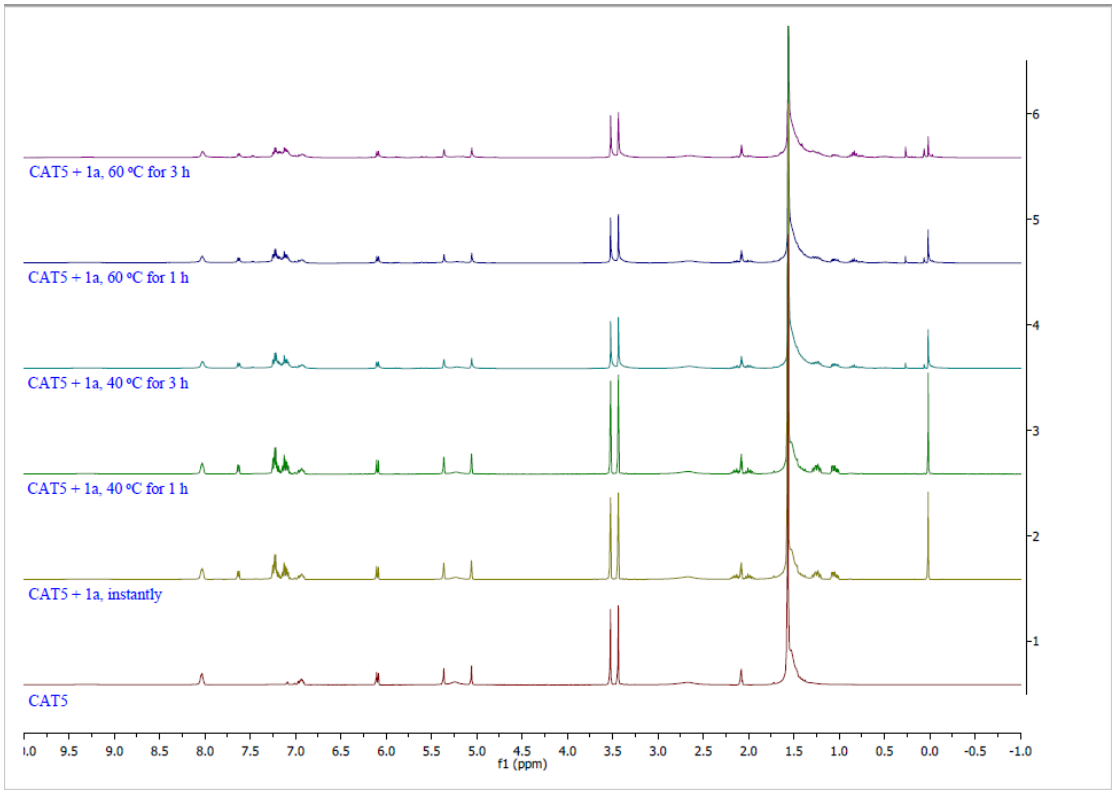


Figure S22. Time-course ^{1}H NMR monitoring on the reaction of **1a** with **CAT5**.

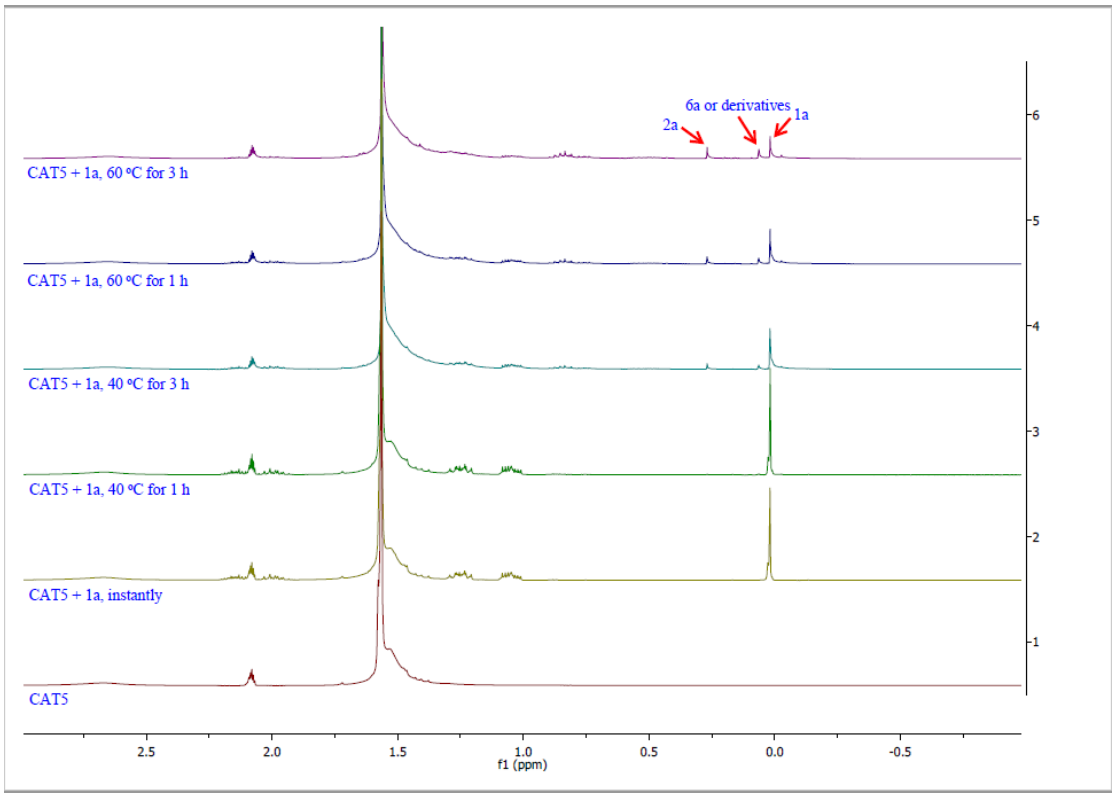


Figure S23. Zoom-in time-course ^{1}H NMR monitoring on the reaction of **1a** with **CAT5** (alkyl region).

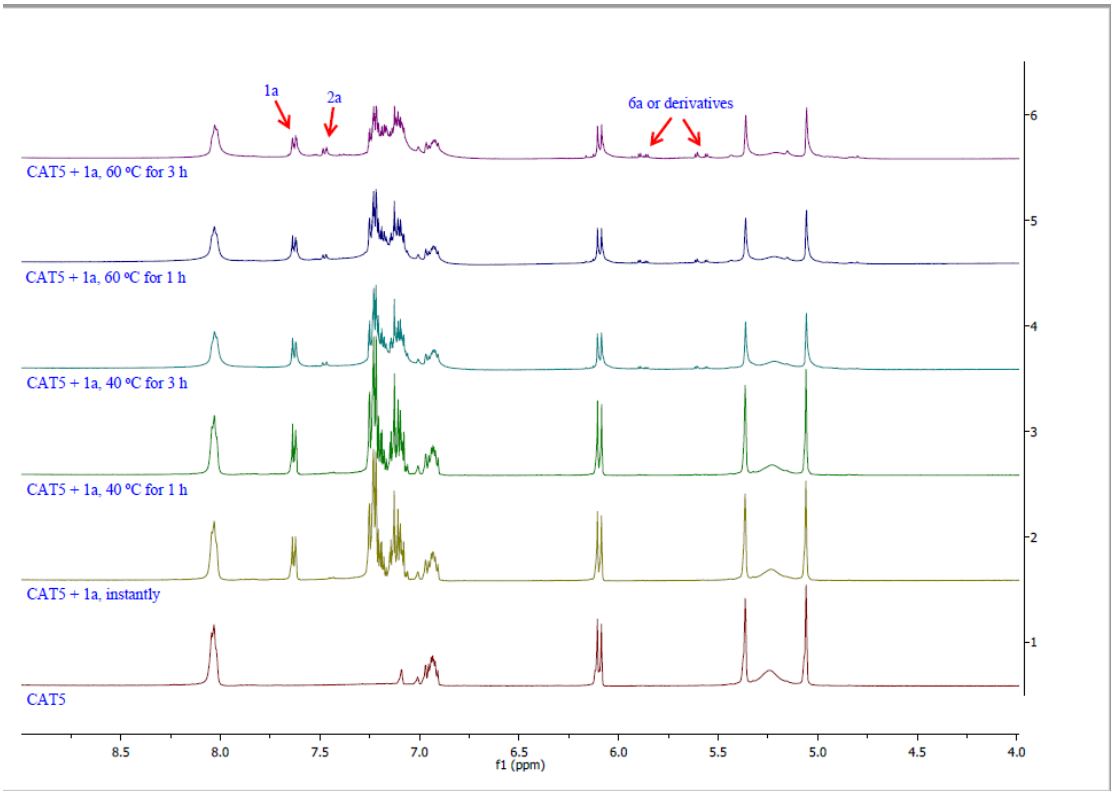


Figure S24. Zoom-in time-course ^{1}H NMR monitoring on the reaction of **1a** with **CAT5** (aryl region).

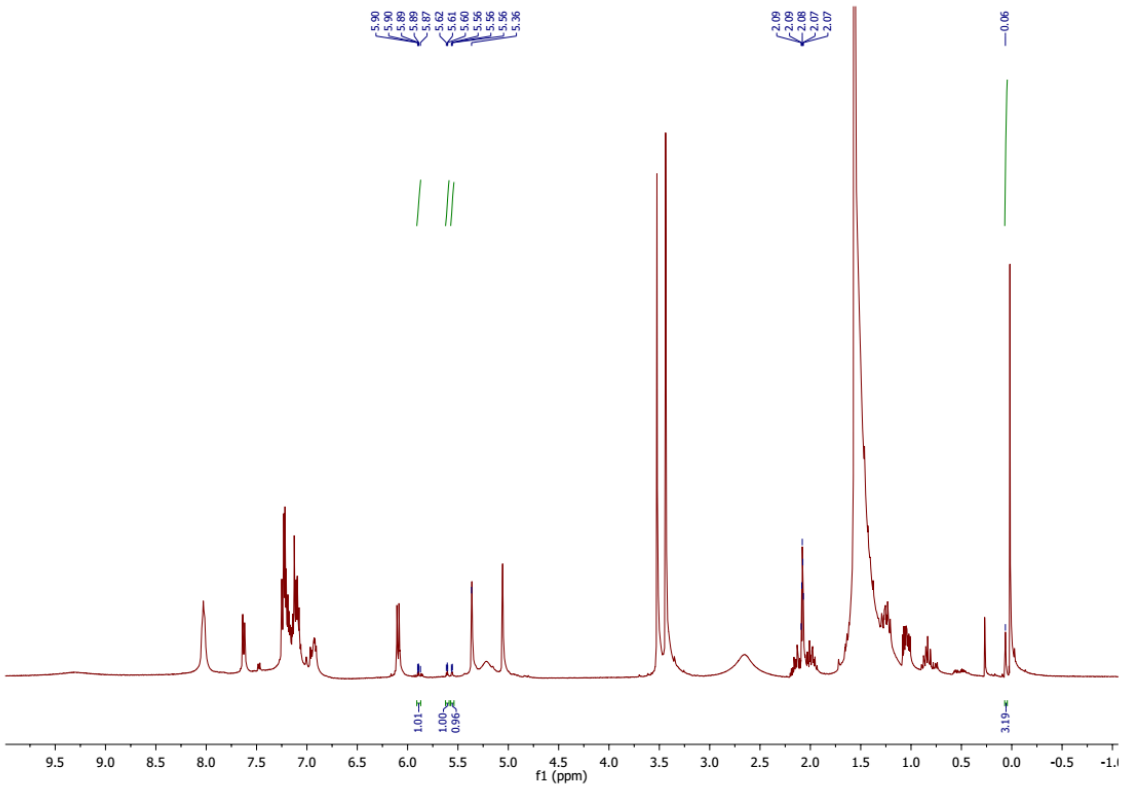


Figure S25. ^{1}H NMR spectrum of the sample corresponding to line 4.

Considering the low abundance of **6a** or its derivatives observed in ^{1}H NMR spectrum, we thus pursued GC–MS characterization for its higher sensitivity (Figure S26). The results gave signals corresponding to the hydrolyzed product of chlorosilane **6a**, silanol **6b**, which further supported the formation of **6a**. As depicted in Figure S27, peak (a) with the retention time of 8.2 minutes gave an *m*/*z* value of 253 [M(**6b**)−H] (negative mode).

Figure S26. GC spectrum of the sample corresponding to line 6.

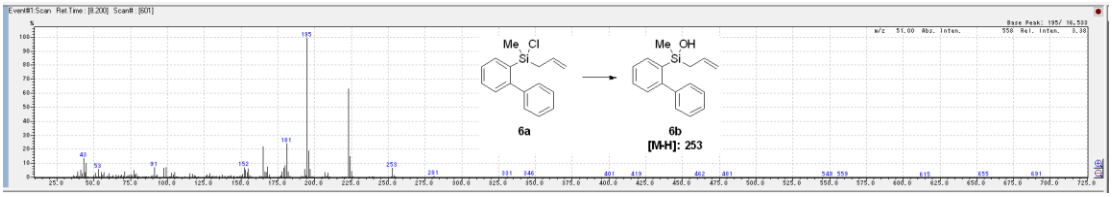


Figure S27. Mass spectrum of peak (a).

S16. References

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