Electronic Supplementary Material (ESI) for Chemical Science

Structural and Mechanistic Investigation of a Cationic Hydrogen-Substituted Ruthenium Silylene Catalyst for Alkene Hydrosilation

Supporting Information

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Contents:

General Considerations. All experiments were carried out under a nitrogen atmosphere using standard Schlenk techniques or an inert atmosphere (N_2) glovebox. Olefin impurities were removed from pentane by treatment with concentrated H_2SO_4, 0.5 N $KMnO_4$ in 3 M H_2SO_4, and then $NaHCO_3$. Pentane was then dried over $MgSO_4$ and stored over activated 4 Å molecular sieves, and dried over alumina. Thiophene impurities were removed from benzene and toluene by treatment with H_2SO_4 and saturated $NaHCO_3$. Benzene and toluene were then dried over $CaCl_2$ and further dried over alumina. Tetrahydrofuran, diethyl ether, dichloromethane, and hexanes were dried over alumina. Fluorobenzene was dried over P_2O_5, degassed and distilled under N_2. Methylene chloride-d_2 was dried by vacuum distillation from CaH_2. Benzene-d_6 was dried by vacuum distillation from Na/K alloy. Bromobenzene-d_5 was refluxed over CaH_2 for 20 h and then distilled under nitrogen. $Cp^*(^iPr_3P)RuH_2(SiHMesOTf)$[11] and $[Et_3Si][B(C_6F_5)_4]$[12] were prepared according to literature methods. All other chemicals were purchased from commercial sources and used without further purification.

NMR spectra were recorded using Bruker AVB 400, AV-500 or AV-600 spectrometers equipped with a 5 mm BB probe. Spectra were recorded at room temperature and referenced to the residual protonated solvent for ^1H. $^{31}P\{^1H\}$ NMR spectra were referenced relative to 85% H_3PO_4 external standard ($\delta = 0$). $^{13}C\{^1H\}$ NMR spectra were calibrated internally with the resonance for the solvent relative to tetramethylsilane. For $^{13}C\{^1H\}$ NMR spectra, resonances obscured by the solvent signal are omitted. ^{29}Si NMR spectra were referenced relative to a tetramethylsilane standard and obtained via 2D ^1H ^{29}Si HMBC unless specified otherwise. The following abbreviations have been used to describe peak multiplicities in the reported NMR

spectroscopic data: "m" for complex multiplet, and "br" for broadened resonances. Elemental analyses were performed by the College of Chemistry Microanalytical Laboratory at the University of California, Berkeley.

[Cp*(^{i}Pr$_3$P)RuH$_2$(=SiHMes)][CB$_{11}$H$_6$Br$_6$] (2). A solution of [Et$_3$Si][CB$_{11}$H$_6$Br$_6$] (0.052 g, 0.07 mmol) in 0.5 mL of C$_6$H$_5$F was added to a solution of Cp*(^{i}Pr$_3$P)RuH$_2$(SiHMesOTf) (0.050 g, 0.07 mmol) in 1 mL of C$_6$H$_5$F. After stirring 5 min at room temperature, 15 mL of pentane was added to the bright orange solution and the resulting mixture was placed in the −30 °C freezer. After 1 h, an orange solid settled to the bottom of the vial. The solution was carefully decanted and the resulting orange solid was dried under vacuum for 1 h to afford **2** in 89% yield (0.075 g). ^{1}H NMR (C$_6$D$_5$Br, 600 MHz): δ 8.15 (1H, br s, $^{1}J_{SiH}$ = 224.5 Hz, Si*H*), 6.97 (2H, s, Ar*H*), 3.17 – 2.97 (6H, br s, carborane), 2.43 (6H, s, ArC*H*$_3$), 2.41 (3H, s, ArC*H*$_3$), 2.11 (3H, sept, *J* = 7.1 Hz, C*H*(CH$_3$)$_2$), 1.59 (15H, s, C$_5$*Me*$_5$), 1.13 (18H, dd, *J* = 7.1 Hz, J_{PH} = 13.9 Hz, CH(C*H*$_3$)$_2$), -11.35 (2H, d, $^{2}J_{PH}$ = 14.5 Hz, $^{2}J_{SiH}$ = 62.3 Hz, Ru*H*). ^{13}C{^{1}H} NMR (C$_6$D$_5$Br, 150.9 MHz): 144.7 (Ar*C*), 143.2 (Ar*C*), 139.8 (Ar*C*), 97.7 (*C*$_5$Me$_5$), 41.3 (carborane), 26.1 (*C*H(CH$_3$)$_2$), 25.9 (*C*H(CH$_3$)$_2$), 22.3 (Ar*Me*), 21.7 (Ar*Me*), 19.4 (CH(*C*H$_3$)$_2$), 11.0 (C$_5$*Me*$_5$). ^{31}P{^{1}H} NMR (C$_6$D$_5$Br, 163.0 MHz): δ 65.1. ^{29}Si NMR (C$_6$D$_5$Br, 99.4 MHz): δ 228.7. Anal. Calcd for C$_{29}$H$_{56}$B$_{11}$Br$_6$PRuSi: C, 29.94; H, 4.85. Found: C, 29.64; H, 4.65.

[Cp*(^{i}Pr$_3$P)RuD$_2$(=SiDMes)][CB$_{11}$H$_6$Br$_6$] (2-*d*$_3$). By a procedure analogous to that for **2**, complex **2-*d*$_3$** was obtained using MesSiD$_3$.

[Cp*(^{i}Pr$_3$P)RuH$_2$(=SiMes(Hex)][CB$_{11}$H$_6$Br$_6$] (3). An excess of 1-hexene (0.008 g, 0.04 mmol) was added to a solution of **2** (0.050 g, 0.04 mmol) in 1 mL of C_6H_5F to give a yellow solution. After 5 min, the reaction mixture was dried under vacuum. The resulting oil was washed with 3 aliquots of hexanes (ca. 10 mL) and then dried under vacuum to give a yellow solid in 96% yield (0.055 g). ^{1}H NMR (C_6D_5Br, 600 MHz): δ 6.96 (2H, s, Ar*H*), 3.16 – 2.81 (6H, br s, carborane), 2.60 (3H, m, C*H*$_3$), 2.49 (6H, s, ArC*H*$_3$), 2.38 (3H, s, ArC*H*$_3$), 2.09 (3H, sept, J = 6.8 Hz, C*H*(CH$_3$)$_2$), 1.60 (15H, s, C$_5$*Me*$_5$), 1.35 (4H, m, C*H*$_2$), 1.28 (6H, m, C*H*$_2$), 1.17 (18H, dd, J = 6.8 Hz, J_{PH} = 13.7 Hz, CH(C*H*$_3$)$_2$), -11.62 (2H, d, $^{2}J_{PH}$ = 15.6 Hz, Ru*H*). ^{13}C{^{1}H} NMR (C_6D_5Br, 150.9 MHz): 142.1 (Ar*C*), 138.7 (Ar*C*), 132.9 (Ar*C*), 98.4 (*C*$_5$Me$_5$), 41.4 (carborane), 32.7 (*C*H$_2$), 31.3 (*C*H$_2$), 27.5 (*C*H(CH$_3$)$_2$), 27.3 (*C*H(CH$_3$)$_2$), 24.0 (*C*H$_2$), 23.3 (*C*H$_2$), 22.7 (Ar*Me*), 21.6 (Ar*Me*), 19.8 (CH(*C*H$_3$)$_2$), 17.6 (*C*H$_3$), 11.1 (C$_5$*Me*$_5$). ^{31}P{^{1}H} NMR (C_6D_5Br, 163.0 MHz): δ 68.9. ^{29}Si NMR (C_6D_5Br, 99.4 MHz): δ 264.7. Anal. Calcd for $C_{35}H_{68}B_{11}Br_6PRuSi$: C, 33.70; H, 5.49. Found: C, 33.50; H, 5.19.

General Procedure for Catalytic Hydrosilation Reactions. Hydrosilation catalytic runs were performed in Teflon capped J. Young NMR tubes. In a representative catalytic run, **1** (10 mg, 0.007 mmol, 1 mol%) was dissolved in 0.5 mL of bromobenzene-d_5, and the resulting solution was added to hexamethylbenzene (14.3 mg, 0.14 mmol) (as a standard) followed by alkene (0.14 mmol) and silane (0.14 mmol). The solution was transferred to a Teflon–capped J. Young NMR tube, and heated to 80 °C in an oil bath with a temperature-controlled hotplate for 1 – 18 h. The progress of the reaction was monitored

via ^{1}H NMR spectroscopy and yields were obtained by integration against a standard. For kinetic runs, the sample was placed in an NMR probe preheated to 353.0 K. Single-scan spectra were obtained using an automated acquisition program that was started immediately after placing the sample in the probe, and the peaks were integrated relative to the internal standard.

X-ray Crystallography. The single-crystal X-ray analysis of compound **1** was carried out at the UC Berkeley CHEXRAY crystallographic facility. Measurements were made on a Bruker APEX II CCD area detector with micro-focus sealed source Mo Kα radiation (λ = 0.71069 Å). Data was integrated and analyzed for agreement using Bruker APEX2 v. 2009.1. Empirical absorption correction were made using SADABS. Structures were solved by direct methods using the SHELX program package.

Figure S1. Plot of rate versus [**2**].

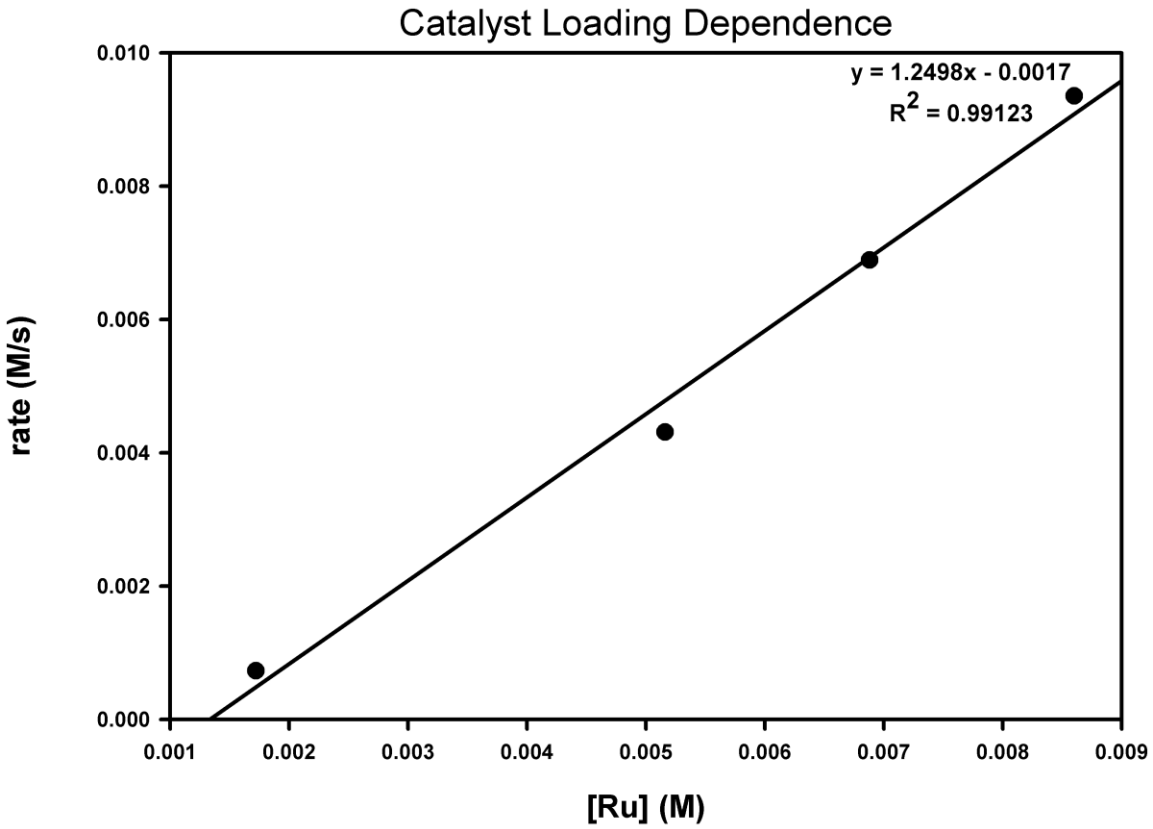


Figure S2. Plot of 1/rate versus [olefin].

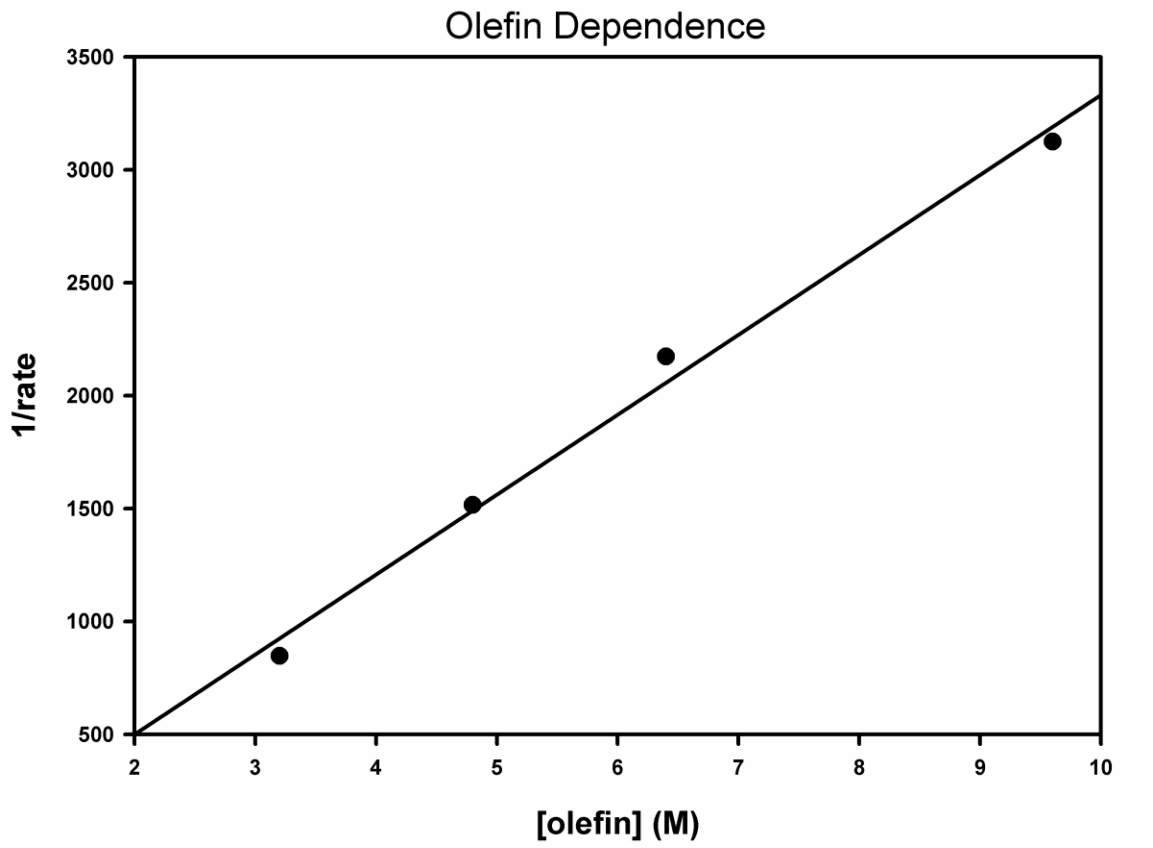


Figure S3.

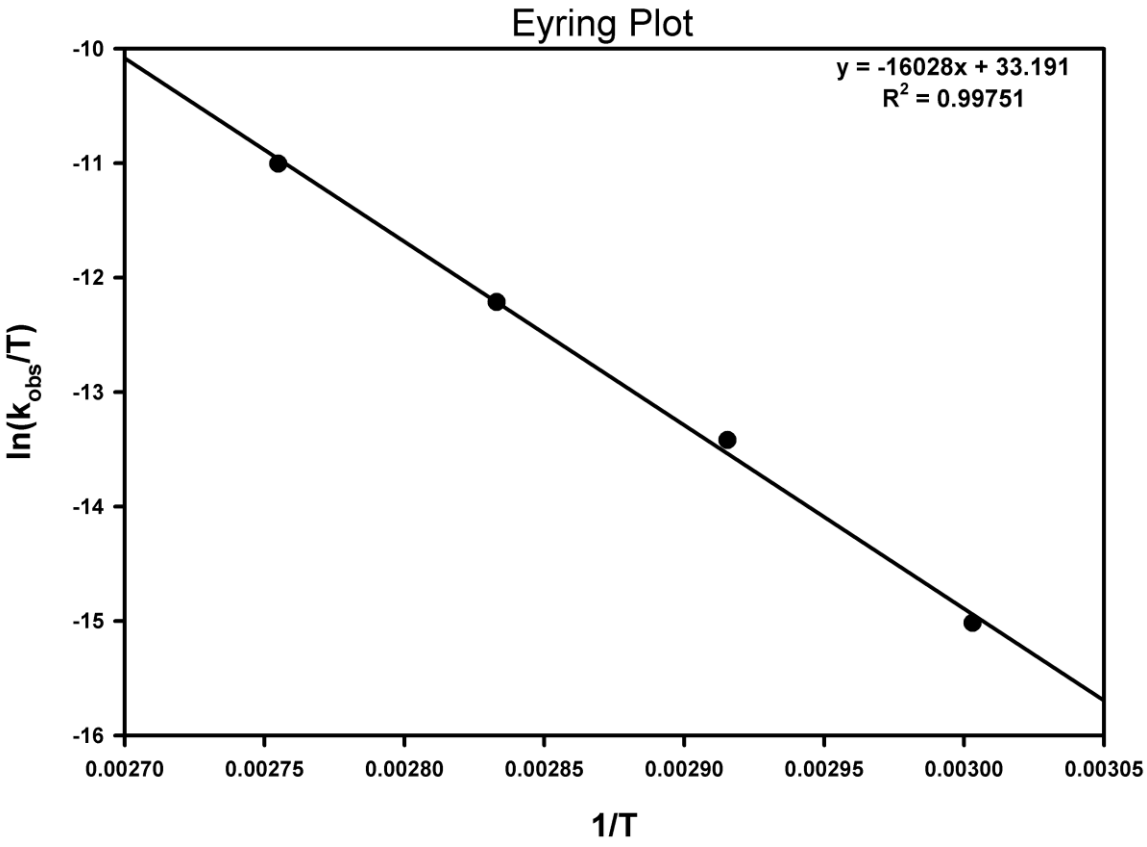


Figure S4. Plot of [$CySiH_3$] vs time under conditions of 0.16 M 1-octene, 0.14 M $CySiH_3$, and 1 mol % **2**.

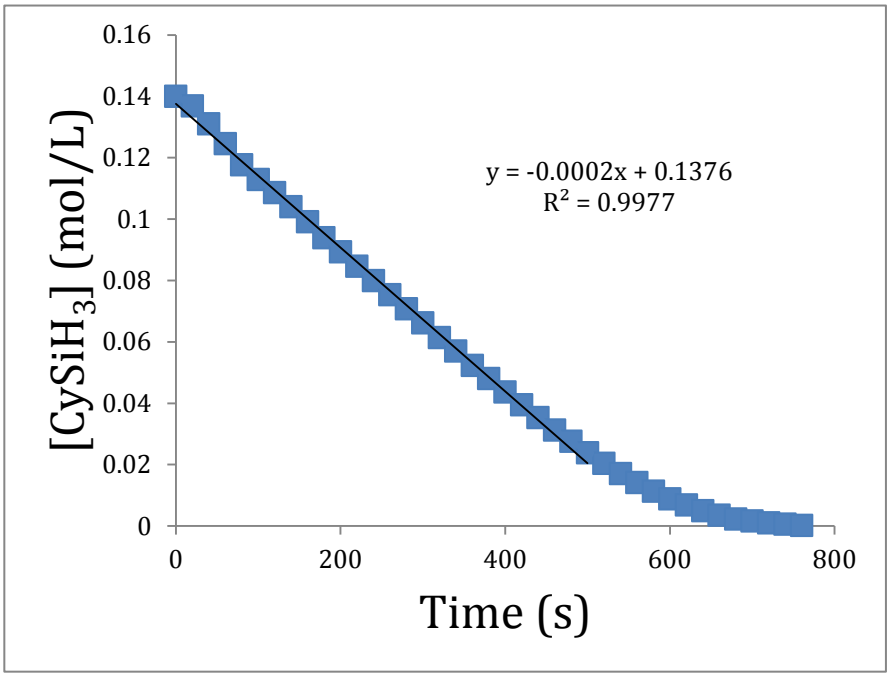


Figure S5. Plot of [1-octene] vs time under conditions of 0.16 M 1-octene, 0.14 M $CySiH_3$, and 1 mol % **2**.

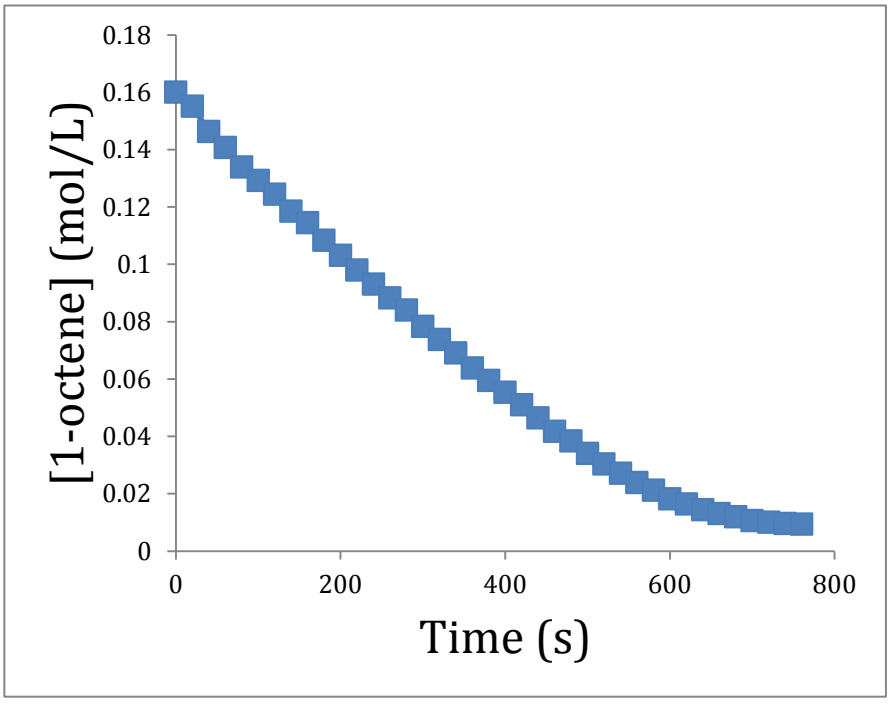


Figure S6. Plot of [$CySiH_3$] vs time under conditions of 3.2 M 1-octene, 0.16 M $CySiH_3$, and 1 mol % **2**.

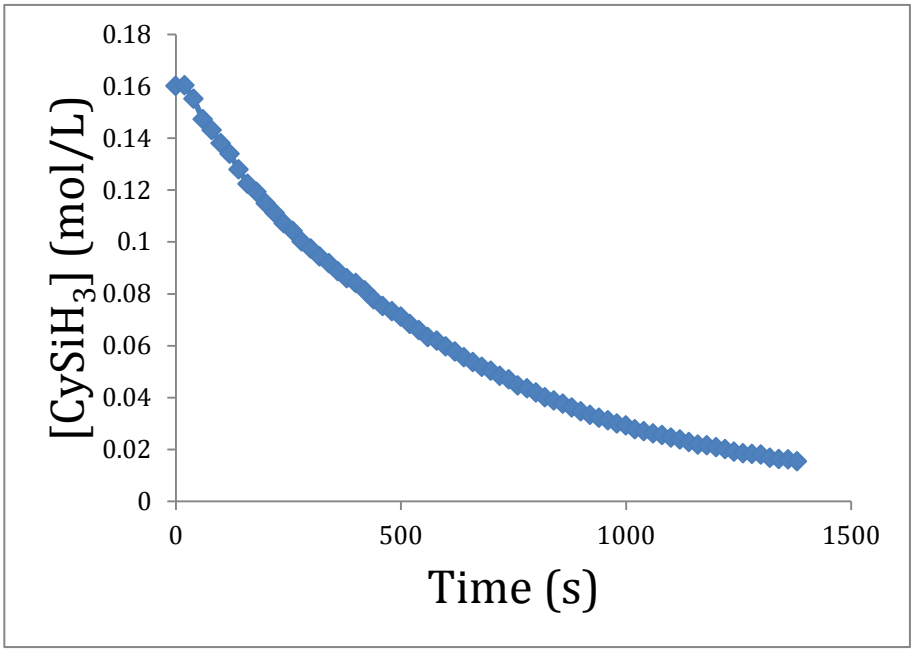


Figure S7. Plot of –ln([$CySiH_3$]/[$CySiH_3$]$_i$) vs time under conditions of 3.2 M 1-octene, 0.16 M $CySiH_3$, and 1 mol % **2**.

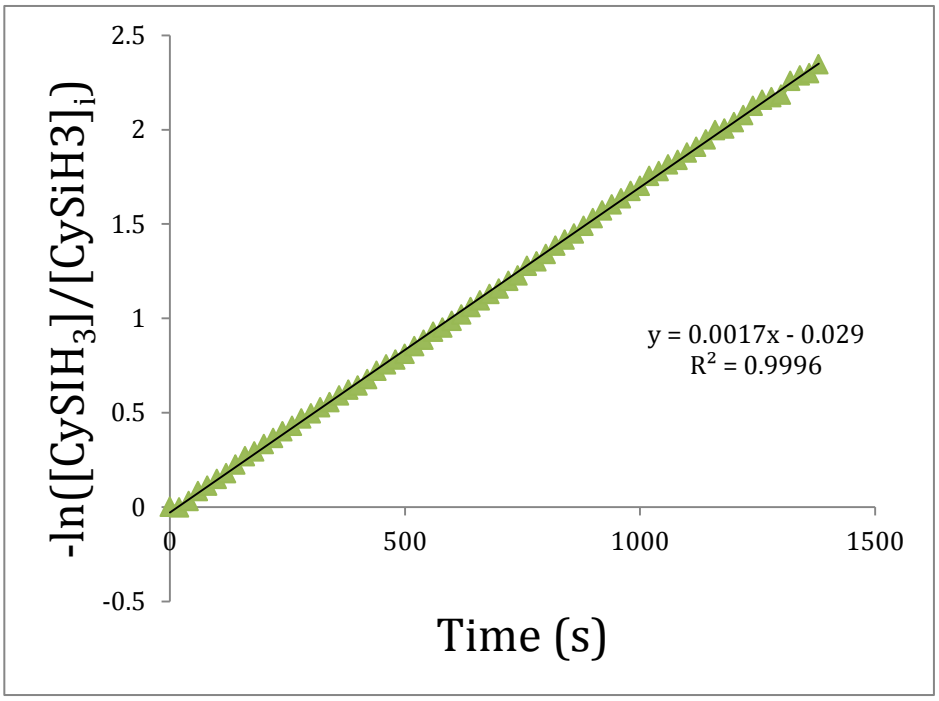


Figure S8. Plot of rate versus [silane] under conditions of 3.2 M 1-octene.

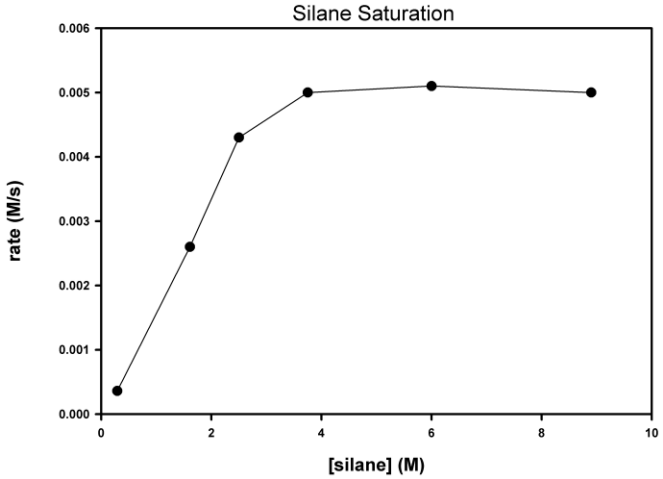
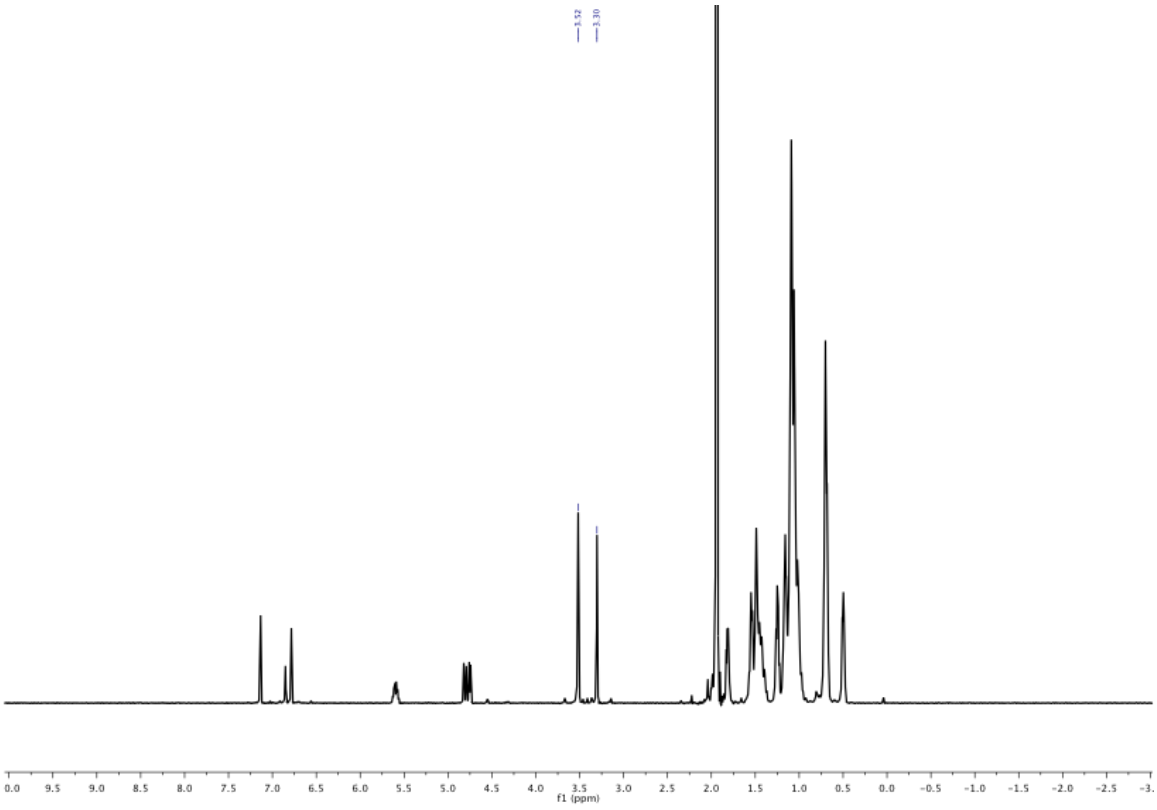


Figure S9. Example ^{1}H NMR spectrum from data used for Figures S4 and S5. The peaks marked at 3.52 and 3.30 ppm correspond to the Si—H bonds of $CyOctSiH_2$ and $CySiH_3$, respectively.



Rate Law Determination

The reaction mechanism shown in Scheme 3 can be simplified and written in the following form:

(1) **A** + olefin → **B**

(2) **B** ⇆ **C**

(3) **C** ⇆ **D** + product

(4) **D** + alkene ⇆ **E**

(5) **D** + silane ⇆ **A**

The reaction rate, in terms of silane consumption, is: d[silane]/dt = $-k_5$[**D**][silane]

Using the steady state approximation and assuming that an equilibrium between **B** and **C** is fully established during the reaction (i.e., [**C**] = K_2[**B**]), then [**D**] is given by:

d[**D**]/dt = k_3K_2[**B**] + k_{-4}[**E**] – k_{-3}[**D**][product] – k_4[**D**][alkene] – k_5[**D**][silane] = 0

or [**D**] = k_3K_2[**B**] + k_{-4}[**E**] / (k_{-3}[product] + k_4[alkene] + k_5[silane])

Substitution of this expression for [**D**] into the rate equation gives:

$$\frac{d[silane]}{dt} = \frac{-k_5[silane](k_3K_2[\mathbf{B}] + k_{-4}[\mathbf{E}])}{(k_{-3}[product] + k_4[alkene] + k_5[silane])}$$

When k_4[alkene] >> (k_{-3}[product] + k_5[silane]), then [**E**] is the resting state and the rate expression can be simplified in experimental terms with [**E**] = [**2**] ([**2**] = concentration of **2** initially added to the reaction):

$$\frac{d[silane]}{dt} = \frac{-k_{obs}[silane][\mathbf{2}]}{[alkene]}$$

Under these conditions, the plot of ln[silane] vs. time is linear (Figure S7) and the plot of 1/rate vs. [alkene] is linear (Figure S2).

When k_5[silane] >> k_{-3}[product] + k_4[olefin], then [**B**] = [**2**] and the rate expression can be simplified as:

$$\frac{d[silane]}{dt} = -k_{obs}[\mathbf{2}]$$

This predicts saturation behavior with respect to silane when the concentration is sufficiently high with respect to the product and alkene (Figure S8). Under these conditions, the plot of [silane] vs. time and [alkene] vs. time are both linear (Figure S4 and S5).

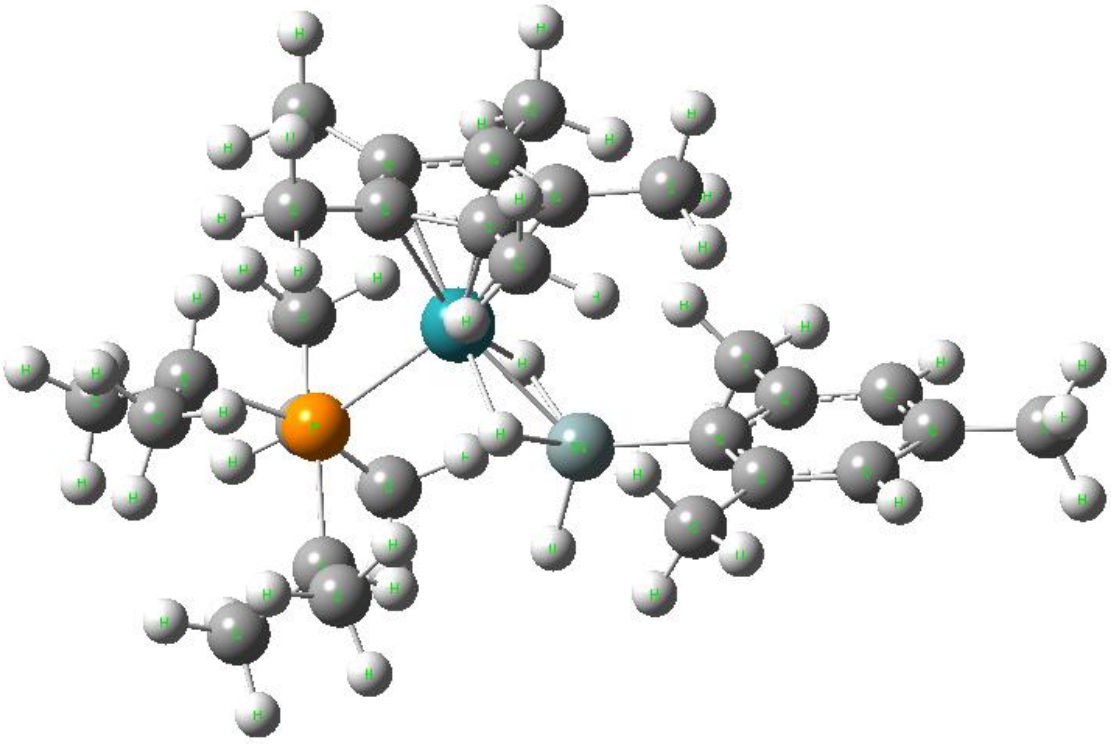
When k_{-3}[product] >> k_4[olefin] + k_5[silane], then [**B**] = [**2**] and the rate expression can be simplified to:

$$\frac{d[silane]}{dt} = \frac{-k_{obs}[silane][\mathbf{2}]}{[product]}$$

Under these conditions, the reaction rate should exhibit first order dependence in [silane] and inverse dependence in [product], which is consistent with a decrease in the reaction rate at high conversions (Figure S4, data past 500 s).

Computational Details

All calculations were performed using Gaussian '09 suite of programs (geometry optimization and NBO calculations[6]) in the molecular graphics and computing facility of the College of Chemistry, University of California, Berkeley. The crystallographically determined atomic coordinates of **2** were used as starting points for geometry optimization calculations for **2-DFT** using the B3PW91 hybrid functional with the 6-31G(d,p) basis set for all main-group elements and the LANL 2DZ basis set for ruthenium. Vibrational frequencies were calculated for the optimized structure and indicate that this structures lies on a minimum (no imaginary frequencies were determined). The optimized coordinates and select NLMO's for **2-DFT** are provided:



Optimized coordinates for **2-DFT**:

C	-0.90051800	2.34988400	-0.07040000
C	-0.14161600	2.29540700	-1.28626400
C	1.25785100	2.39574000	-0.96661700
C	1.36708800	2.52177300	0.46948400
C	0.04106000	2.47813900	1.01170000
C	-2.38772200	2.46428800	0.03971600
H	-2.68605400	3.51862400	-0.01129000
H	-2.76078500	2.06022900	0.98270400
H	-2.90128400	1.93276600	-0.76363700
C	-0.70268900	2.26613800	-2.67109600
H	-1.71303500	1.85350600	-2.69213000
H	-0.07678500	1.68210600	-3.34979600
H	-0.75656900	3.28736500	-3.06838100
C	2.33677000	2.68189000	-1.96109500
H	2.17668000	2.15563300	-2.90432100
H	3.32759300	2.41797000	-1.58926800
H	2.34990800	3.75638000	-2.18537600
C	2.58409400	2.94347800	1.22914200
H	2.62437500	4.03969100	1.26758200
H	3.51046200	2.60971400	0.75765500
H	2.57531800	2.58148400	2.25869900
C	-0.30868100	2.67765500	2.45073000
H	0.44968300	2.26093800	3.11705000
H	-1.27129500	2.22907100	2.70366900
H	-0.38185500	3.75111400	2.66584000
C	2.77982400	-0.35911400	2.82549000
H	1.82115000	0.16096400	2.92147000
H	3.52668300	0.36605600	2.49052500
H	3.07773500	-0.70291200	3.82189300
C	2.64980300	-1.55511000	1.88015600
H	3.61893500	-2.06540000	1.83501700
C	1.62534400	-2.55262900	2.42456500
H	1.91100000	-2.83936100	3.44233100
H	1.56511100	-3.47127800	1.83559500
H	0.62375400	-2.11531100	2.48404400
C	5.22770100	-0.76939600	0.27708800
H	5.38934000	-1.83084600	0.07244700
H	5.22384000	-0.62719900	1.36001400
H	6.09787000	-0.22987100	-0.11353600
C	3.96628300	-0.22580700	-0.40576100
H	3.84838400	0.81740900	-0.09459800
C	4.14155700	-0.24507300	-1.92881900
H	4.93649100	0.45054300	-2.21818400
H	3.23271100	0.04067000	-2.46335000

H	4.44304700	-1.23656100	-2.27710200
C	3.27699600	-3.61446200	-0.62479200
H	2.98238900	-4.58510100	-1.03865900
H	3.54866600	-3.77752600	0.42094800
H	4.17264700	-3.29616800	-1.16512500
C	2.12224000	-2.62037600	-0.80174700
H	1.24880200	-3.04008300	-0.28723500
C	1.74551700	-2.50174900	-2.28409700
H	2.61448200	-2.29474600	-2.91176800
H	1.00548200	-1.71931500	-2.46912800
H	1.32137200	-3.45247600	-2.62451400
C	-3.01407200	-0.96783700	0.04957600
C	-3.70310200	-1.07814500	-1.18032700
C	-5.09223900	-0.95198700	-1.19535200
H	-5.61788000	-1.03331600	-2.14442800
C	-5.82640700	-0.73618700	-0.02577600
C	-5.13112800	-0.65787000	1.18356100
H	-5.68765900	-0.50801500	2.10617400
C	-3.74197400	-0.77622800	1.24554300
C	-2.96877500	-1.35580000	-2.46926700
H	-2.41757500	-2.30413700	-2.42270000
H	-2.24766100	-0.56732100	-2.71560900
H	-3.66170800	-1.43415300	-3.31044000
C	-7.32601700	-0.63390000	-0.06447700
H	-7.78231400	-1.62869200	0.00459900
H	-7.67361000	-0.18161300	-0.99738300
H	-7.71067900	-0.04032400	0.76908600
C	-3.05667700	-0.73616800	2.58919600
H	-2.61358500	-1.70804800	2.84178400
H	-3.76251100	-0.49232200	3.38688200
H	-2.25315500	0.00873200	2.62455200
Si	-1.16120600	-1.13835900	0.07274800
P	2.31968800	-0.98521100	0.11589200
Ru	0.42283600	0.52376200	-0.04014400
H	-0.26419300	-0.56386100	-1.22965900
H	-0.78398600	-2.57195100	0.15619100
H	-0.26603500	-0.41272400	1.28998400

Select NMLO's for **2-DFT**:

83. (2.00000) 79.3617% BD (1)Si 76- H 79
1.576% C 1 s(2.69%)p36.08(97.19%)d 0.04(0.12%)
3.921% C 2 s(1.88%)p52.10(98.08%)d 0.02(0.04%)
0.662% C 3 s(5.41%)p17.41(94.27%)d 0.06(0.32%)
1.142% C 4 s(3.86%)p24.92(96.12%)d 0.01(0.03%)
0.153% C 5 s(0.29%)p99.99(99.06%)d 2.25(0.65%)
0.033% C 10 s(9.00%)p 9.55(85.94%)d 0.56(5.06%)
0.035% H 13 s(99.83%)p 0.00(0.17%)
0.025% C 18 s(18.61%)p 4.31(80.27%)d 0.06(1.11%)
0.015% H 19 s(99.87%)p 0.00(0.13%)
0.011% H 25 s(99.84%)p 0.00(0.16%)
0.051% C 30 s(34.16%)p 1.92(65.48%)d 0.01(0.36%)
0.068% C 50 s(30.17%)p 2.29(69.22%)d 0.02(0.61%)
0.023% C 52 s(34.28%)p 1.88(64.48%)d 0.04(1.24%)
0.066% H 54 s(99.02%)p 0.01(0.98%)
0.104% C 56 s(25.00%)p 2.97(74.23%)d 0.03(0.77%)
0.020% C 57 s(35.27%)p 1.81(63.97%)d 0.02(0.76%)
0.033% C 63 s(28.55%)p 2.46(70.23%)d 0.04(1.22%)
0.014% C 64 s(2.20%)p41.96(92.50%)d 2.40(5.30%)
0.018% H 66 s(97.94%)p 0.02(2.06%)
29.996% Si 76 s(30.12%)p 2.29(69.00%)d 0.03(0.88%)
0.740% P 77 s(11.95%)p 7.25(86.68%)d 0.11(1.37%)
11.301% Ru 78 s(26.71%)p 0.01(0.16%)d 2.74(73.12%)
49.711% H 79 s(99.92%)p 0.00(0.08%)
0.020% H 80 s(98.22%)p 0.02(1.78%)
0.149% H 81 s(99.29%)p 0.01(0.71%)

84. (2.00000) 98.3344% BD (1)Si 76- H 80
0.029% C 1 s(0.38%)p99.99(99.34%)d 0.72(0.28%)
0.017% C 3 s(30.91%)p 2.23(68.99%)d 0.00(0.09%)
0.022% C 4 s(28.40%)p 2.52(71.51%)d 0.00(0.08%)
0.025% C 50 s(31.71%)p 2.14(67.82%)d 0.01(0.47%)
0.052% H 51 s(98.91%)p 0.01(1.09%)
0.276% C 56 s(22.86%)p 3.36(76.82%)d 0.01(0.32%)
0.068% C 57 s(0.55%)p99.99(99.13%)d 0.59(0.32%)
0.029% C 60 s(2.68%)p36.34(97.31%)d 0.00(0.01%)
0.066% C 63 s(3.34%)p28.86(96.29%)d 0.11(0.38%)
42.028% Si 76 s(35.76%)p 1.77(63.43%)d 0.02(0.81%)
0.033% P 77 s(27.43%)p 2.64(72.28%)d 0.01(0.29%)
0.165% Ru 78 s(5.41%)p 1.96(10.58%)d15.53(84.01%)
0.078% H 79 s(98.73%)p 0.01(1.27%)
56.957% H 80 s(99.88%)p 0.00(0.12%)
0.079% H 81 s(98.75%)p 0.01(1.25%)

85. (2.00000) 80.7625% BD (1)Si 76- H 81
1.655% C 1 s(2.33%)p41.80(97.56%)d 0.05(0.11%)
0.165% C 2 s(0.28%)p99.99(98.87%)d 3.06(0.85%)
2.311% C 3 s(3.10%)p31.21(96.87%)d 0.01(0.02%)
0.075% C 4 s(12.56%)p 6.71(84.23%)d 0.26(3.21%)
3.221% C 5 s(2.39%)p40.74(97.56%)d 0.02(0.05%)
0.030% C 14 s(13.89%)p 6.06(84.16%)d 0.14(1.95%)
0.029% H 17 s(99.83%)p 0.00(0.17%)
0.029% C 22 s(8.01%)p10.91(87.34%)d 0.58(4.65%)
0.031% H 25 s(99.82%)p 0.00(0.18%)
0.088% C 30 s(37.15%)p 1.67(62.18%)d 0.02(0.67%)
0.015% C 32 s(31.35%)p 2.14(67.01%)d 0.05(1.64%)
0.042% H 35 s(98.96%)p 0.01(1.04%)
0.051% C 40 s(24.13%)p 3.13(75.59%)d 0.01(0.28%)
0.099% C 56 s(25.96%)p 2.82(73.14%)d 0.03(0.90%)
0.031% C 57 s(33.50%)p 1.94(65.01%)d 0.04(1.49%)
0.019% C 63 s(40.10%)p 1.47(59.13%)d 0.02(0.77%)
0.014% C 72 s(5.01%)p17.99(90.20%)d 0.95(4.79%)
0.021% H 75 s(98.00%)p 0.02(2.00%)
30.763% Si 76 s(31.39%)p 2.16(67.76%)d 0.03(0.85%)
0.898% P 77 s(13.44%)p 6.33(85.10%)d 0.11(1.46%)
9.718% Ru 78 s(29.04%)p 0.01(0.22%)d 2.44(70.74%)
0.043% H 79 s(98.08%)p 0.02(1.92%)
0.029% H 80 s(98.67%)p 0.01(1.33%)
50.503% H 81 s(99.92%)p 0.00(0.08%)

129. (2.00000) 97.1032% LP (1)Ru 78
0.056% C 1 s(55.17%)p 0.56(30.79%)d 0.25(14.05%)
0.063% C 2 s(54.89%)p 0.59(32.12%)d 0.24(12.98%)
0.082% C 3 s(51.28%)p 0.76(38.73%)d 0.19(9.98%)
0.086% C 4 s(57.09%)p 0.59(33.44%)d 0.17(9.47%)
0.068% C 5 s(47.95%)p 0.84(40.34%)d 0.24(11.71%)
0.048% C 6 s(43.78%)p 1.26(55.02%)d 0.03(1.20%)
0.050% C 10 s(46.26%)p 1.14(52.57%)d 0.03(1.17%)
0.011% H 13 s(99.89%)p 0.00(0.11%)
0.060% C 14 s(38.87%)p 1.56(60.52%)d 0.02(0.61%)
0.061% C 18 s(37.22%)p 1.67(62.12%)d 0.02(0.66%)
0.048% C 22 s(44.78%)p 1.21(54.24%)d 0.02(0.97%)
0.132% C 40 s(40.76%)p 1.43(58.29%)d 0.02(0.96%)
0.084% C 50 s(36.12%)p 1.73(62.56%)d 0.04(1.32%)
0.111% C 56 s(32.33%)p 2.06(66.70%)d 0.03(0.96%)
0.011% H 75 s(99.64%)p 0.00(0.36%)
0.914% Si 76 s(8.19%)p 9.65(79.02%)d 1.56(12.79%)
0.484% P 77 s(1.80%)p47.42(85.58%)d 6.99(12.61%)
97.109% Ru 78 s(0.14%)p 0.13(0.02%)d99.99(99.84%)

0.090% H 79 s(95.06%)p 0.05(4.94%)
0.187% H 80 s(99.37%)p 0.01(0.63%)
0.091% H 81 s(95.42%)p 0.05(4.58%)

130. (2.00000) 94.1633% LP (2)Ru 78
0.034% C 1 s(1.09%)p70.32(76.31%)d20.83(22.60%)
0.621% C 2 s(8.39%)p10.80(90.56%)d 0.12(1.05%)
1.517% C 3 s(5.38%)p17.55(94.46%)d 0.03(0.16%)
1.534% C 4 s(4.15%)p23.07(95.67%)d 0.04(0.18%)
0.145% C 5 s(17.72%)p 4.37(77.39%)d 0.28(4.89%)
0.014% C 10 s(2.71%)p34.60(93.89%)d 1.25(3.40%)
0.015% H 12 s(99.95%)p 0.00(0.05%)
0.043% C 14 s(27.45%)p 2.49(68.24%)d 0.16(4.32%)
0.035% H 17 s(99.71%)p 0.00(0.29%)
0.028% C 18 s(17.78%)p 4.30(76.39%)d 0.33(5.83%)
0.033% H 19 s(99.74%)p 0.00(0.26%)
0.010% C 22 s(2.40%)p39.86(95.49%)d 0.88(2.11%)
0.010% C 26 s(54.46%)p 0.77(42.06%)d 0.06(3.48%)
0.266% C 30 s(31.54%)p 2.14(67.62%)d 0.03(0.84%)
0.012% H 35 s(99.78%)p 0.00(0.22%)
0.035% C 40 s(19.01%)p 4.22(80.19%)d 0.04(0.80%)
0.138% C 50 s(30.32%)p 2.28(69.10%)d 0.02(0.57%)
0.018% C 52 s(48.98%)p 1.03(50.51%)d 0.01(0.51%)
0.019% H 54 s(99.24%)p 0.01(0.76%)
0.203% Si 76 s(0.54%)p99.99(78.12%)d39.62(21.34%)
0.832% P 77 s(0.08%)p99.99(87.42%)d99.99(12.50%)
94.246% Ru 78 s(0.00%)p 0.00(0.00%)d 1.00(100.00%)
0.042% H 79 s(86.22%)p 0.16(13.78%)
0.034% H 81 s(83.68%)p 0.19(16.32%)

131. (2.00000) 91.7332% LP (3)Ru 78
0.639% C 1 s(6.48%)p14.40(93.28%)d 0.04(0.24%)
0.495% C 2 s(4.54%)p20.88(94.90%)d 0.12(0.56%)
0.220% C 3 s(12.22%)p 6.95(85.00%)d 0.23(2.78%)
0.234% C 4 s(13.69%)p 6.11(83.64%)d 0.20(2.67%)
1.094% C 5 s(4.15%)p23.02(95.62%)d 0.06(0.23%)
0.027% C 6 s(17.73%)p 4.41(78.13%)d 0.23(4.14%)
0.024% H 7 s(99.82%)p 0.00(0.18%)
0.016% H 13 s(99.82%)p 0.00(0.18%)
0.014% C 22 s(12.62%)p 6.35(80.11%)d 0.58(7.27%)
0.018% H 25 s(99.77%)p 0.00(0.23%)
0.012% C 32 s(39.66%)p 1.51(59.75%)d 0.01(0.59%)
0.017% H 35 s(99.53%)p 0.00(0.47%)
0.044% C 40 s(28.68%)p 2.44(69.87%)d 0.05(1.45%)
0.015% C 50 s(33.53%)p 1.95(65.49%)d 0.03(0.98%)
0.016% C 52 s(38.02%)p 1.62(61.57%)d 0.01(0.41%)

0.026% H 54 s(99.35%)p 0.01(0.65%)
0.192% C 56 s(33.93%)p 1.94(65.82%)d 0.01(0.24%)
0.031% C 57 s(1.57%)p62.16(97.88%)d 0.34(0.54%)
0.015% C 60 s(5.05%)p18.79(94.93%)d 0.00(0.02%)
0.037% C 63 s(0.62%)p99.99(98.97%)d 0.65(0.41%)
3.473% Si 76 s(46.61%)p 1.05(48.95%)d 0.10(4.44%)
0.172% P 77 s(9.05%)p 8.42(76.24%)d 1.62(14.71%)
91.796% Ru 78 s(0.00%)p 1.00(0.02%)d99.99(99.97%)
0.715% H 79 s(99.56%)p 0.00(0.44%)
0.106% H 80 s(98.35%)p 0.02(1.65%)
0.446% H 81 s(99.19%)p 0.01(0.81%)