

Electronic Supplemental Information

Hydroboration of Carbonyl Compounds Catalysed by a Molybdenum Germylyne Complex: Metal–Ligand Cooperative Mechanism

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Experimental Procedures

1. General experimental details

All manipulations were performed using vacuum line techniques or in a drybox (MBraun UNILab workstation) under an argon atmosphere, unless otherwise specified.

1.1. Materials

Benzaldehyde (**2a**, TCI Chemicals), 4-fluorobenzaldehyde (**2b**, TCI Chemicals), *p*-cyanobenzaldehyde (**2c**, Sigma Aldrich), *p*-tolualdehyde (**2d**, TCI Chemicals), *p*-anisaldehyde (**2e**, TCI Chemicals), pivalaldehyde (**2f**, TCI Chemicals), *n*-butyraldehyde (**2g**, TCI Chemicals), isobutyraldehyde (**2h**, TCI Chemicals), terephthalaldehyde (**2i**, TCI Chemicals), acetophenone (**4a**, TCI Chemicals), benzophenone (**4b**, TCI Chemicals), 2-adamantanone (**4c**, TCI Chemicals), 2-butanone (**4d**, TCI Chemicals), acetylcyclohexane (**4e**, Sigma Aldrich) and pinacolone (**4f**, Sigma Aldrich) were purchased and used without purification. Molybdenum-germylyne complex (η^5 -Cp*)(OC)₂Mo≡Ge(Tsi) (**1**) was synthesized according to literature procedures.¹ DBpin was synthesized according to literature procedures.² Benzene-*d*₆ was dried over CaH₂ and degassed using the freeze-pump-thaw technique, then stored with molecular sieves 4Å in a drybox.

1.2. Spectroscopic Measurements

¹H, ¹¹B{¹H}, ¹³C{¹H} and ¹⁹F{¹H} NMR spectra were recorded on a Bruker AVANCE-400 FT spectrometer using J. Young valve-equipped NMR tubes containing C₆Me₆ (>1.0 mg) as internal standard. ¹H and ¹³C{¹H} NMR spectra were referenced to the residual proton (C₆D₅H: δ = 7.15 ppm) and the carbon (C₆D₆: δ = 128.0 ppm) of deuterated solvents, respectively. ¹¹B{¹H} NMR spectra were referenced to an external standard of BF₃•Et₂O (δ = 0.0 ppm). ¹⁹F{¹H} spectra were referenced to an external standard of trifluoroacetic acid (δ = 0.0 ppm). ¹³C{¹H} NMR spectra were referenced to an external standard of tetramethylsilane (δ = 0.0 ppm).

2. Control Reactions

2.1 Hydroboration of benzaldehyde 2a with HBpin without catalyst 1

A solution of **2a** (2.7 mg, 0.025 mmol, 1.0 eq.), HBpin (4.8 mg, 0.038 mmol, 1.5 eq.) and C₆Me₆ (>1.0 mg) as an internal standard in C₆D₆ (0.50 mL) was prepared. The reaction was monitored by ¹H NMR at 300 K. After 40 min, PhCH₂OBpin (**3a**) was observed in 9% NMR yield. The reaction ceased completely after 19 hours, at which point the NMR yield of **3a** reached 26%.

2.2 Hydroboration of benzaldehyde 2a with HBpin in the presence of 1

A solution of **2a** (2.7 mg, 0.025 mmol, 1.0 eq.), HBpin (4.8 mg, 0.038 mmol, 1.5 eq.), **1** (1.5 mg, 2.5 μ mol, 10 mol%) and C₆Me₆ (>1.0 mg) as an internal standard in C₆D₆ (0.50 mL) was prepared.

Initial rate constants (k_0) were obtained by monitoring the reaction at 300 K. After 40 min, the formation of PhCH₂OBpin (**3a**) was observed in 27% NMR yield, representing a partial conversion during the early stage of the reaction. The reaction reached completion after 20 h to give **3a** in 98% NMR yield.

Figure S1 shows the time-dependent formation of PhCH₂OBpin (**3a**) over the initial 40 minutes of the reactions, comparing runs conducted in the absence of a catalyst and in the presence of catalyst **1**.

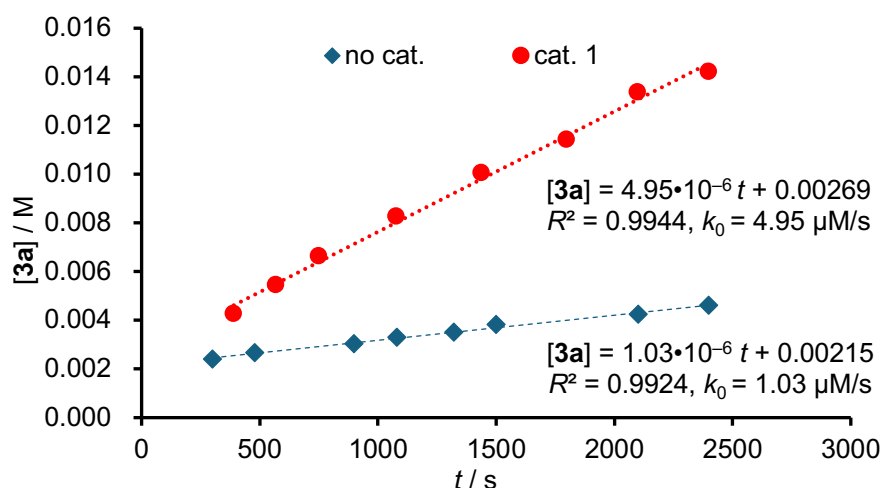
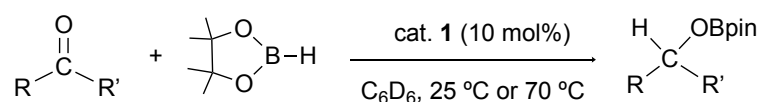


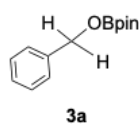
Fig. S1 Determination of k_0 for control and catalytic hydroboration of benzaldehyde **2a** (300 K). **[3a]** indicates the concentration of product **3a**.

3. Substrate Scope

General procedure for catalytic hydroboration of aldehydes and ketones.

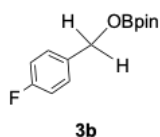


In a typical experiment, a solution of substrate (**2a–2i** for aldehydes, **4a–4f** for ketones; 0.034 mmol), HBpin (6.5 mg, 0.051 mmol, 1.5 eq.),* **1** (2.0 mg, 3.4 μmol , 10 mol%) and C₆Me₆ (>1.0 mg) as an internal standard in C₆D₆ (0.34 mL) was prepared in an NMR tube. The reactions of aldehydes were carried out at 25 °C, whereas those of ketones were performed at 70 °C. Product formation (**3a–3i** from aldehydes, **5a–5f** from ketones) was monitored by ¹H, ¹³C{¹H}, ¹¹B{¹H} and ¹⁹F{¹H} NMR spectroscopy. For each reaction, the reaction endpoint was defined as the time at which the growth of the product signals ceased, as determined by periodic NMR analysis. *For aldehyde **2i**, 3 equivalents of HBpin were used.



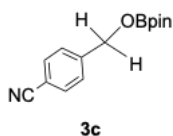
3a

3a³: ¹H NMR (400 MHz, C₆D₆): δ 7.31 (d, ³J_{H-H} = 7.5 Hz, 2H, *o*-Ar), 7.13 (t, ³J_{H-H} = 7.5 Hz, 2H, *m*-Ar), 7.05 (t, ³J_{H-H} = 7.5 Hz, 2H, *p*-Ar), 4.96 (s, 2H, OCH₂Ar), 1.03 (s, 12H, OBpin); ¹³C{¹H} NMR (C₆D₆, 101 MHz): 145.35 (ipso), 128.24 (*m*-Ar), 127.7 (*p*-Ar), 125.6 (*o*-Ar), 82.5 (OBpin), 72.9 (OCH₂Ar), 24.6 (OBpin-Me), ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.7 (OBpin).



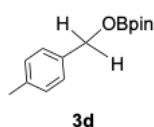
3b

3b³: ¹H NMR (400 MHz, C₆D₆): δ 7.06 (t, ³J_{H-H} = 6.5 Hz, 2H, *o*-Ar), 6.75 (t, ³J_{H-H} = 8.6 Hz, 2H, *m*-Ar), 4.80 (s, 2H, OCH₂Ar), 1.03 (s, 12H, OBpin); ¹³C{¹H} NMR (C₆D₆, 101 MHz): δ 162.6 (d, ¹J_{C-F} = 244 Hz, *p*-Ar), 135.7 (*ipso*), 128.8 (d, ³J_{C-F} = 8.4 Hz, *o*-Ar), 115.3 (d, ²J_{C-F} = 21 Hz, *m*-Ar), 82.8 (OBpin), 66.2 (OCH₂), 24.6 (OBpin-Me), ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.6 (OBpin); ¹⁹F{¹H} NMR (C₆D₆, 376 MHz): δ -115 (*p*-F).



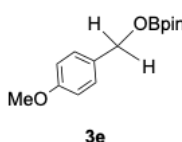
3c

3c³: ¹H NMR (400 MHz, C₆D₆): δ 6.96 (d, ³J_{H-H} = 8.0 Hz, 2H, *o*-Ar), 6.85 (d, ³J_{H-H} = 8.0 Hz, 2H, *p*-Ar), 4.65 (s, 2H, OCH₂), 1.02 (s, 12H, OBpin); ¹³C{¹H} NMR (C₆D₆, 101 MHz): δ 144.4 (*ipso*), 132.0 (*m*-Ar), 118.8 (*p*-CN), 111.7 (*p*-Ar), 83.0 (OBpin-C_q), 65.8 (OCH₂), 24.9, 24.6 (OBpin-Me); ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.6 (OBpin).



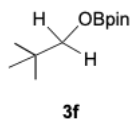
3d

3d³: ¹H NMR (400 MHz, C₆D₆): δ 7.27 (d, ³J_{H-H} = 8.0 Hz, 2H, *o*-Ar), 6.96 (d, ³J_{H-H} = 8.0 Hz, 2H, *m*-Ar), 4.97 (s, 2H, OCH₂), 2.07 (s, 3H, *p*-Me), 1.04 (s, 12H, OBpin); ¹³C{¹H} NMR (C₆D₆, 101 MHz): δ 129.3 (*m*-Ar), 127.2 (*o*-Ar), 82.63 (OBpin-C_q), 66.9 (OCH₂), 24.6 (OBpin-Me), 21.0 (*p*-Me); ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.7 (OBpin).



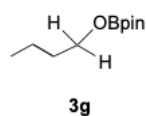
3e

3e³: ¹H NMR (400 MHz, C₆D₆): δ 7.27 (d, ³J_{H-H} = 9.0 Hz, 2H, *o*-Ar), 6.75 (d, ³J_{H-H} = 9.0 Hz, 2H, *m*-Ar), 4.94 (s, 2H, OCH₂), 3.26 (s, 2H, *p*-OMe), 1.04 (s, 12H, OBpin); ¹³C{¹H} NMR (C₆D₆, 101 MHz): δ 159.6 (*p*-Ar), 132.2 (*ipso*), 128.8 (*o*-Ar), 114.1 (*m*-Ar), 82.6 (OBpin-C_q), 66.8 (OCH₂), 54.7 (*p*-OMe), 24.7 (OBpin-Me), ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.8 (OBpin).



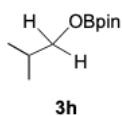
3f

3f⁴: ¹H NMR (400 MHz, C₆D₆): δ 3.66 (s, 4H, OCH₂), 1.06 (s, 12H, OBpin), 0.90 (s, 3H, Me); ¹³C{¹H} NMR (C₆D₆, 101 MHz): 82.3 (OBpin-C_q), 75.1 (OCH₂), 32.5 (C_q), 26.2 (Me), 24.7 (OBpin-Me); ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.5 (OBpin).

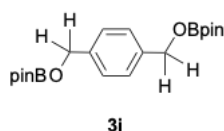


3g

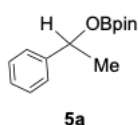
3g⁵: ¹H NMR (400 MHz, C₆D₆): δ 3.93 (d, ³J_{H-H} = 6.5 Hz, 2H, CH₂O), 1.54-1.47 (m, 2H, CH₂), 1.35-1.25 (m, 2H, CH₂), 1.06 (OBpin), 0.80 (t, ³J_{H-H} = 7.3 Hz, 3H, Me); ¹³C{¹H} NMR (C₆D₆, 101 MHz): 83.1, 82.3 (OBpin-C_q), 64.8 (OCH₂), 35.0 (CH₂), 24.9 (OBpin-Me), 19.1 (CH₂), 13.9 (Me); ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.5 (OBpin).



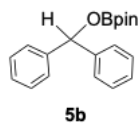
3h⁶: ¹H NMR (400 MHz, C₆D₆): δ 3.73 (d, ³J_{H-H} = 6.7 Hz, 2H, CH₂O), 1.83-1.74 (m, 1H, CH), 1.06 (OBpin), 0.84 (d, ³J_{H-H} = 6.9 Hz, 6H, Me); ¹³C{¹H} NMR (C₆D₆, 101 MHz): 83.1, 82.3 (OBpin-C_q), 71.5 (OCH₂), 30.3 (CH), 24.9, 24.8 (OBpin-Me), 18.9 (Me); ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.8 (OBpin).



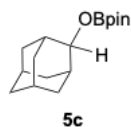
3i⁷: ¹H NMR (400 MHz, C₆D₆): δ 7.27 (s, Ar), 4.92 (s, 4H, OCH₂), 1.03 (OBpin); ¹³C{¹H} NMR (C₆D₆, 101 MHz): 139.1 (*ipso*), 127.1 (Ar), 82.7 (OBpin-C_q), 66.7 (OCH₂), 24.9, 24.6 (OBpin-Me); ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.8 (OBpin).



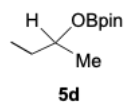
5a⁸: ¹H NMR (400 MHz, C₆D₆): δ 7.37 (d, ³J_{H-H} = 7.2 Hz, 1H, *o*-Ar), 7.12 (d, ³J_{H-H} = 7.2 Hz, 1H, *m*-Ar), 7.04 (t, ³J_{H-H} = 7.2 Hz, 1H, *p*-Ar), 5.41 (q, ³J_{H-H} = 6.6 Hz, 1H, OCH), 1.45 (d, ³J_{H-H} = 6.6 Hz, 3H, OCMe), 1.02 (OBpin), 1.01 (OBpin); ¹³C{¹H} NMR (C₆D₆, 101 MHz): 145.4 (*ipso*), 128.5 (*m*-Ar), 127.3 (*o*-Ar), 125.7 (*p*-Ar), 82.5 (OBpin-C_q), 72.9 (OCH), 25.7 (OCMe), 24.9, 24.6, 24.5 (OBpin-Me); ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.4 (OBpin).



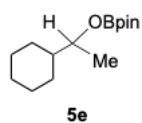
5b³: ¹H NMR (400 MHz, C₆D₆): δ 7.44 (d, ³J_{H-H} = 7.7 Hz, 4H, *o*-Ar), 7.09 (t, ³J_{H-H} = 7.7 Hz, 4H, *m*-Ar), 7.00 (d, ³J_{H-H} = 7.7 Hz, 1H, *p*-Ar), 6.43 (s, OCH), 0.97 (OBpin); ¹³C{¹H} NMR (C₆D₆, 101 MHz): 143.9 (*ipso*), 128.5 (*m*-Ar), 127.5 (*o*-Ar), 126.9 (*p*-Ar), 82.8 (OBpin-C_q), 78.5 (OCH), 24.5 (OBpin-Me); ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.6 (OBpin).



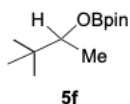
5c³: ¹H NMR (400 MHz, C₆D₆): δ 4.48 (broad pseudo-singlet, 1H, OCH), 2.41–2.38 (br pseudo-doublet, 2H, Ad), 2.08 (br pseudo-singlet, 2H, Ad), 1.71-1.43 (br pseudo-quintet, 10H, Ad), 1.07 (s, 12H, OBpin); ¹³C{¹H} NMR (C₆D₆, 100 MHz): 82.2 (Bpin-C_q), 77.1 (OCH), 37.8, 36.6, 34.6, 31.5, 27.9, 27.4 (Ad), 24.7 (Bpin-Me); ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.16 (OBpin).



5d⁸: ¹H NMR (400 MHz, C₆D₆): δ 4.26 (sextet, ³J_{H-H} = 6.3 Hz, 1H, OCH), 1.58-1.34 (m, 2H, CH₂), 1.17 (d, ³J_{H-H} = 6.3 Hz, 3H, OCMe), 1.06 (s, 12H, OBpin), 0.87 (t, ³J_{H-H} = 7.8 Hz, 3H, CH₃); ¹³C{¹H} NMR (C₆D₆, 101 MHz): 82.1 (OBpin-C_q), 72.2 (OCH), 31.4(CH₂), 24.9, 24.6 (OBpin-Me), 22.3 (OCMe), 10.0 (CH₃); ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.4 (OBpin).



5e⁹: ¹H NMR (400 MHz, C₆D₆): δ 4.16 (quintet, ³*J*_{H-H} = 6.0 Hz, 1H, OCH), 1.91–1.88 (m, 1H, Cy), 1.69–1.62 (m, 3H, Cy), 1.57–1.55 (m, 1H, Cy), 1.37–1.27 (m, 1H, Cy), 1.19 (d, ³*J*_{H-H} = 6.0 Hz, 3H, OCM*e*), 1.15–1.12 (m, 2H, Cy), 1.08 (s, 12H, OB*pin*), 1.00 (s, 3H); ¹³C{¹H} NMR (101 MHz, C₆D₆): δ 82.1 (OBpin-C_q), 75.0 (OCH), 44.7 (Cy), 29.1 (Cy), 28.6 (Cy), 26.8 (Cy), 26.5 (Cy), 26.4 (Cy), 24.7 (OBpin-Me), 20.0 (OC*Me*); ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.4 (OBpin).



5f⁷: ¹H NMR (400 MHz, C₆D₆): δ 4.12–4.07 (q, ³*J*_{H-H} = 6.3 Hz, 1H, CH), 1.07 (s, 12H, OB*pin*), 1.01 (s, 3H, OCM*e*), 0.91 (s, 9H, ^tBu); ¹³C{¹H} NMR (C₆D₆, 101 MHz): 82.1 (OBpin-C_q), 78.2 (OCH), 35.0 (^tBu-C_q), 24.7 (OBpin-Me), 17.6 (OC*Me*); ¹¹B{¹H} NMR (162 MHz, C₆D₆): δ 22.4 (OBpin).

4. Eyring Plot

According to the methodology described in the literature,¹⁰ the kinetic experiments were conducted.

Two sets of five solutions of benzaldehyde **2a** (2.7 mg, 0.025 mmol, 1.0 eq.) and HBpin (4.8 mg, 0.038 mmol, 1.5 eq.) in C₆D₆ (2.0 mL) were prepared. One set was added with **1** (1.5 mg, 2.5 μmol, 10 mol%) and was labelled Experiment A, while the other set was kept catalyst-free and labelled Experiment B. These solutions were heated to 305, 307, 310, 315, and 320 K.

The apparent initial rate constants for Experiment A (k_{A0}) and Experiment B (k_{B0} , blank) were obtained from linear plots of [**3a**] versus time (s). Since a small background reaction occurred under catalyst-free conditions, the intrinsic catalytic rate constant (k_0) was determined by subtracting the blank rate (k_{B0} , blank) from the apparent rate (k_0) obtained under catalytic conditions (Table S1).

Table S1 Eyring plot data

2a + HBpin (1.5 eq.) $\xrightarrow[\text{C}_6\text{D}_6, 300-320 \text{ K, 30 min}]{\text{1 (10 mol\%)}}$ **3a**

Temp. [K]	Experiment A k_{A0} [μM/s]	Experiment A [k_{A0}] – B [k_{B0}] k_0 [μM/s]	1000/ T [K ⁻¹]	ln (k_0/T)
305	7.56	4.33	3.17	-17.74
307	8.21	4.53	3.23	-17.91
310	8.83	5.16	3.26	-18.03
315	9.85	6.21	3.28	-18.07
320	10.4	7.11	3.13	-17.62

The Eyring plot (Fig. S2) was constructed using these corrected rate constants (k_0). Activation parameters were obtained from the slope and intercept of the linear plots of ln(k_0/T) versus 1/ T , according to the Eyring equation. The activation parameters were determined from the Eyring plot, as summarized in Table S2.

$$\ln\left(\frac{k_0}{T}\right) = \left(\frac{-\Delta H^\ddagger}{R}\right)\left(\frac{1}{T}\right) + \frac{\Delta S^\ddagger}{R} + \ln\left(\frac{k_B}{h}\right)$$

$R = 8.314 \text{ J/mol}\cdot\text{K}$ (Ideal gas constant)

$k_B = 1.38 \times 10^{-23} \text{ J}\cdot\text{K}^{-1}$ (Boltzman constant)

$h = 6.63 \times 10^{-34} \text{ J}\cdot\text{s}$ (Planck's constant)

Gibbs free energy of activation was determined using the following equation:

$$\Delta G^\ddagger = \Delta H^\ddagger - T\Delta S^\ddagger$$

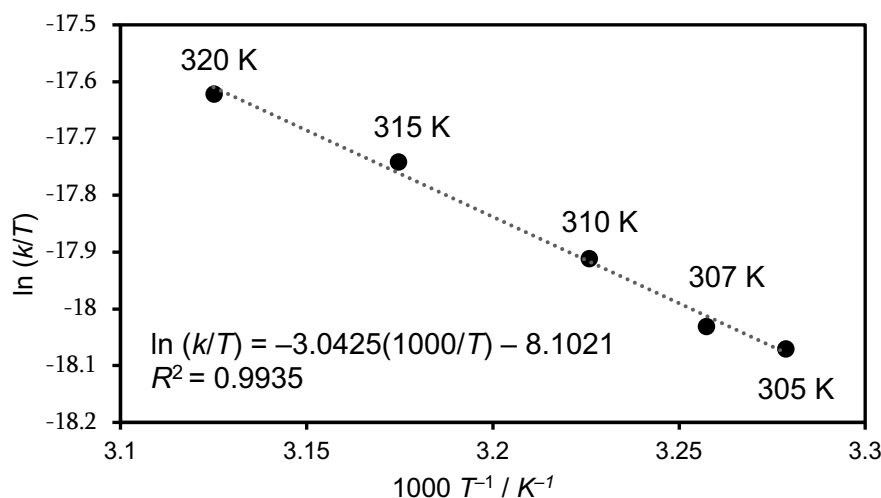


Fig. S2 Eyring plot for benzaldehyde **2a**.

Table S2 Activation parameters for the catalytic hydroboration of **2a** with HBpin mediated by **1**

	$\Delta G^\ddagger_{298.15}$ [kcal/mol]	$\Delta H^\ddagger$ [kcal/mol]	$\Delta S^\ddagger$ [cal/mol · K]
Experiment A	24.5(3)	3.1(3)	-72(1)
Experiment A [k_{A0}] – B [k_{B0}]	24.9(3)	6.0(3)	-63(1)
Theoretical ^[a]	25.0	6.7	-53.1

^[a] The thermodynamic quantities were evaluated at the PW6B95+D3BJ/Def2-TZVPP//PW6B95+D3BJ/Def2-SVP///SMD(C₆H₆) level at 298.15 K and are relative to **b** as shown on.

5. Kinetic Isotope Effect (KIE, k_H/k_D):

5.1 Hydroboration of benzaldehyde **2a** with DBpin without catalyst **1**

Following the procedure described in Section 2.1, a solution of **2a** (2.7 mg, 0.025 mmol, 1.0 eq.), DBpin (6.6 mg, 0.038 mmol, 1.5 eq.) and C₆Me₆ (>1.0 mg) as an internal standard in C₆D₆ (0.50 mL) was prepared. The reaction was monitored by ¹H NMR spectroscopy at 300 K. After 9 hours, PhCH(D)OBpin (**3a-d**) was observed with an NMR yield of 17%.

5.2 Hydroboration of benzaldehyde **2a** with DBpin in the presence of catalyst **1**

Following the procedure described in Section 2.2, a solution of **1** (1.6 mg, 2.8 μmol, 10 mol%), **2a** (2.7 mg, 0.025 mmol, 1.0 eq.), DBpin (6.6 mg, 0.038 mmol, 1.5 eq.) and C₆Me₆ (>1.0 mg) as an internal standard in C₆D₆ (0.50 mL) was prepared. The reaction was monitored by ¹H NMR spectroscopy at 300 K, affording **3a-d** in 83% NMR yield after 12 hours.

3a-d: ¹H NMR (400 MHz, C₆D₆) δ 1.03 (s, 12H, OBpin(CH₃)), 4.93 (s, 1H, OCH(D)Ph), 7.04 (t, ³J_{HH} = 7.5 Hz, 1H, *p*-Ph), 7.12 (t, ³J_{H-H} = 7.5 Hz, 2H, *m*-Ph), 7.31 (d, ³J_{H-H} = 7.5 Hz, 2H, *o*-Ph), ¹¹B{¹H} NMR (MHz, C₆D₆, 300 K) δ 22.8.

Using the same method as described in Section 5, the catalytic rate of **1** was obtained by subtracting the uncatalyzed rate (no cat.) from the observed rate. The processed results are shown in Fig. S3, which presents the time-dependent concentration changes of **3a** and **3a-d** over 40 minutes. From the slopes of these plots, the kinetic isotope effect (KIE) was determined to be 1.8(1).

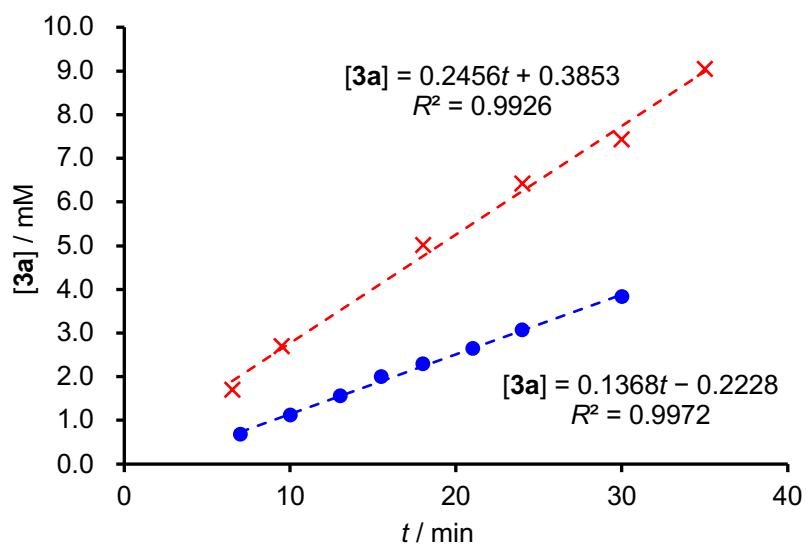


Fig. S3 KIE plot for benzaldehyde **2a**.

6. NMR Spectra of Products

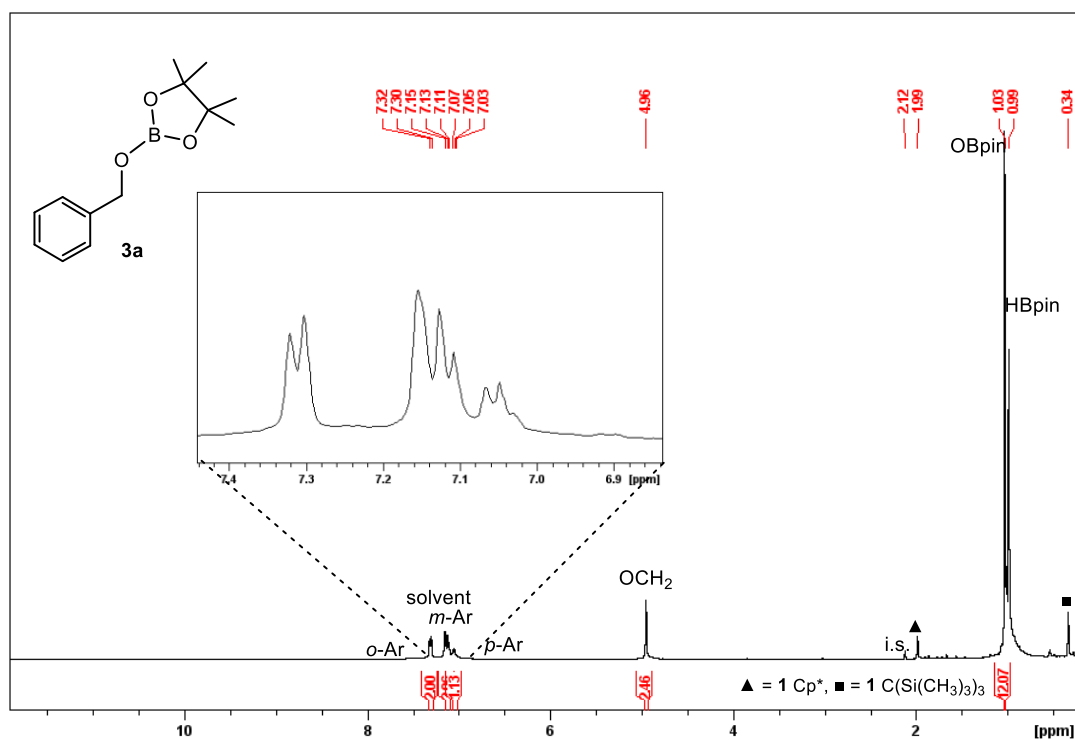


Fig. S4 ^1H NMR spectrum (C_6D_6 , 400 MHz) of **3a**.

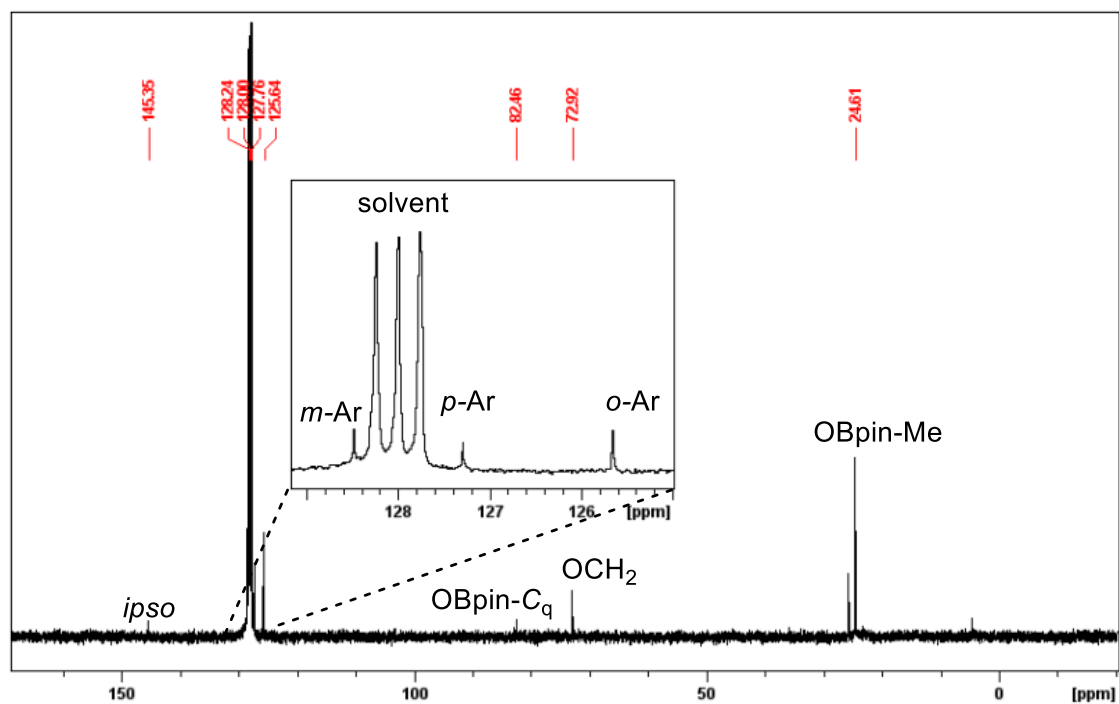


Fig. S5 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 101 MHz) of **3a**.

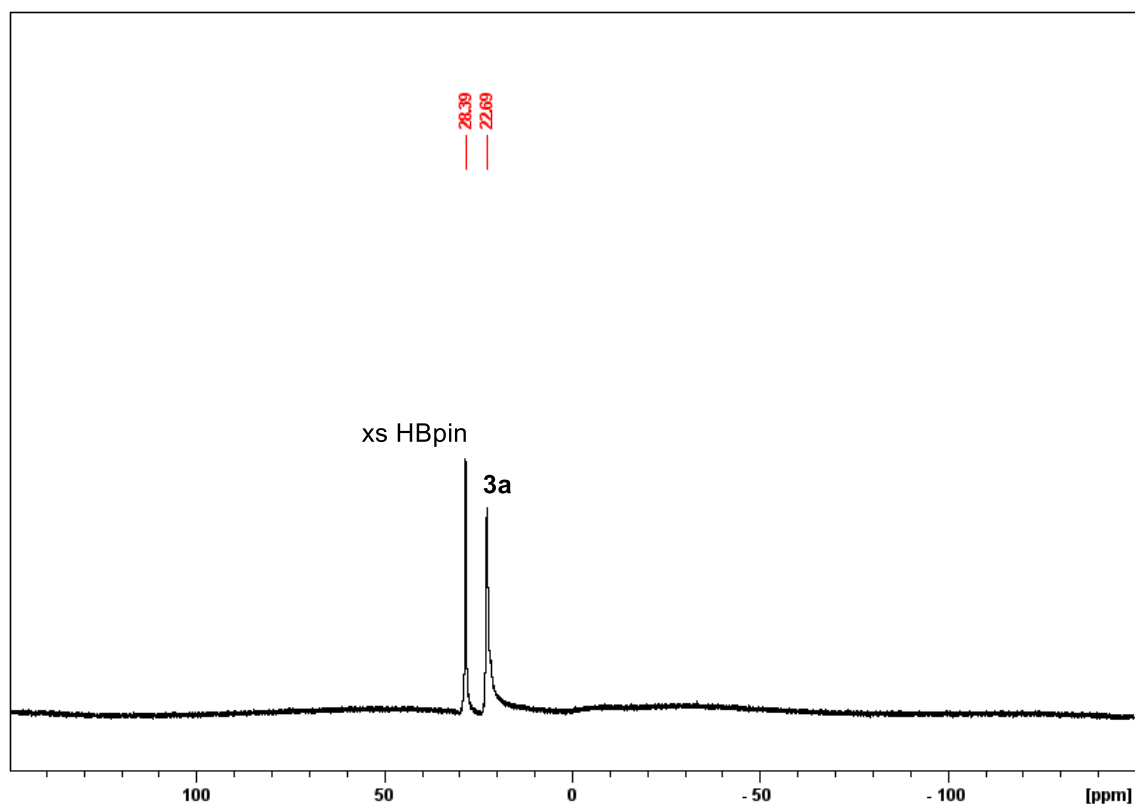


Fig. S6 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 126 MHz) of **3a**.

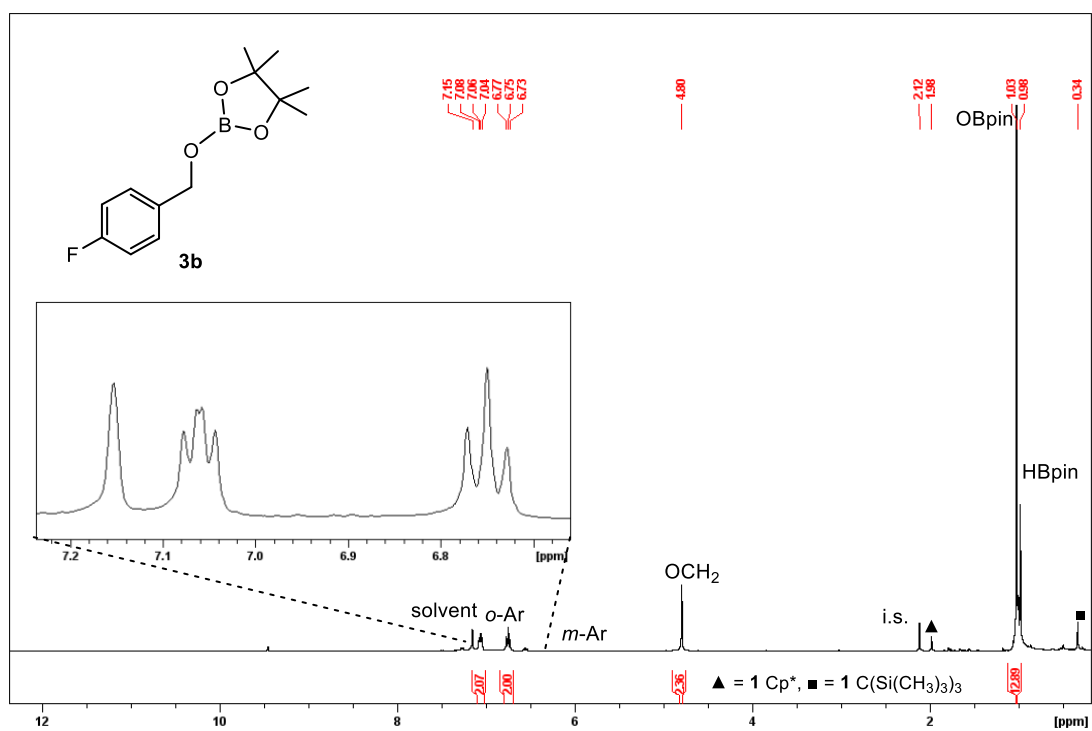


Fig. S7 ^1H NMR spectrum (C_6D_6 , 400 MHz) of **3b**.

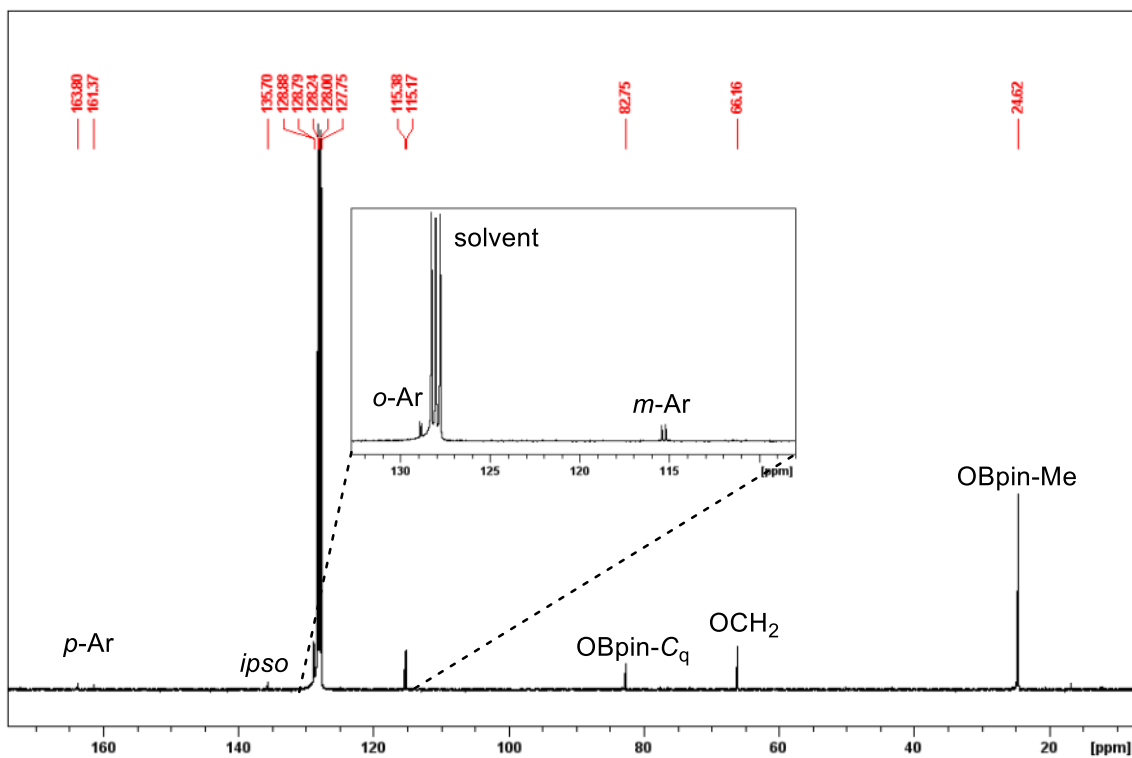


Fig. S8 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (CDCl₃, 101 MHz) of **3b**.

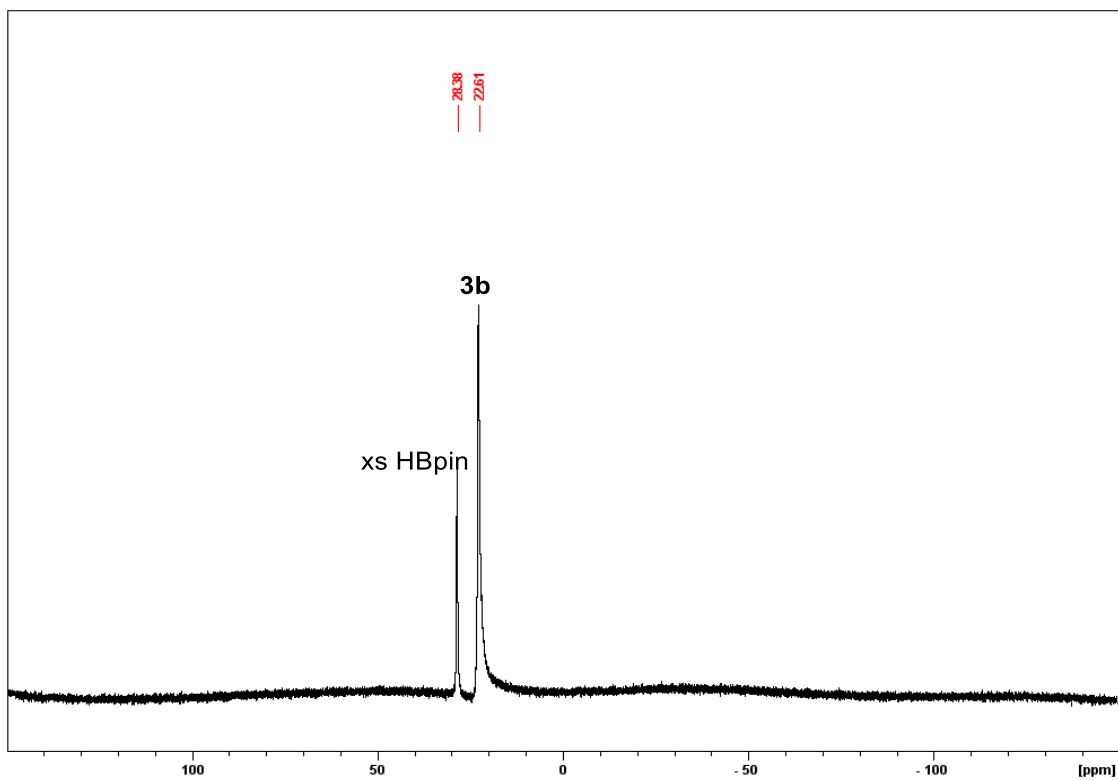


Fig. S9 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (CDCl₃, 126 MHz) of **3b**.

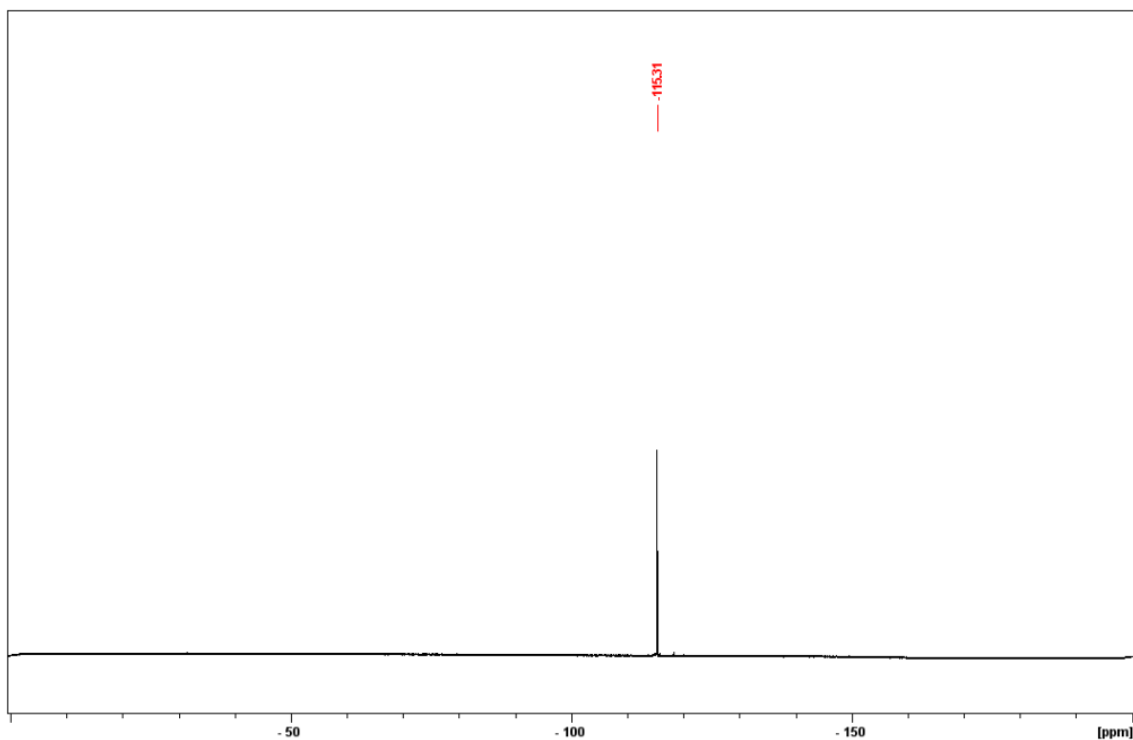


Fig. S10 $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 376 MHz) of **3b**.

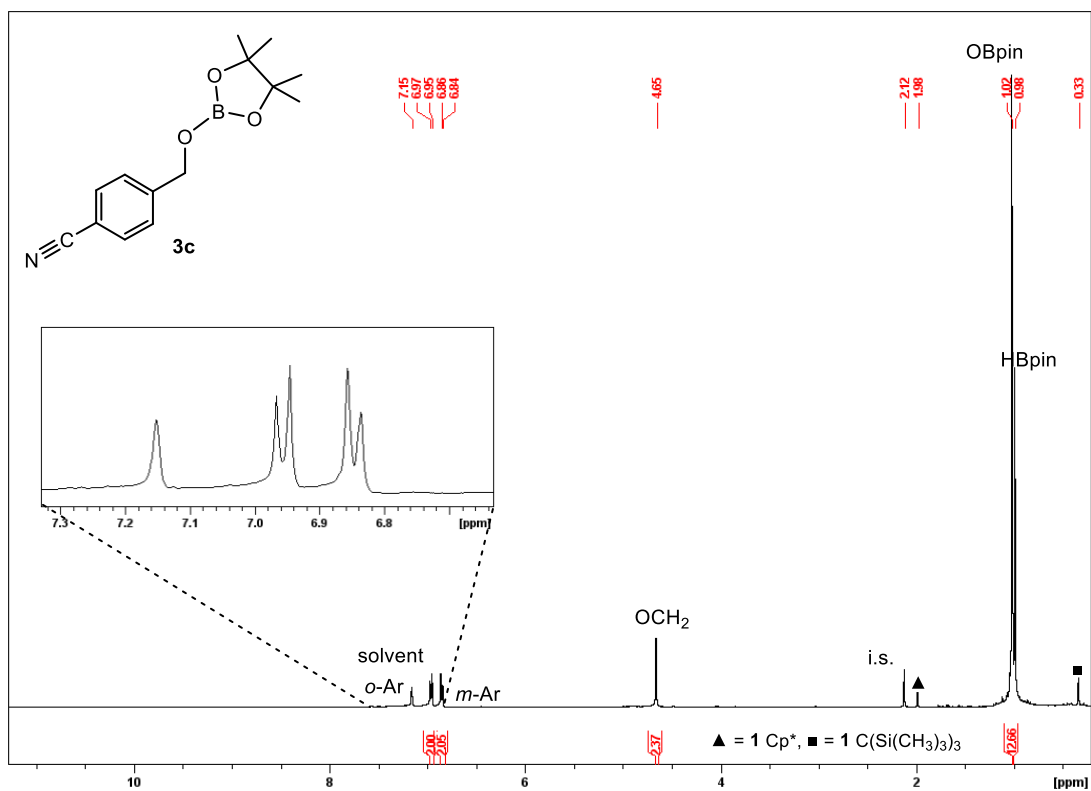


Fig. S11 ^1H NMR spectrum (C_6D_6 , 400 MHz) of **3c**.

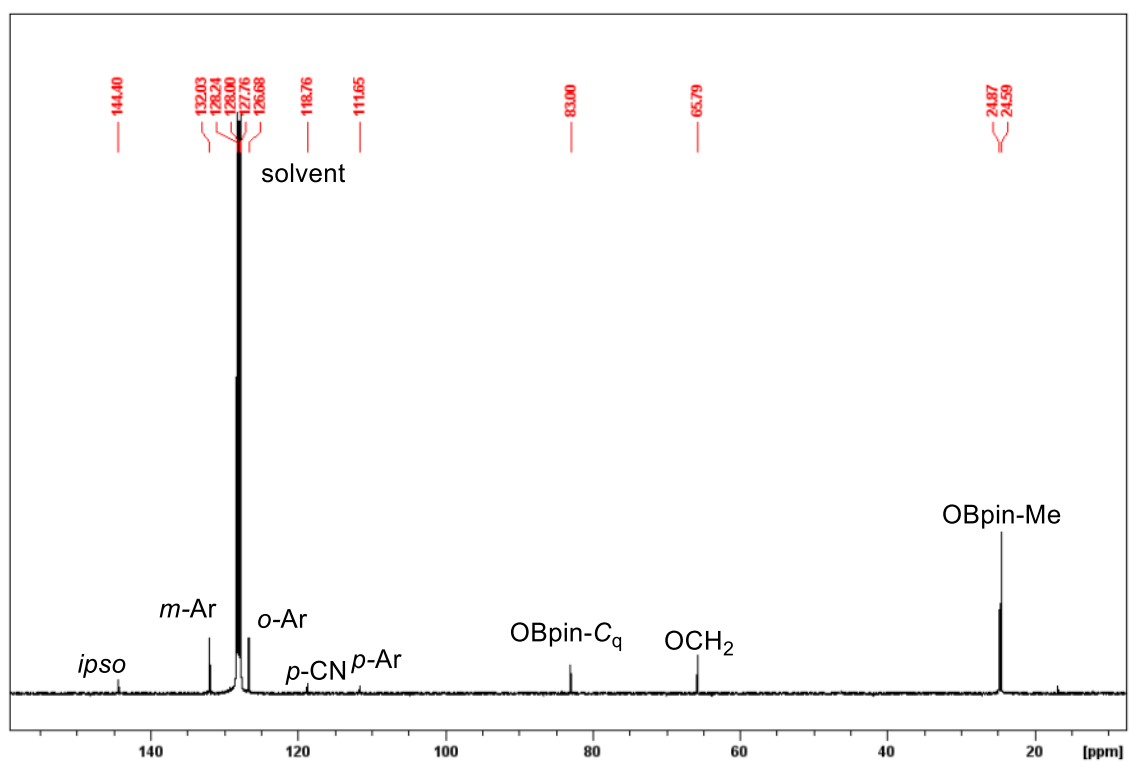


Fig. S12 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 101 MHz) of **3c**.

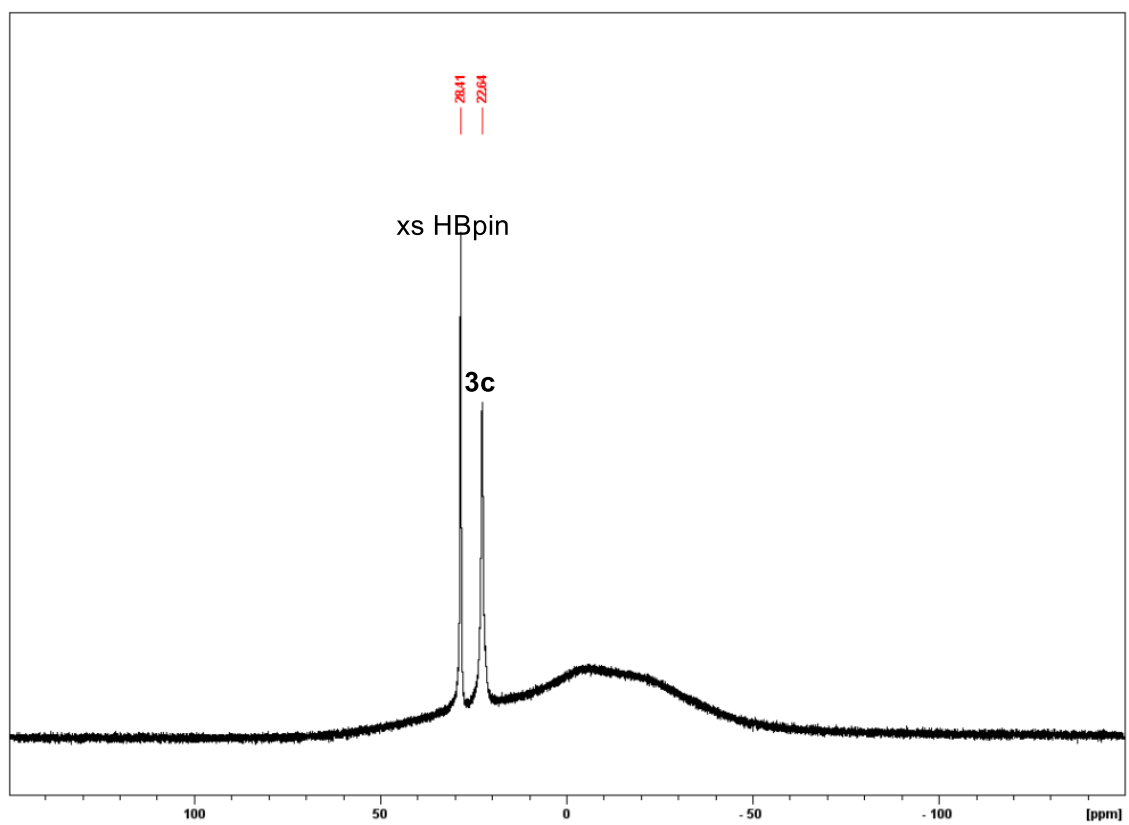


Fig. S13 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 126 MHz) of **3c**.

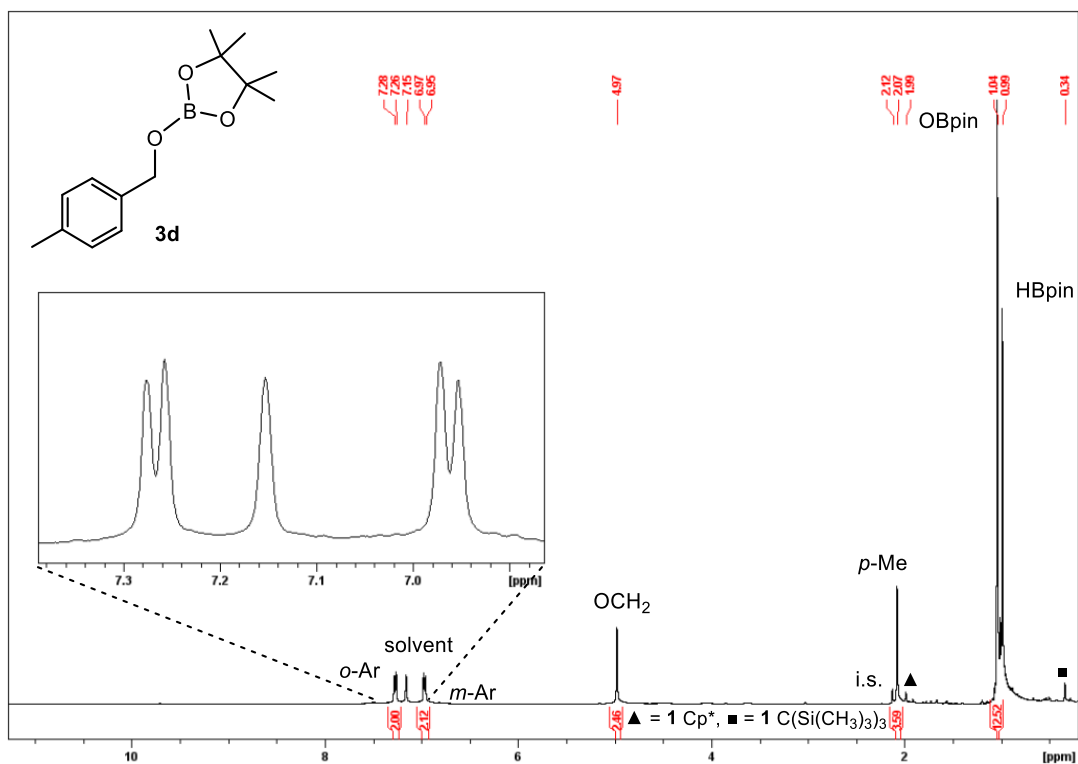


Fig. S14 ¹H NMR spectrum (C₆D₆, 400 MHz) of **3d**.

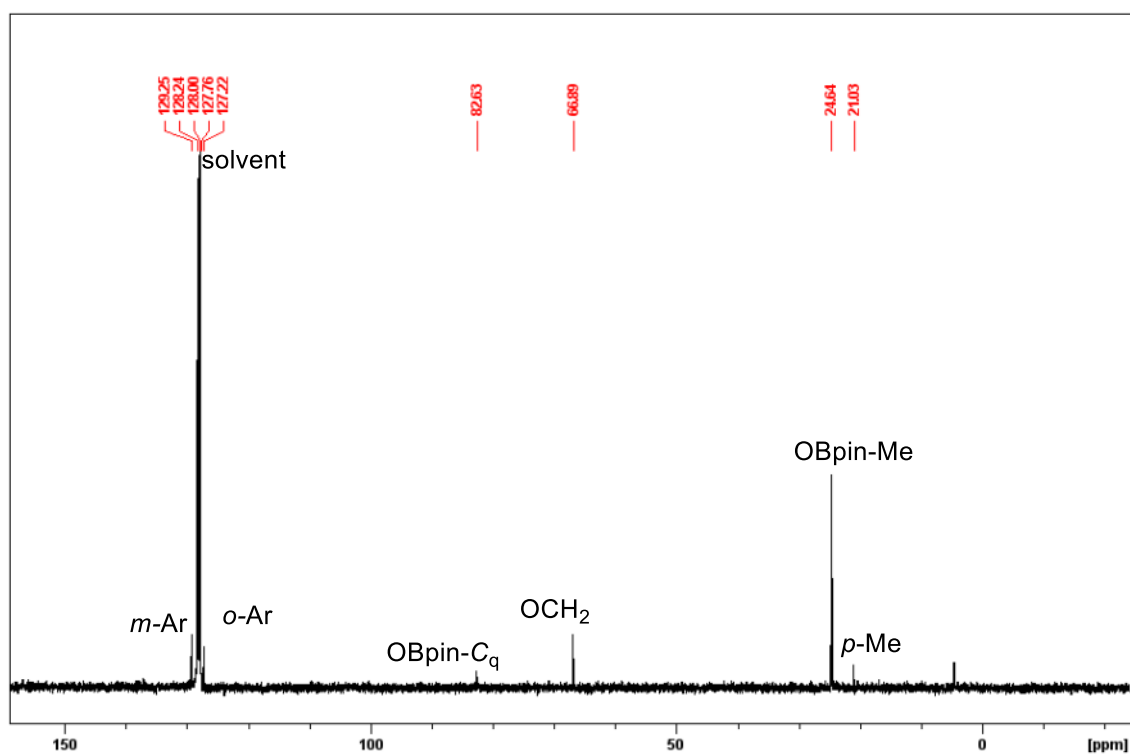


Fig. S15 ¹³C{¹H} NMR spectrum (C₆D₆, 101 MHz) of **3d**.

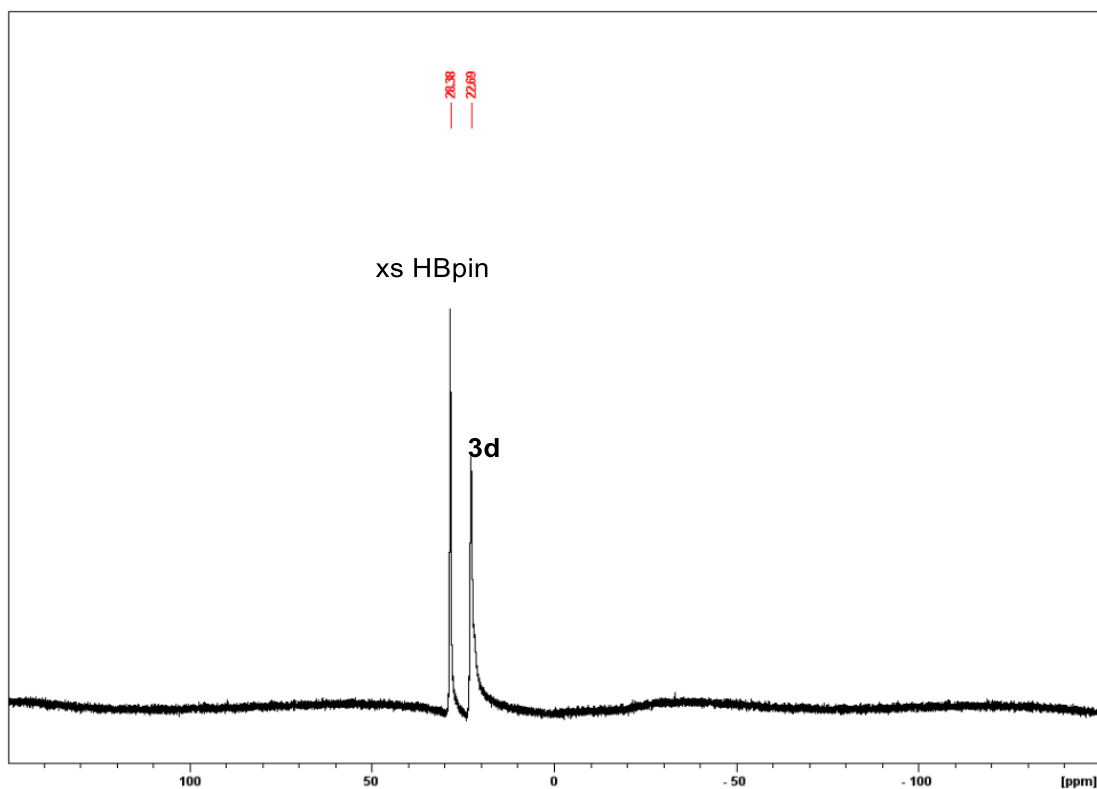


Fig. S16 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 126 MHz) of **3d**.

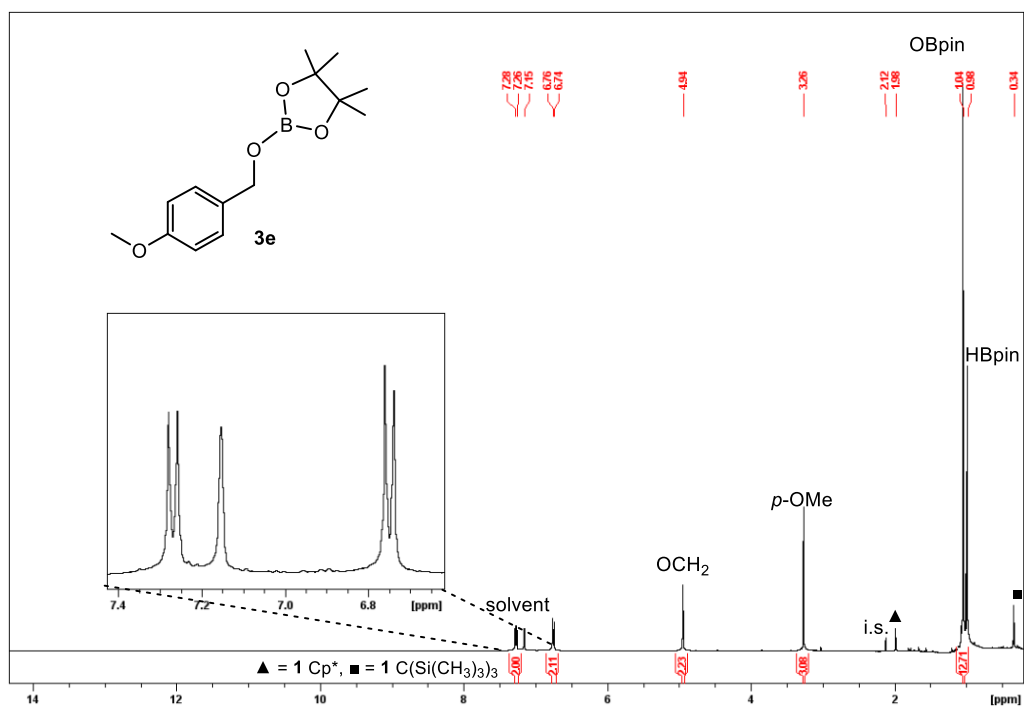


Fig. S17 ^1H NMR spectrum (C_6D_6 , 400 MHz) of **3e**.

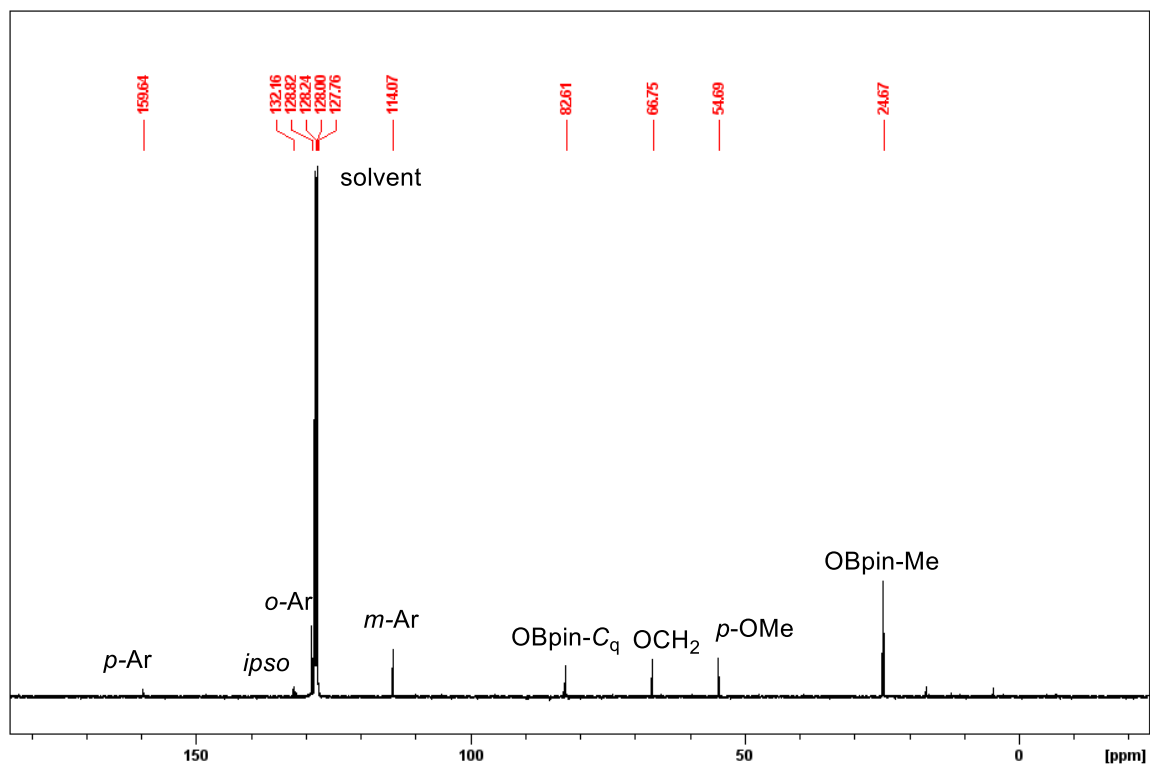


Fig. S18 ¹³C{¹H} NMR spectrum (C₆D₆, 101 MHz) of **3e**.

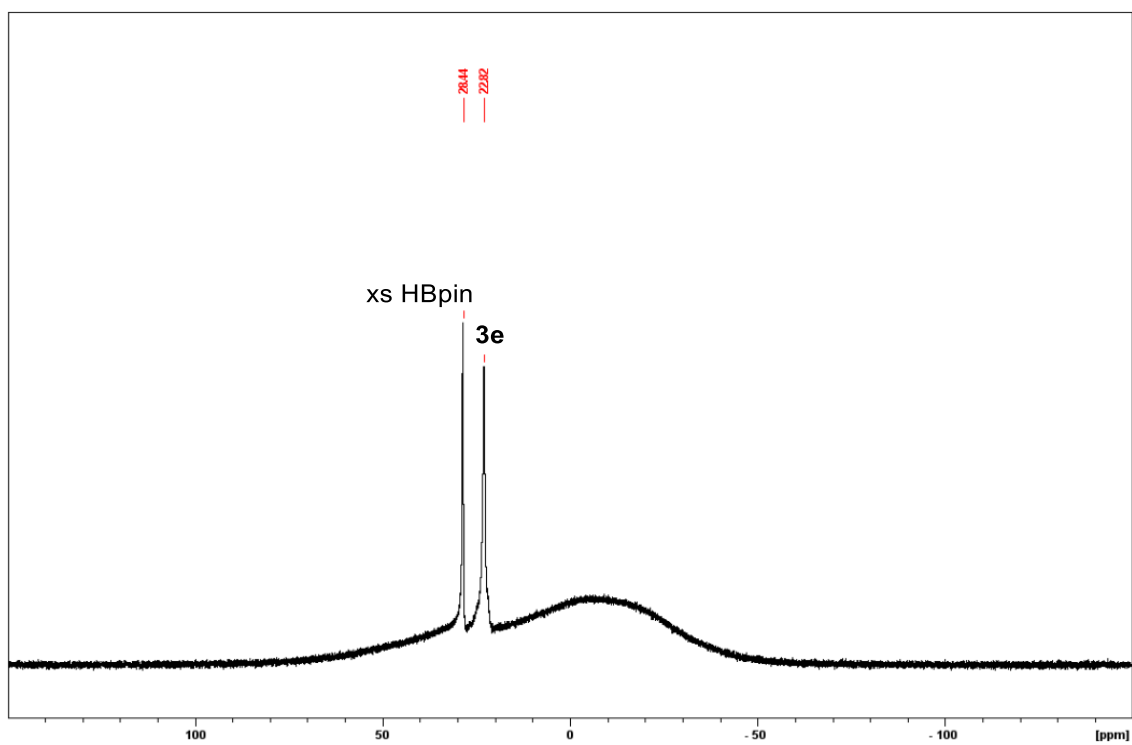


Fig. S19 ¹¹B{¹H} NMR spectrum (C₆D₆, 126 MHz) of **3e**.

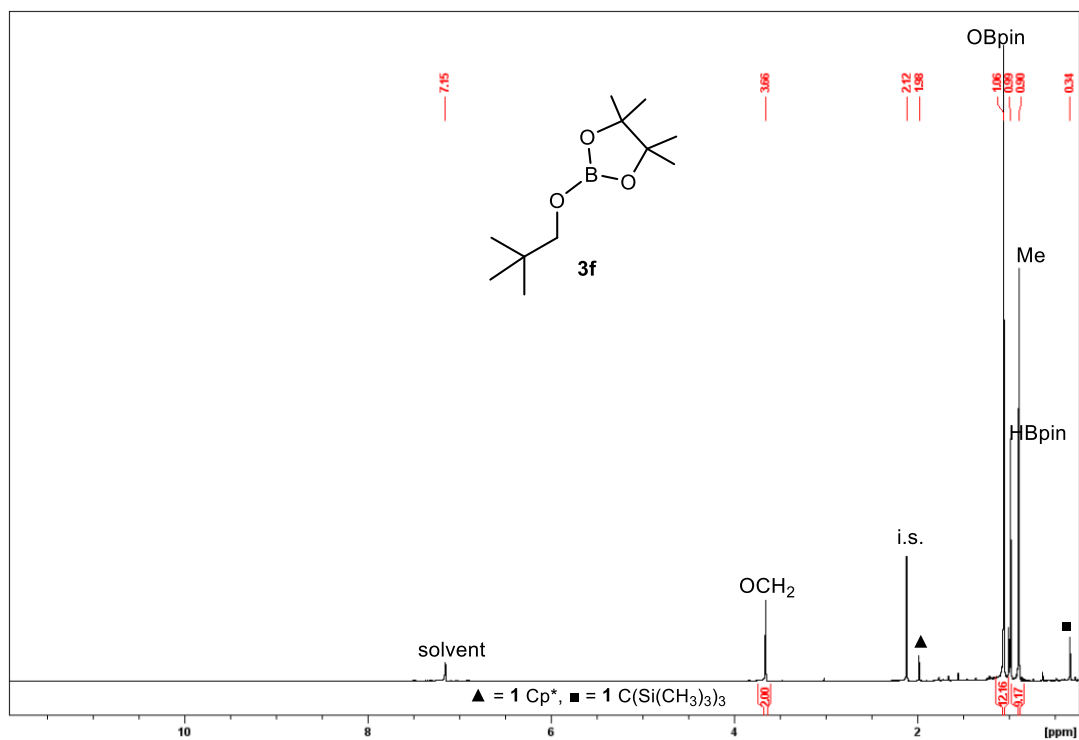


Fig. S20 ¹H NMR spectrum (C₆D₆, 400 MHz) of **3f**.

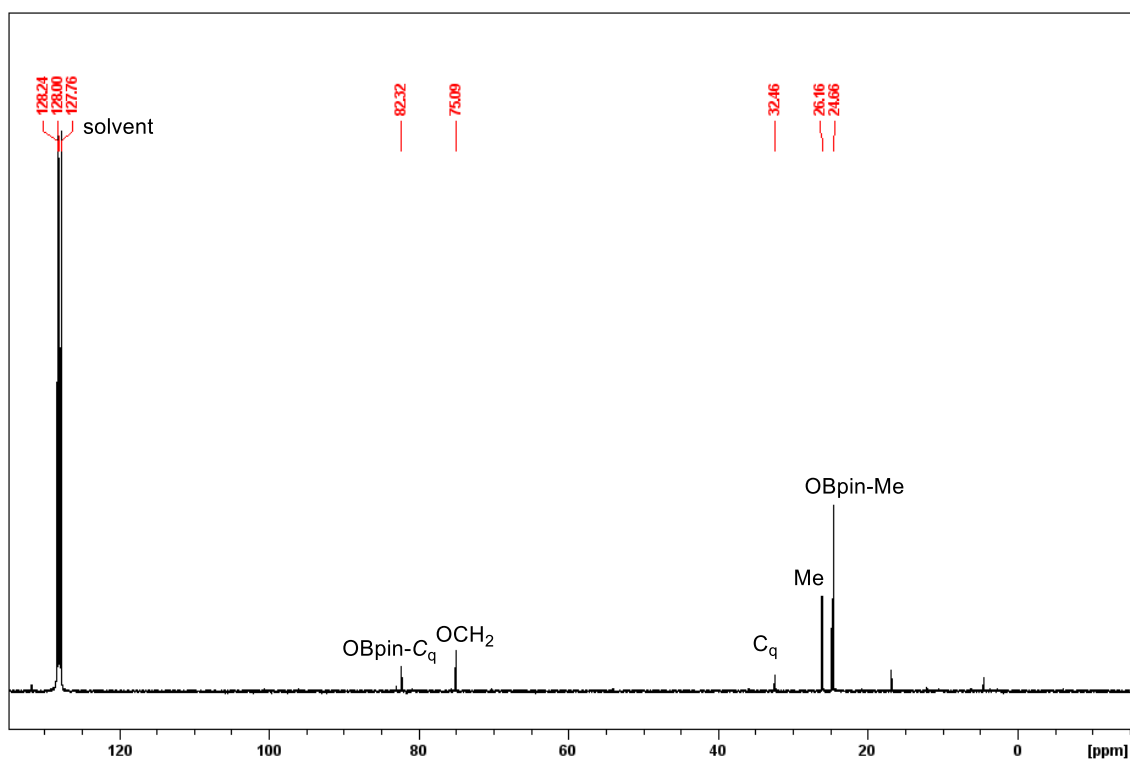
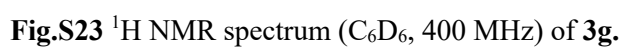
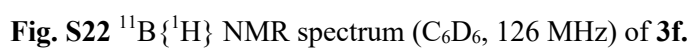


Fig. S21 ¹³C{¹H} NMR spectrum (C₆D₆, 101 MHz) of **3f**.



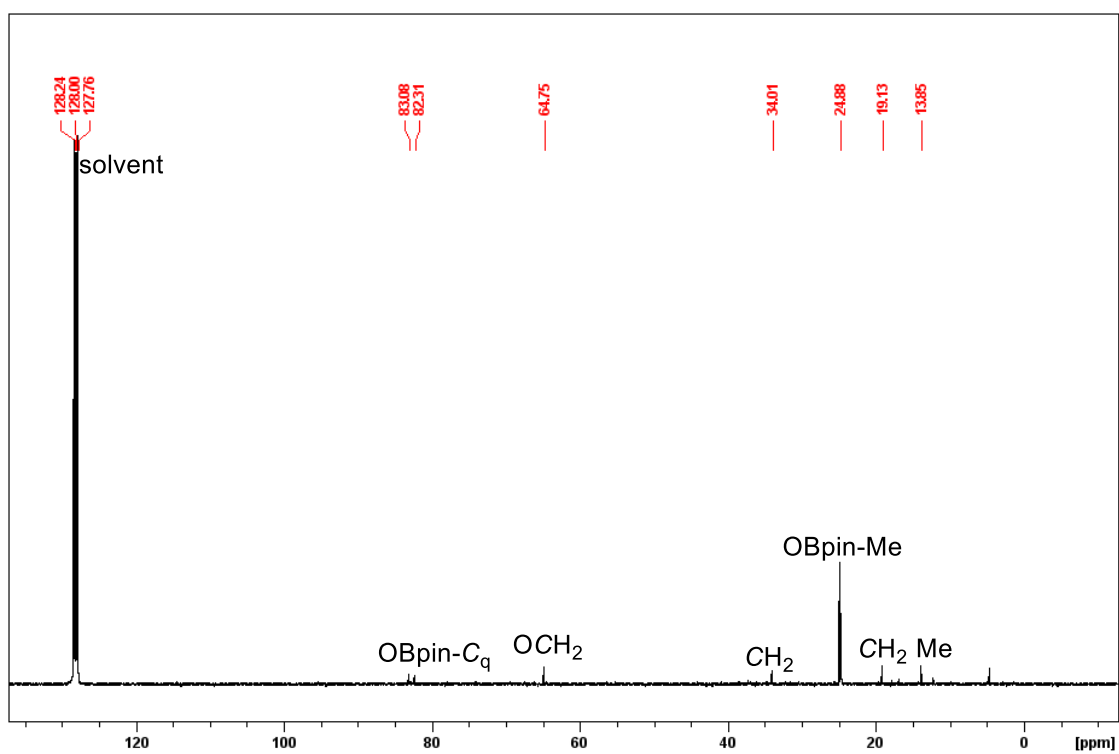


Fig. S24 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 101 MHz) of **3g**.

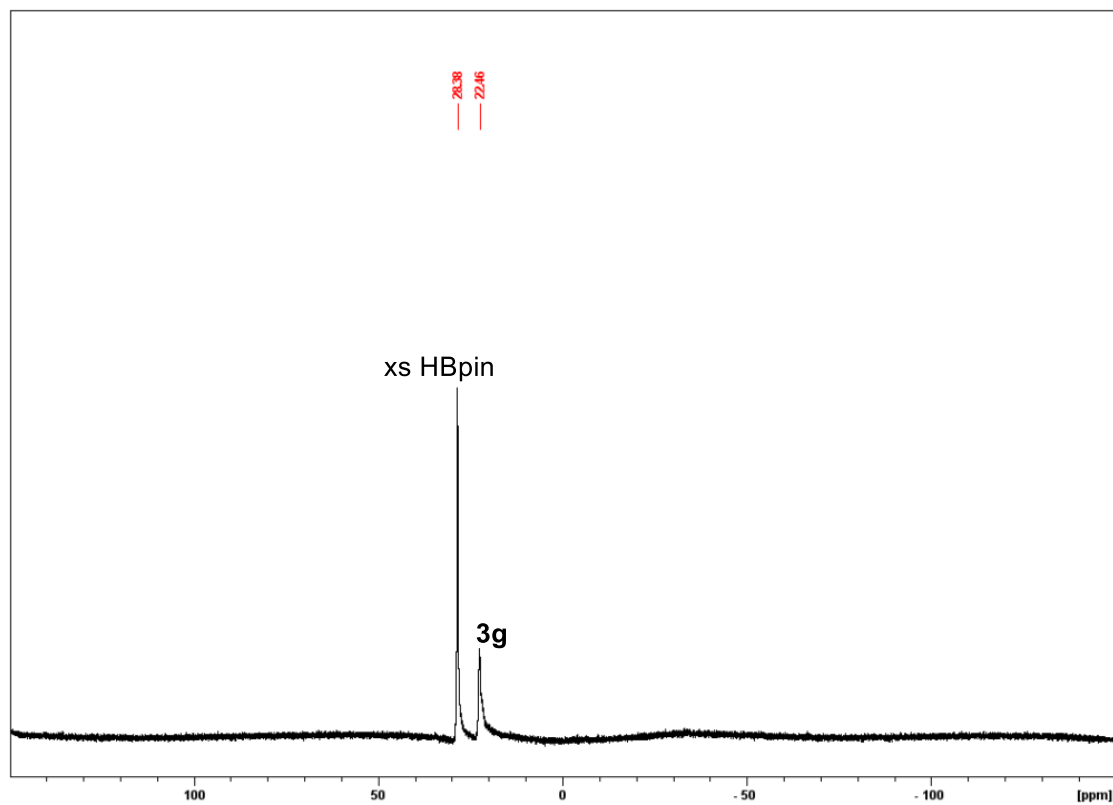


Fig. S25 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 126 MHz) of **3g**.

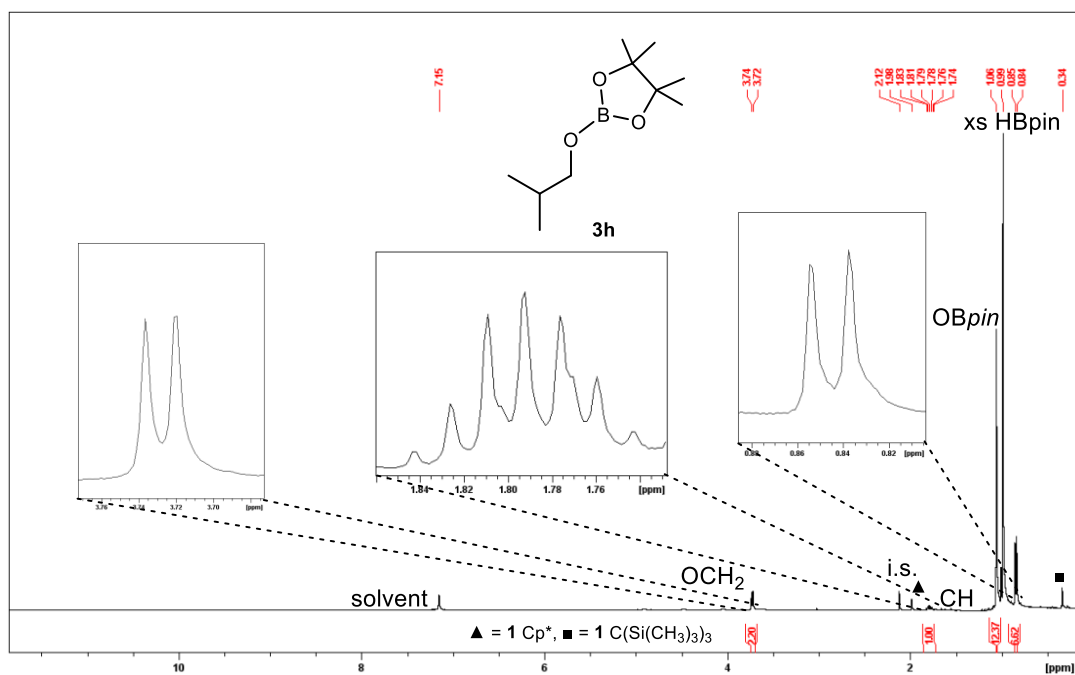


Fig. S26 ^1H NMR spectrum (C_6D_6 , 400 MHz) of **3h**.

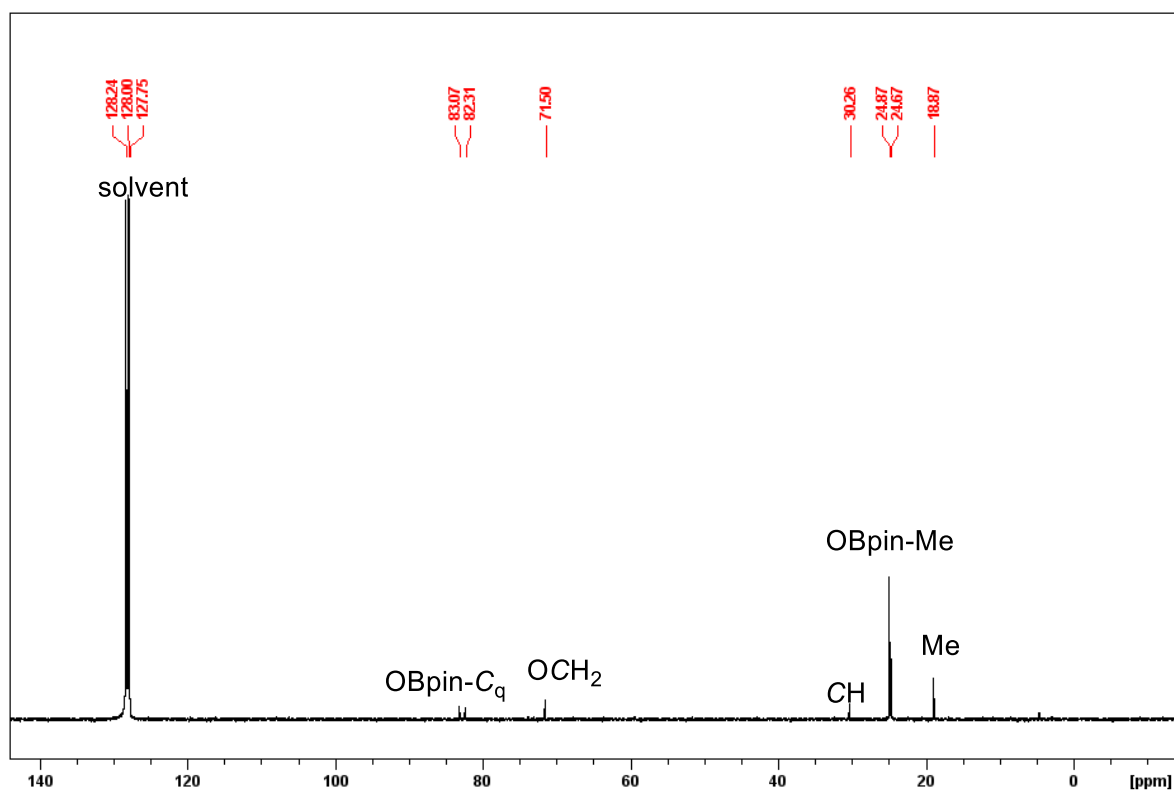


Fig. S27 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 101 MHz) of **3h**.

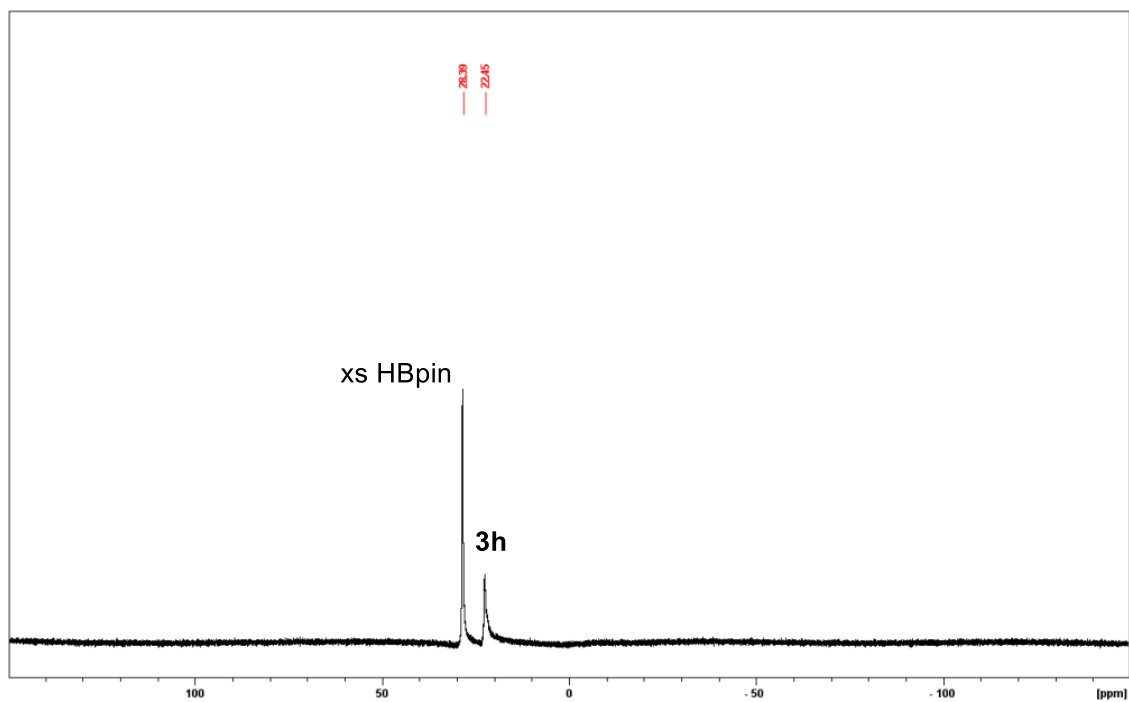


Fig. S28 ¹¹B{¹H} NMR spectrum (C₆D₆, 126 MHz) of **3h**.

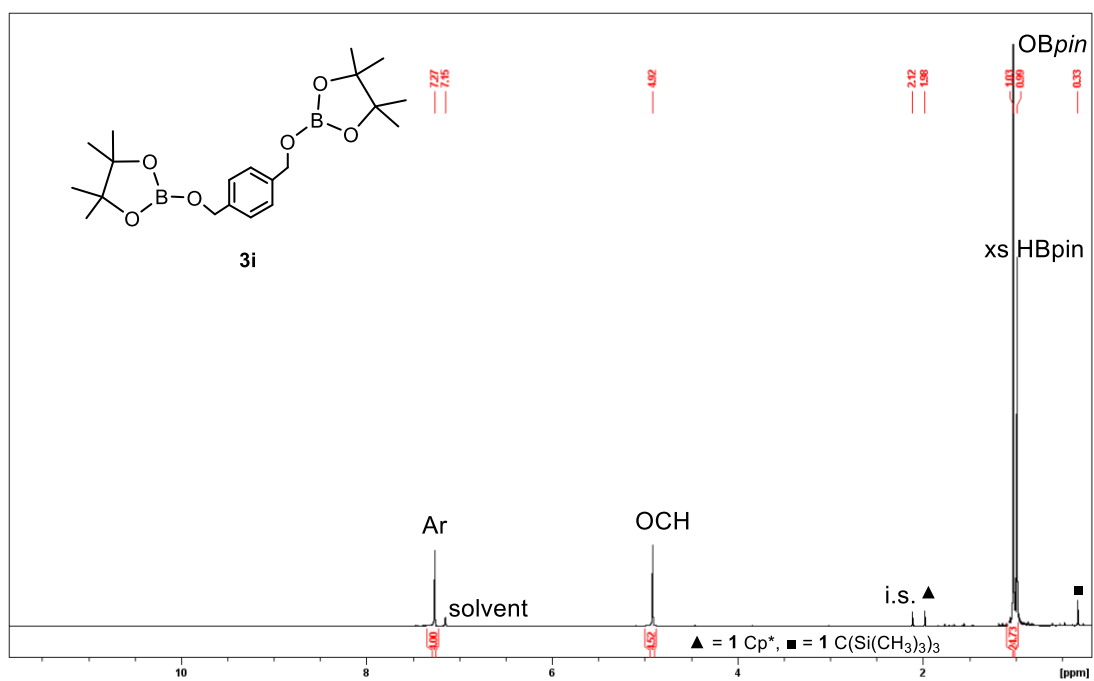


Fig. S29 ¹H NMR spectrum (C₆D₆, 400 MHz) of **3i**.

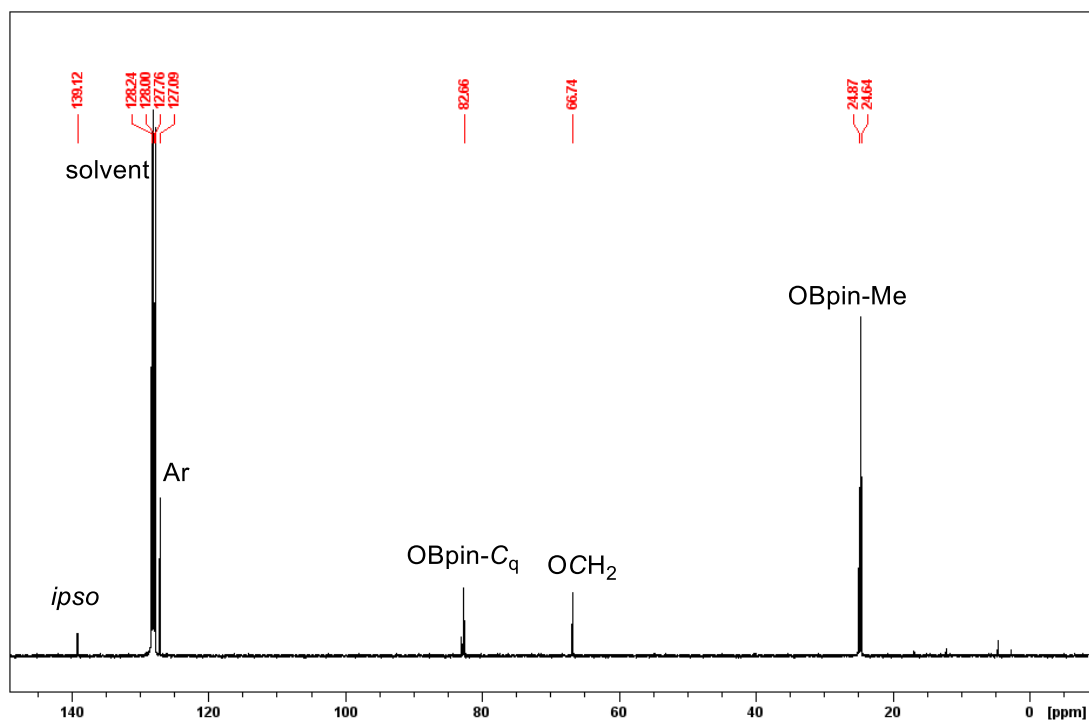


Fig. S30 ¹³C{¹H} NMR spectrum (C₆D₆, 101 MHz) of **3i**.

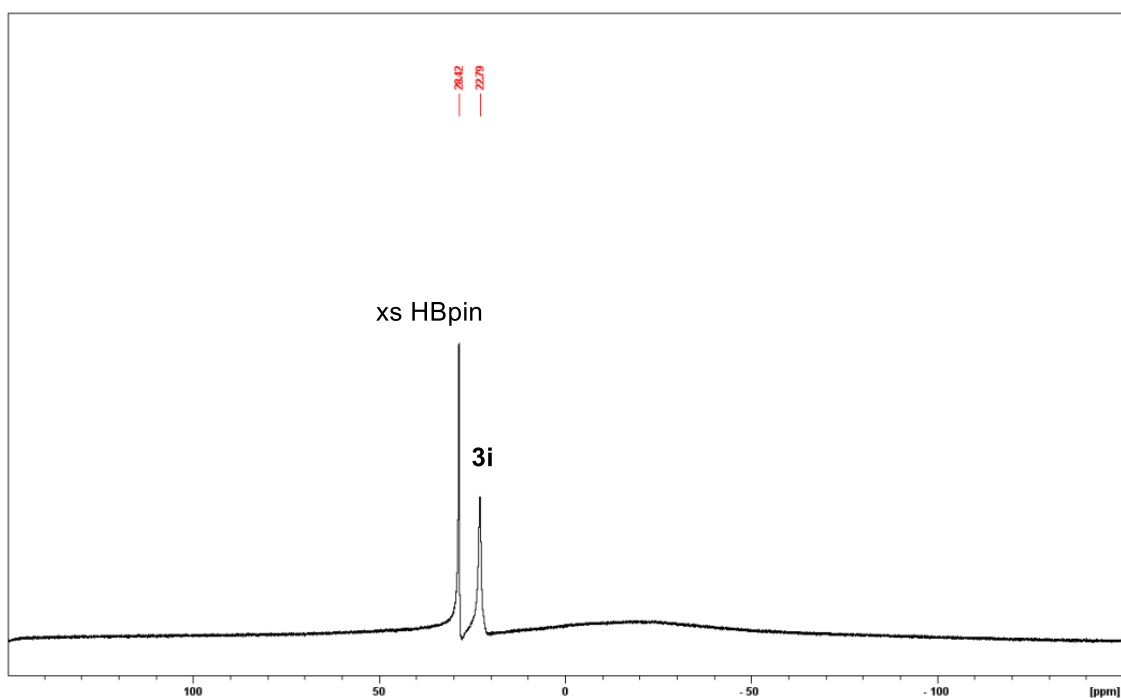


Fig. S31 ¹¹B{¹H} NMR spectrum (C₆D₆, 126 MHz) of **3i**.

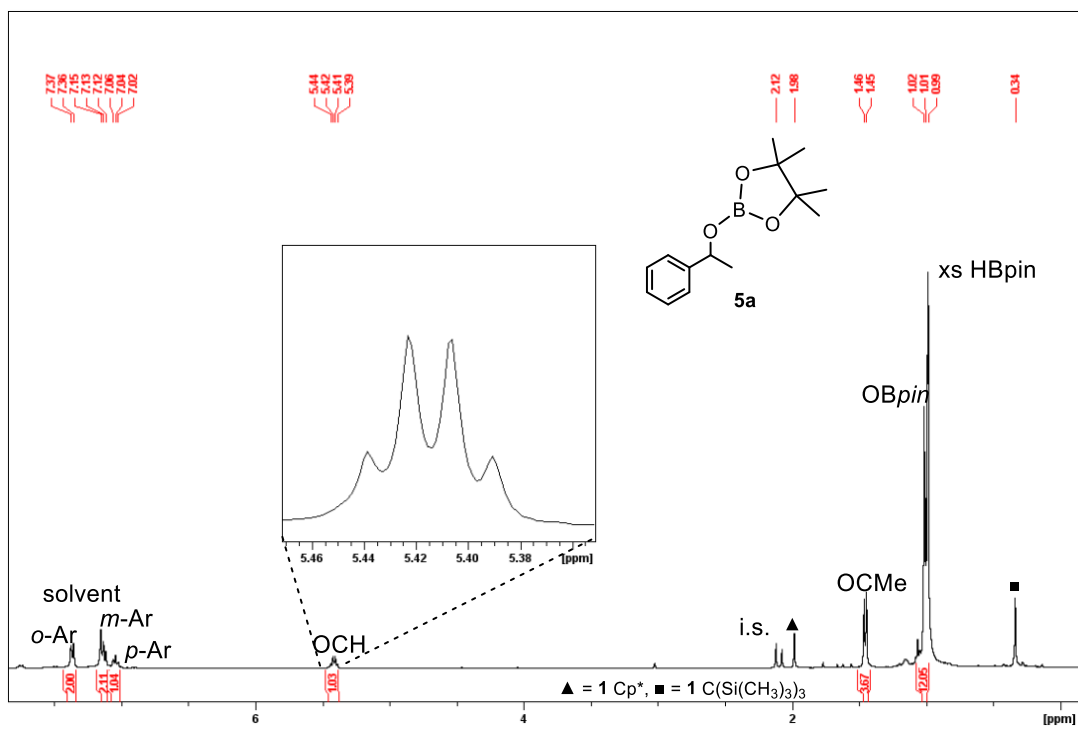


Fig. S32 ¹H NMR spectrum (C₆D₆, 400 MHz) of **5a**.

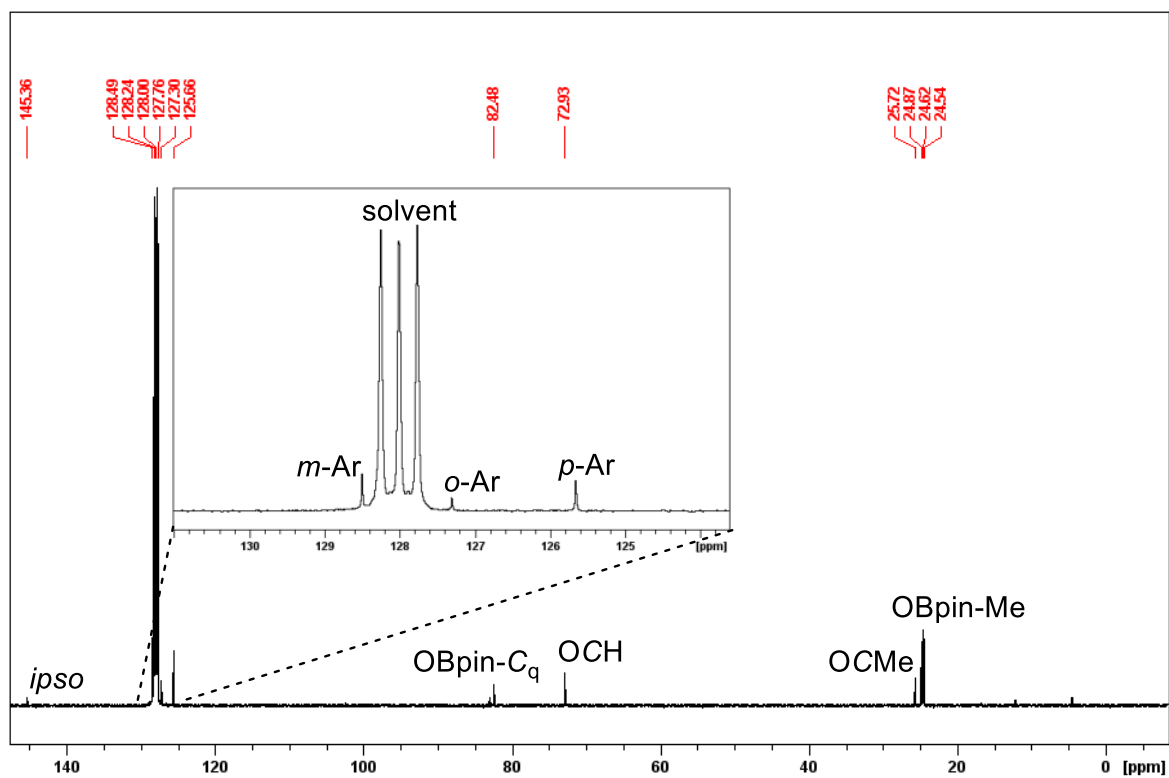


Fig. S33 ¹³C{¹H} NMR spectrum (C₆D₆, 101 MHz) of **5a**.

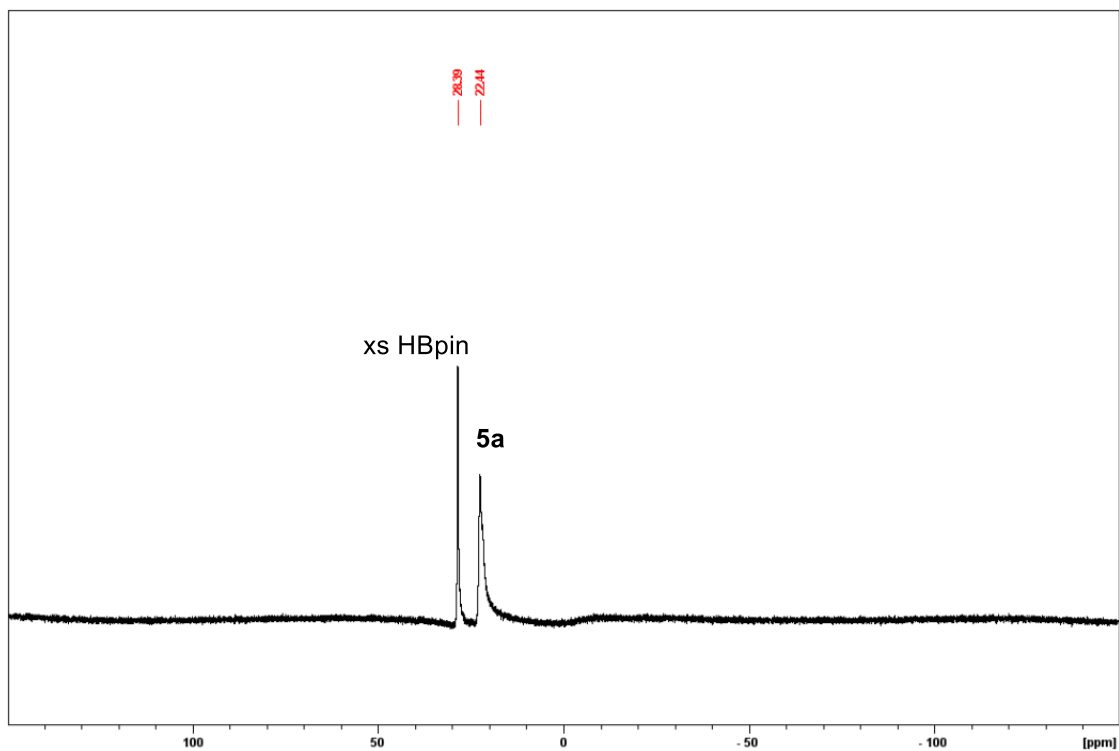


Fig. S34 ¹¹B{¹H} NMR spectrum (C₆D₆, 126 MHz) of **5a**.

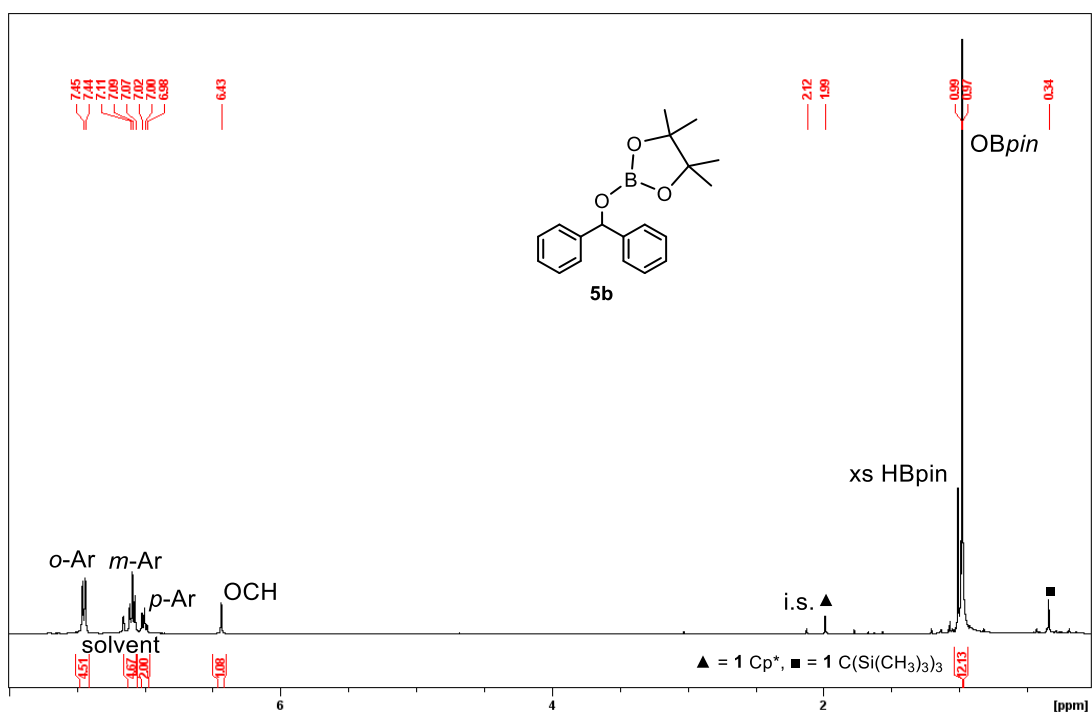


Fig. S35 ¹H NMR spectrum (C₆D₆, 400 MHz) of **5b**.

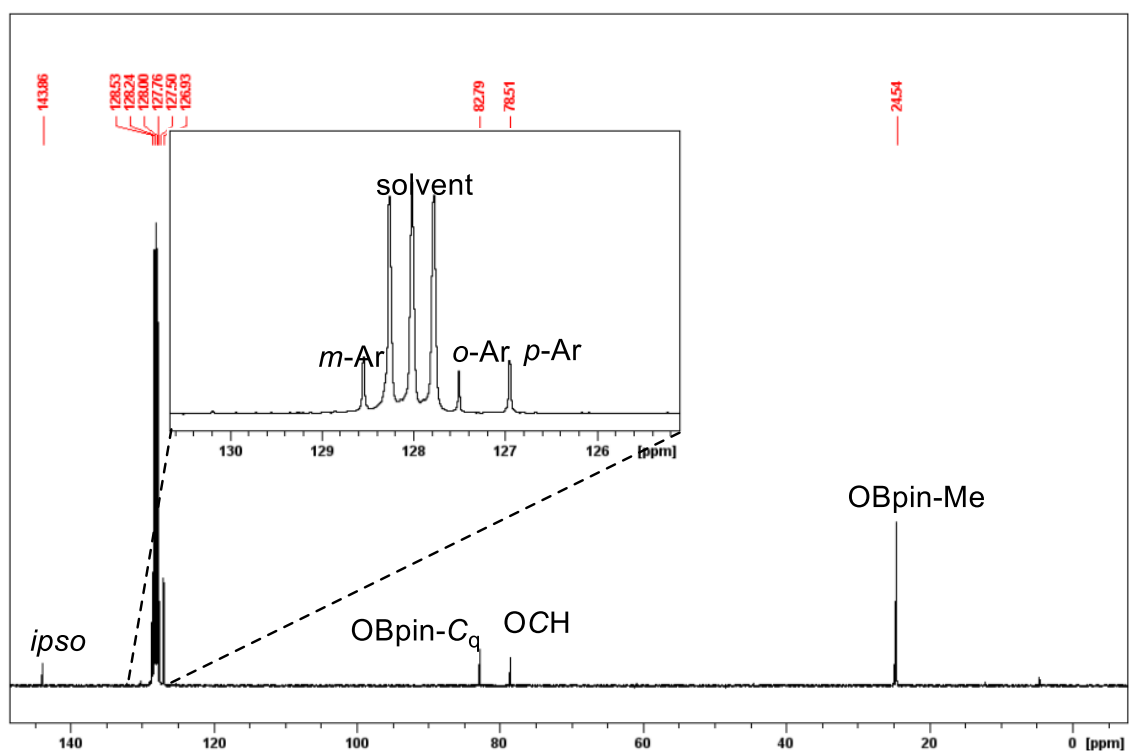


Fig. S36 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 101 MHz) of **5b**.

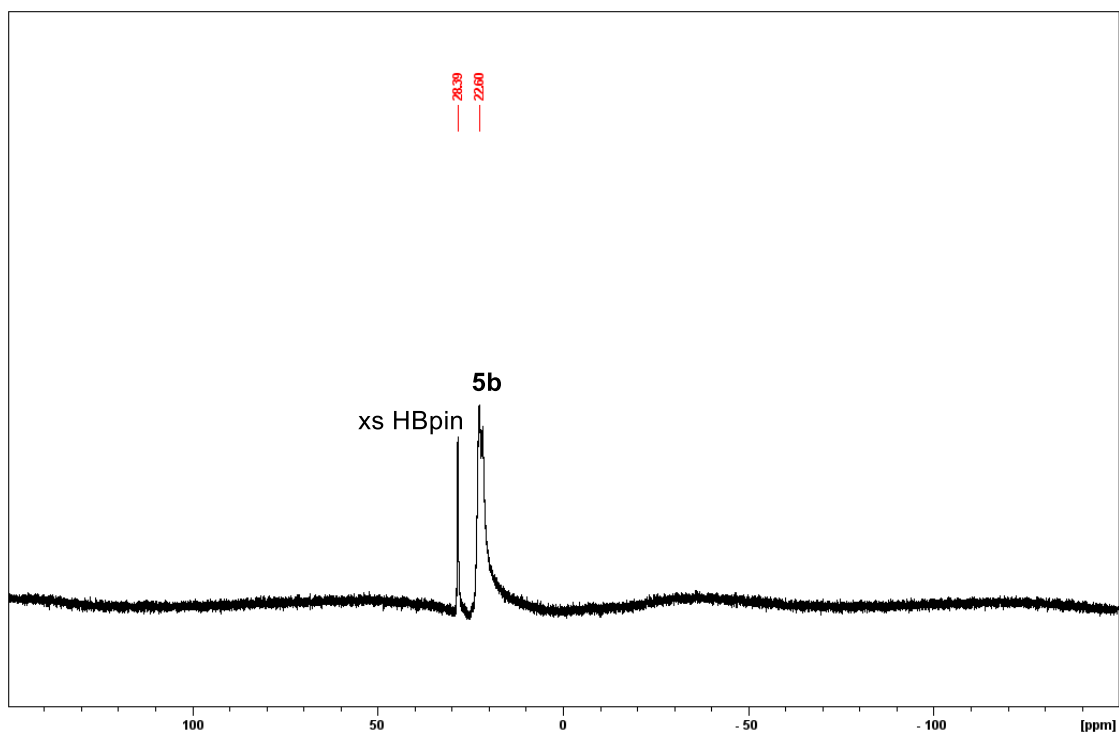


Fig. S37 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 126 MHz) of **5b**.

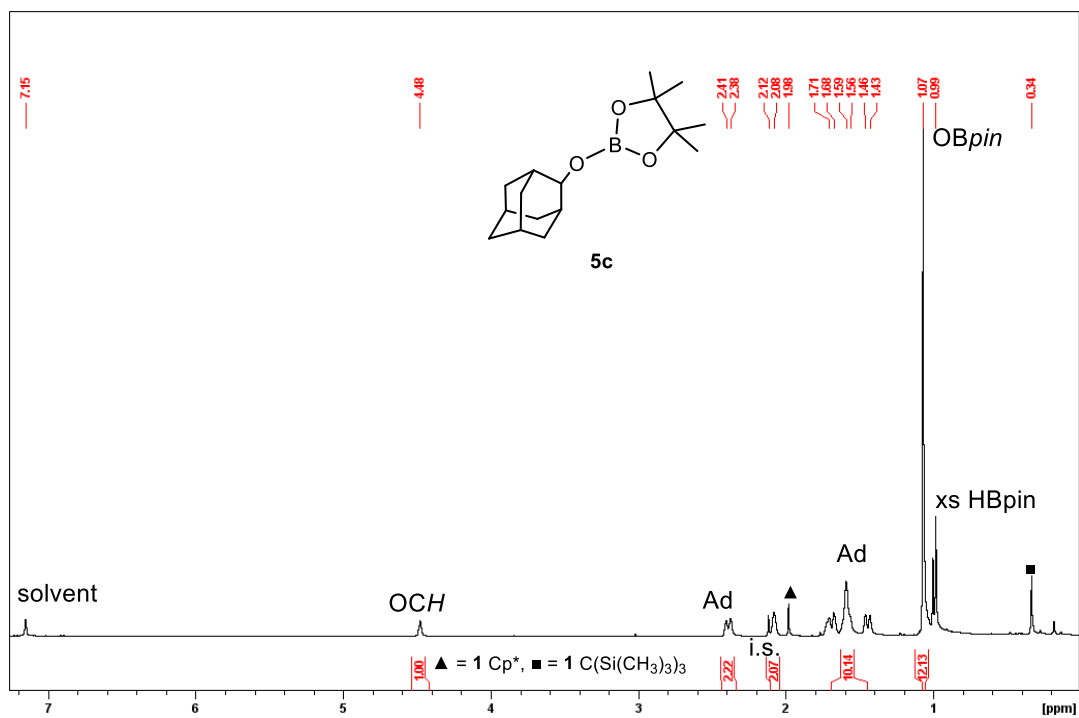


Fig. S38 ¹H NMR spectrum (C₆D₆, 400 MHz) of **5c**.

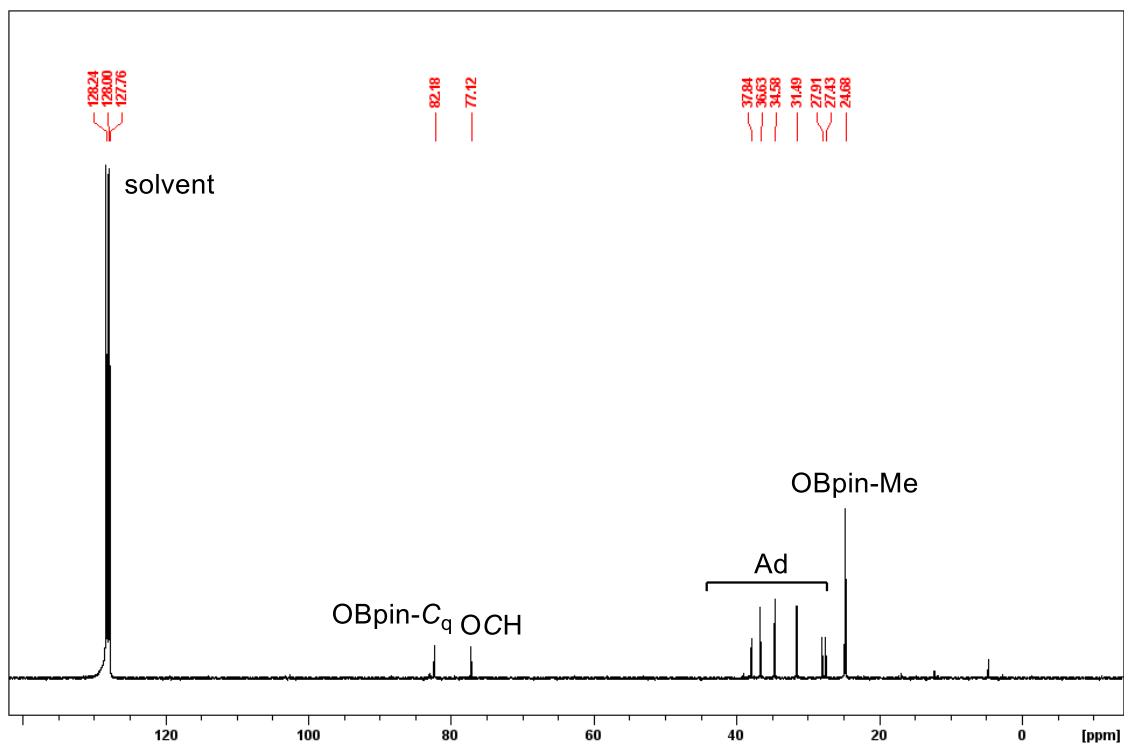


Fig. S39 ¹³C{¹H} NMR spectrum (C₆D₆, 101 MHz) of **5c**.

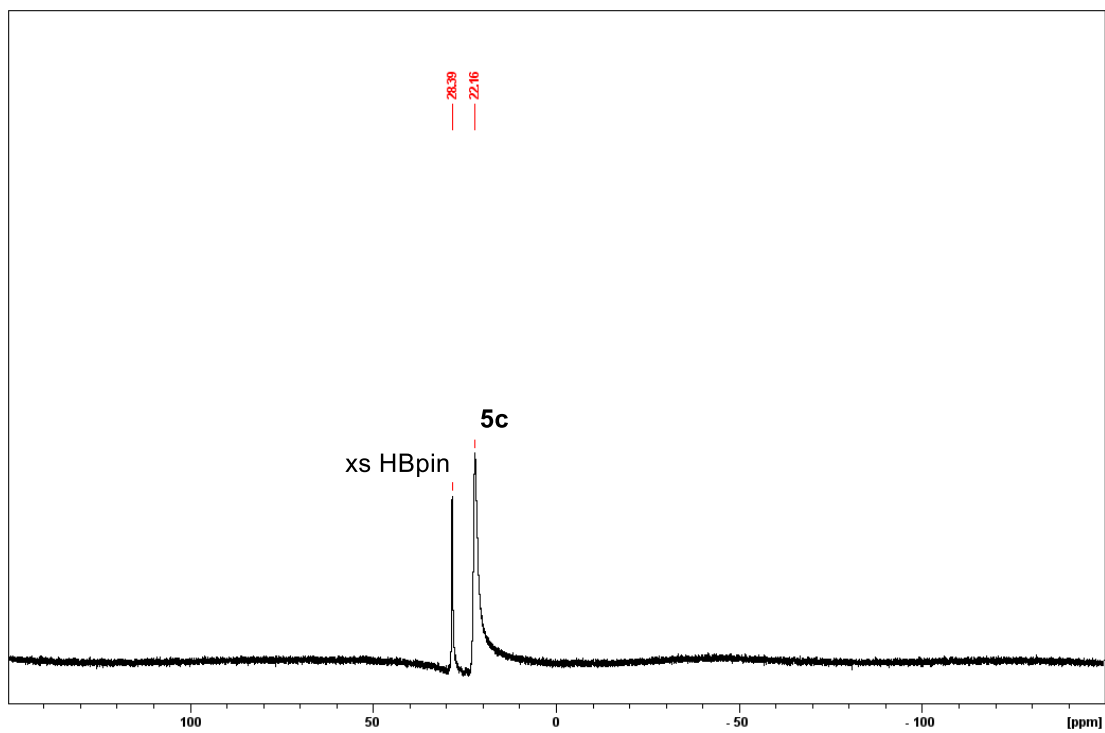


Fig. S40 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 126 MHz) of **5c**.

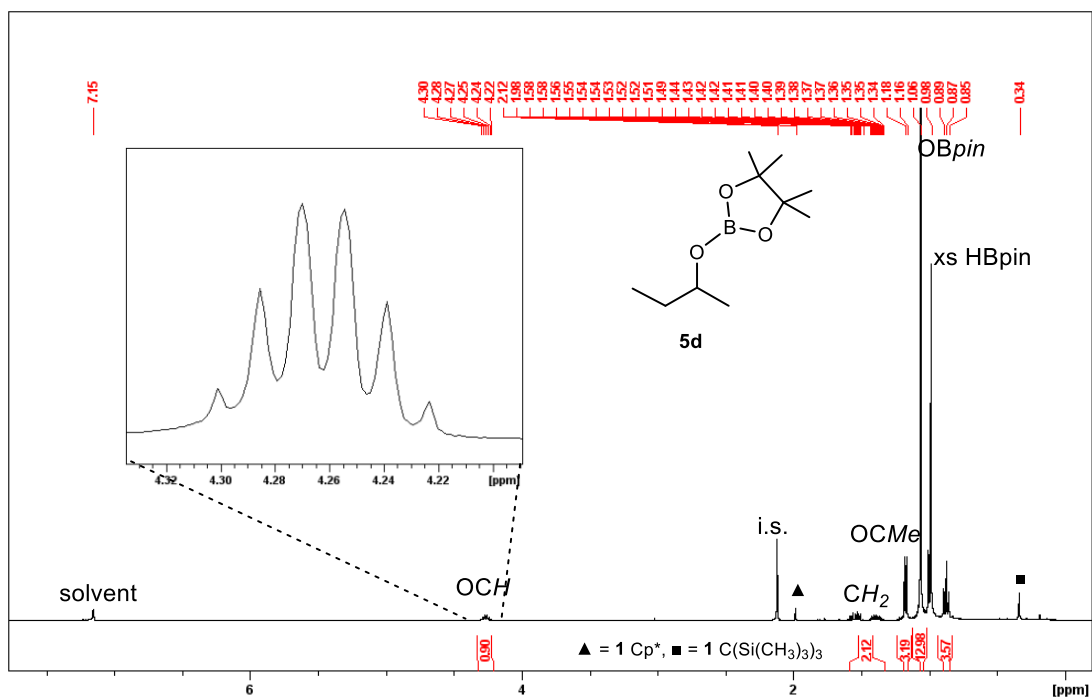


Fig. S41 ^1H NMR spectrum (C_6D_6 , 400 MHz) of **5d**.

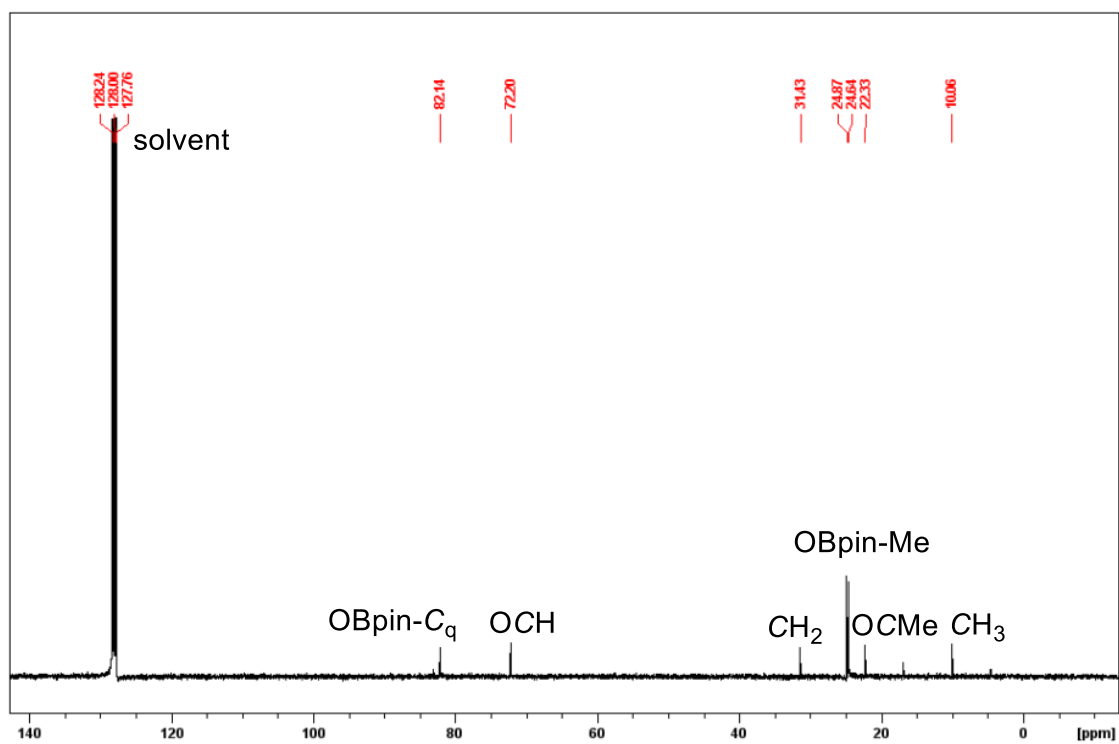


Fig. S42 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (C₆D₆, 101 MHz) of **5d**.

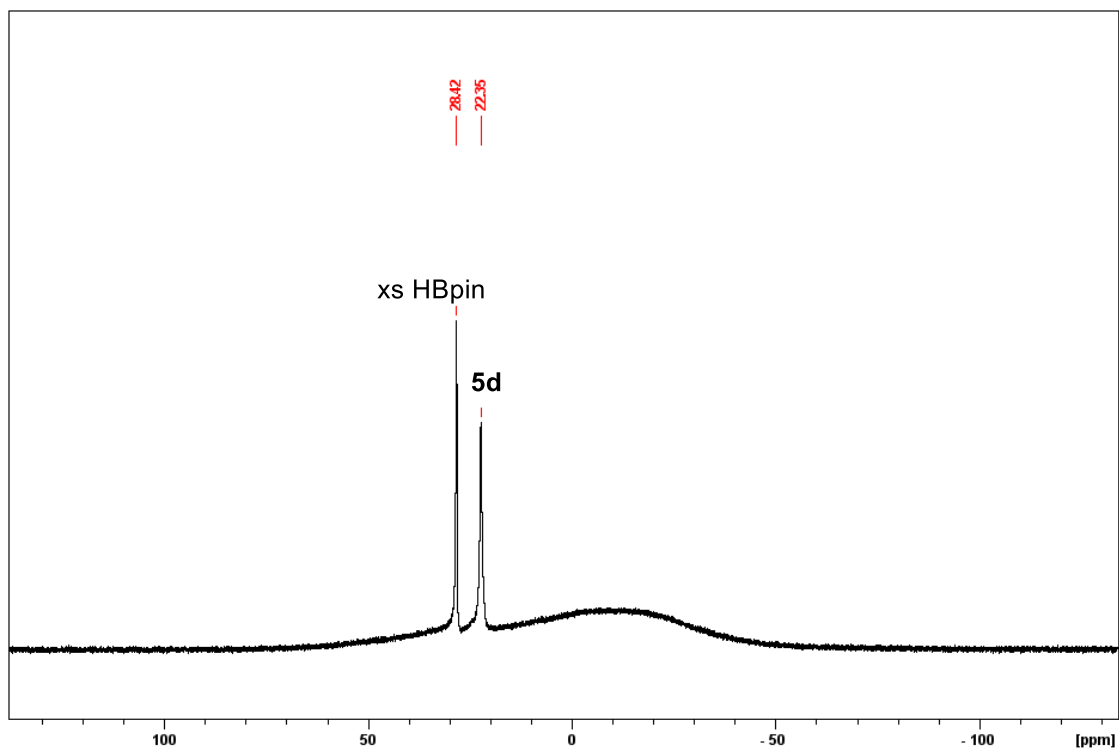


Fig. S43 $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (C₆D₆, 126 MHz) of **5d**.

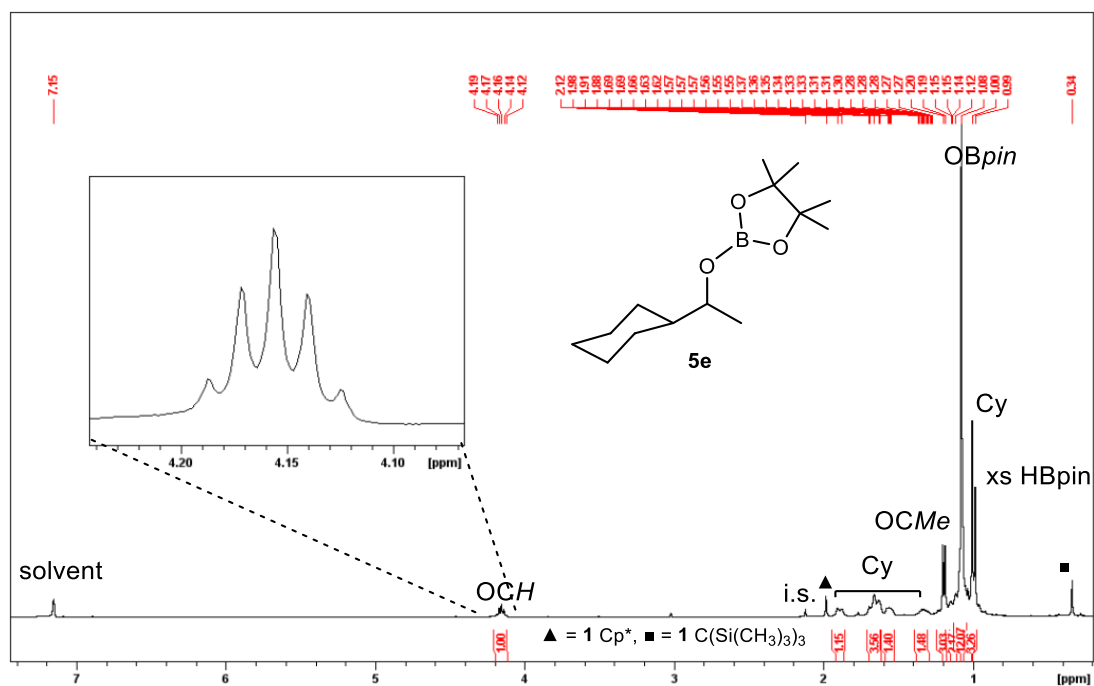


Fig. S44 ^1H NMR spectrum (C_6D_6 , 400 MHz) of **5e**.

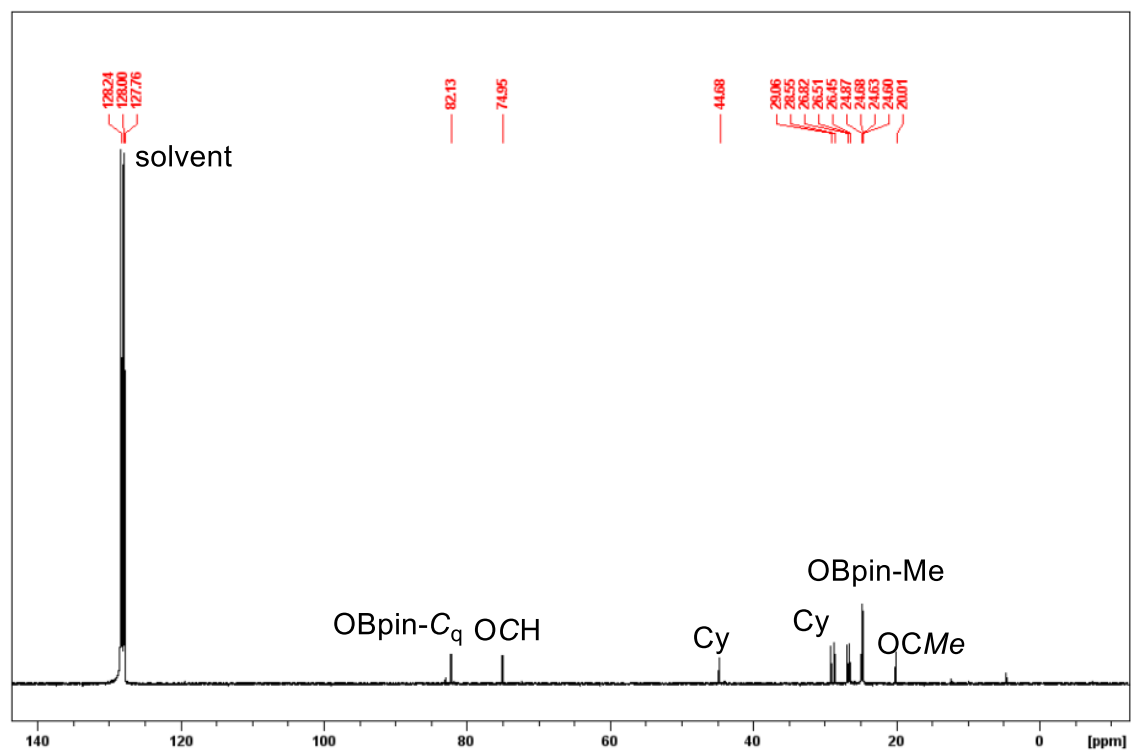


Fig. S45 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (C_6D_6 , 101 MHz) of **5e**.

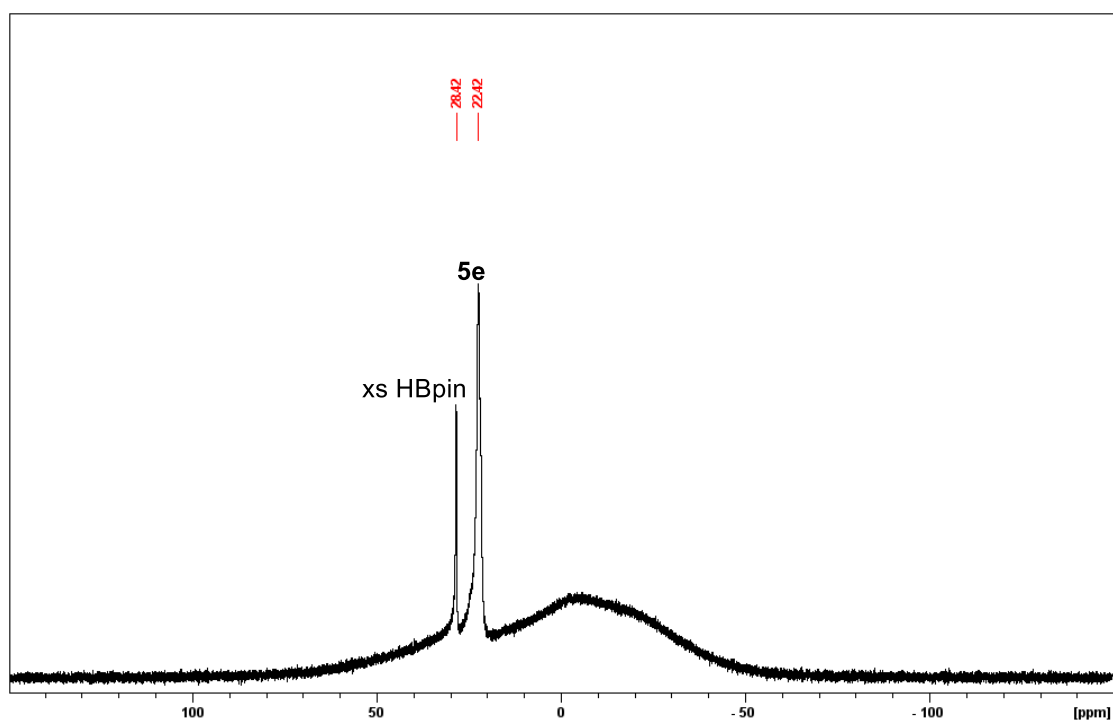


Fig. S46 ¹¹B{¹H} NMR spectrum (C₆D₆, 126 MHz) of **5e**.

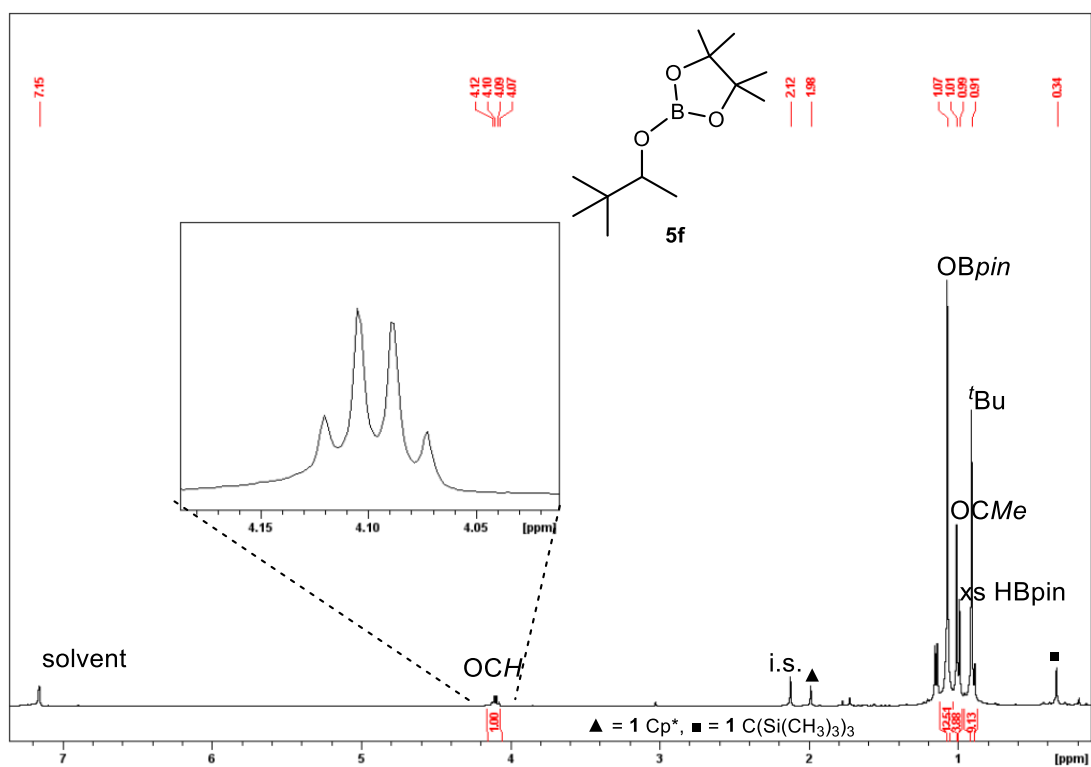


Fig. S47 ¹H NMR spectrum (C₆D₆, 400 MHz) of **5f**.

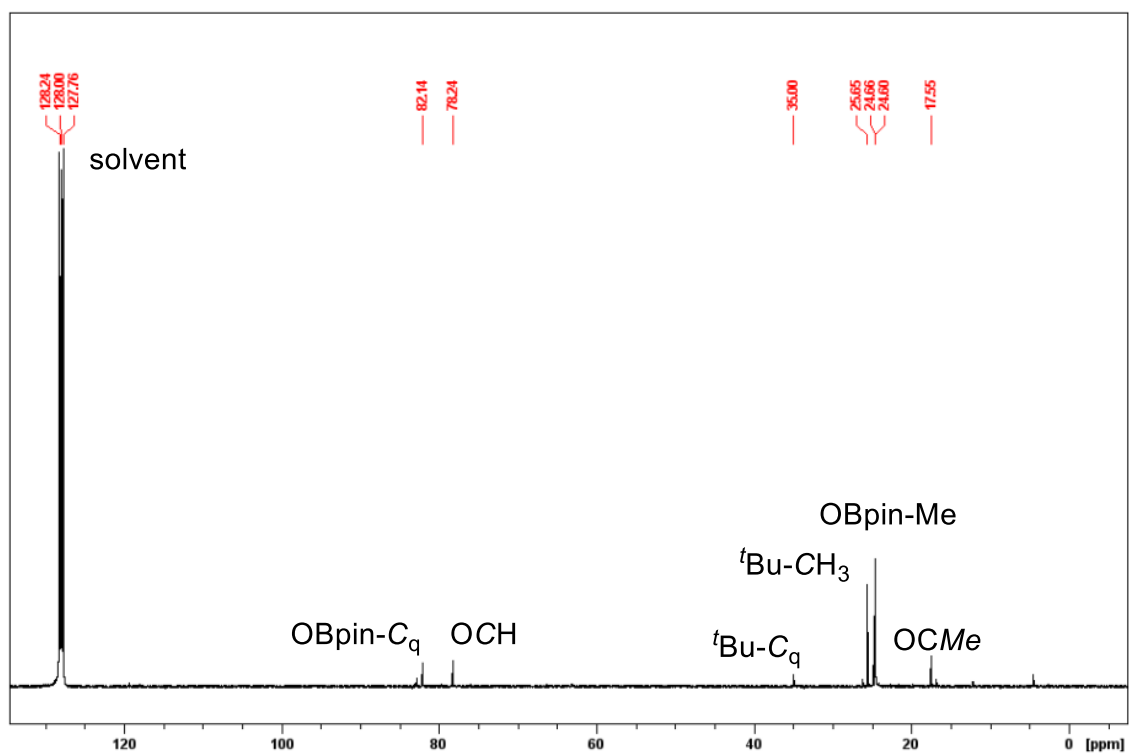


Fig. S48 ¹³C{¹H} NMR spectrum (C₆D₆, 101 MHz) of **5f**.

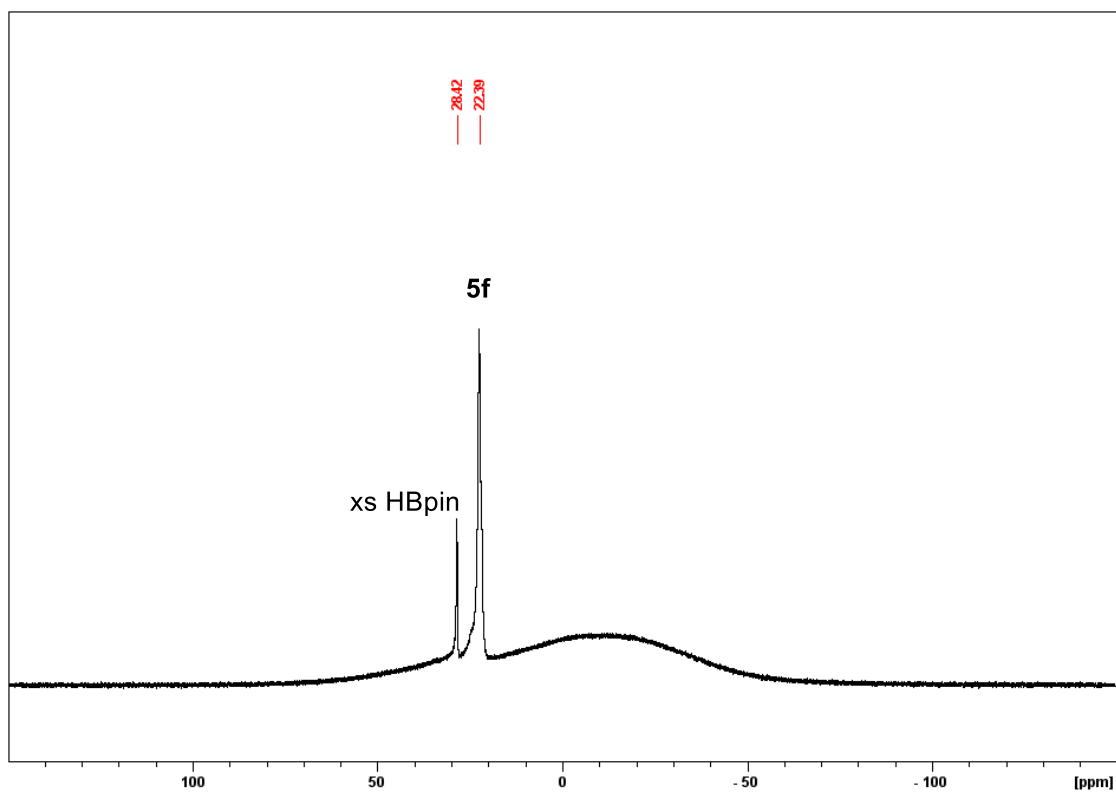


Fig. S49 ¹¹B{¹H} NMR spectrum (C₆D₆, 126 MHz) of **5f**.

7. Computational Details

DFT calculations were performed using the Gaussian 16 (Revision C.02) suite,¹¹ and visualizations were conducted with GaussView program.¹² The real structures of **1**, HBpin, and **2a** were used. Geometries were optimized with the PW6B95-D3BJ functional,¹³ which is a 6-parameter global hybrid meta-generalized gradient approximation (GH meta-GGA) functional based on Perdew-Wang-91 exchange and Becke-95 correlation corrected. The functional was applied with Grimme-D3 dispersion with Becke-Johnson damping¹⁴ and the Solvation Model based on Density (SMD).¹⁵ The Def2-SVP basis set, which is a split-valence triple-zeta Ahlrich basis set,¹⁶ was used. The vibrational frequencies of each stationary state were obtained at the same level to determine whether it was an equilibrium or transition state. The Intrinsic Reaction Coordinate (IRC)¹⁷ calculations were conducted for the optimized transition states to determine if their singular imaginary frequencies connected reactants with products through the transition states. Single-point energy calculations were performed using the Def2-TZVPP basis set,¹⁸ a higher-accuracy Ahlrichs basis set than Def2-SVP, to determine the thermochemical parameters of each stationary state in order to investigate the reaction pathway. Natural Population Analysis (NPA)¹⁹ was performed using the NBO 7.0 program²⁰ on selected stationary states at the same level of theory to determine Natural Bonding Orbitals (NBO), Wiberg Bond Indices (WBI),²¹ and NPA charges. Theoretical kinetics isotope effect studies (KIE, k_H/k_D) were conducted using the PyQuiver program²² with the Wigner tunnel corrections.²³ Energy diagrams were drawn with the mechaSVG suite.²⁴

8. Optimized Structures

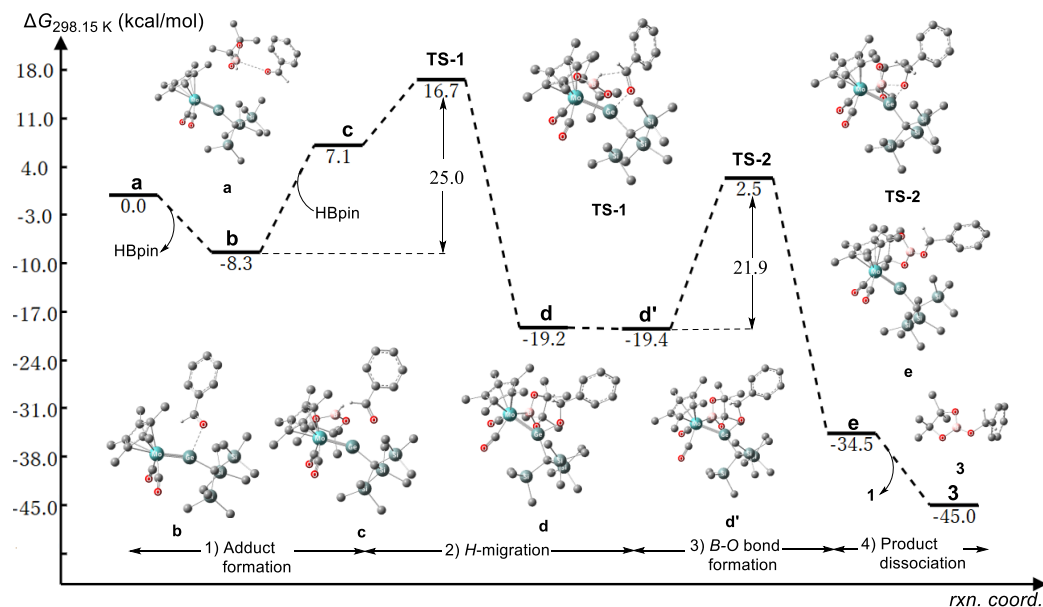


Fig. S50 Gibbs Free Energy Diagram for hydroboration of **2a** by HBpin with **1**.

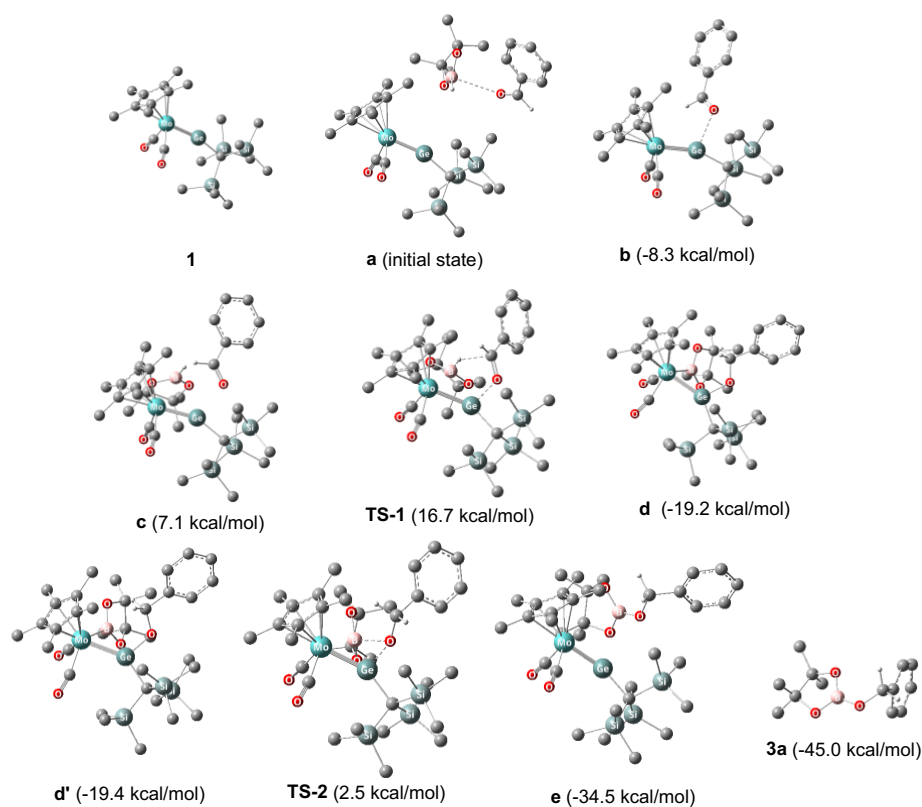


Fig. S51 Optimized structures and their associated $\Delta G_{298.15\text{ K}}$.

Table S3 Energy and structural parameters for the proposed pathway

	HBpin	2a (PhCHO)	1	a	b	c
G [a.u.] = G_{corr} + SPE	-412.39474	-346.08004	-4031.13487	-4789.57730	-4377.19575	-4789.56593
H [a.u.] = H_{corr} + SPE	-412.35146	-346.04233	-4031.01677	-4789.42159	-4377.06319	-4789.41655
ΔG (kcal/mol)	-	-	-	-	-8.3	7.1
ΔH (kcal/mol)	-	-	-	-	4.4	3.2
ΔS (cal/mol*K)	-	-	-	-	36.8	-11.6
Imag. freq., cm^{-1}	-	-	-	-	-	-
FMO Gap, eV	9.12	5.96	4.25	3.60	2.86	2.79
d (Mo-Ge), Å	-	-	2.29	2.3	2.32	2.33
d (Mo-HBpin), Å	-	-	-	4.85	-	4.04
d (Mo-Bpin), Å	-	-	-	5.63	-	4.39
d (H-B), Å	1.2	-	-	1.2	-	1.19
d (Ge-O), Å	-	-	-	5.94	2.46	2.43
θ (Mo-Ge-O)	-	-	-	120.6	108.3	114.3
θ (Mo-Ge-Tsi)	-	-	165.58	162.6	158.3	154.5
μ (D)	3.0271	3.5077	4.3144	7.8766	9.807	8.6521
	TS-1	d	d'	TS-2	e	3a (PhCH ₂ OBpin)
G [a.u.] = G_{corr} + SPE	-4789.55075	-4789.60795	-4789.60829	-4789.57330	-4789.63235	-758.51421
H [a.u.] = H_{corr} + SPE	-4789.40393	-4789.46189	-4789.46204	-4789.42925	-4789.47823	-758.45429
ΔG (kcal/mol)	16.7	-19.2	-19.4	2.5	-34.5	-45.0
ΔH (kcal/mol)	11.1	-25.3	-25.4	-4.8	-35.5	-31.0
ΔS (cal/mol*K)	-16.3	-17.7	-17.3	-21.3	-2.9	40.8
Imag. freq., cm^{-1}	-187.53	-	-	-251.07	-	-
FMO Gap, eV	2.78	4.56	4.54	4.35	4.17	7.02
d (Mo-Ge), Å	2.42	2.47	2.48	2.39	2.3	-
d (Mo-HBpin), Å	2.59	-	-	-	-	-
d (Mo-Bpin), Å	2.83	2.28	2.28	2.56	5.22	-
d (H-B), Å	1.25	-	-	-	-	-
d (Ge-O), Å	1.98	1.82	1.82	1.97	4.28	-
θ (Mo-Ge-O)	113.2	118.6	118.4	102.8	98.6	-
θ (Mo-Ge-Tsi)	150.9	144.8	144.8	152.5	160.9	-
μ (D)	5.6951	3.8985	3.8422	3.7278	4.2627	2.7592

Table S4 Selected NPA charges and WBI

		HBpin	2a	1	a	b	c	TS-1	d	TS-2	e
NPA Charge	Mo	-	-	-1.438	-1.392	-1.455	-1.335	-1.375	-1.476	-1.428	-1.385
	Ge	-	-	1.354	1.341	1.394	1.335	1.546	1.766	1.651	1.318
	O	-	-0.54965	-	-0.562	-0.567	-0.568	-0.73	-0.897	-0.849	-0.77
	C	-	0.43047	-	0.44	0.453	0.472	0.293	-0.054	-0.061	-0.049
	H	-0.116	-	-	-0.116	-	-0.125	-0.053	0.212	0.21	0.219
	B	0.952	-	-	0.968	-	0.975	0.989	1.058	1.108	1.342
WBI	Mo, Ge	-	-	1.4686	1.5779	1.4088	1.4483	1.1078	0.8678	1.0624	1.5758
	Ge, O	-	-	-	0	0.1803	0.1731	0.4051	0.5537	0.352	0.0015
	O, C	-	1.802	-	1.7688	1.1978	1.6656	1.261	0.9126	0.885	0.8887
	C, H	-	-	-	0.0004	-	0.0032	0.1629	0.8866	0.9027	0.9026
	H, B	0.9561	-	-	0.9515	-	0.9455	0.7017	0.0029	0.0019	0.0014
	B, Mo	-	-	-	0.0005	-	0.0073	0.2155	0.6222	0.4647	0.0009
	Mo, C	-	-	-	0	0.0094	0.0088	0.102	0.0091	0.0118	0.0008
	B, O	-	-	-	0.0291	-	0.0013	0.0697	0.0172	0.3285	0.8653
	Mo, O	-	-	-	0	0.021	0.0225	0.0366	0.041	0.044	0.0008

9. Transition State Analysis

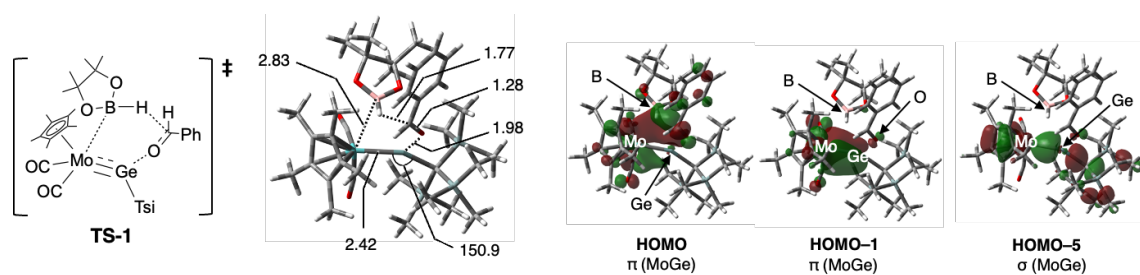


Fig. S52 Structure and main bonding orbitals of the transition state of **TS-1**. Inserted values indicate either bond lengths (Å) or angles (°).

10. Alternative Pathway

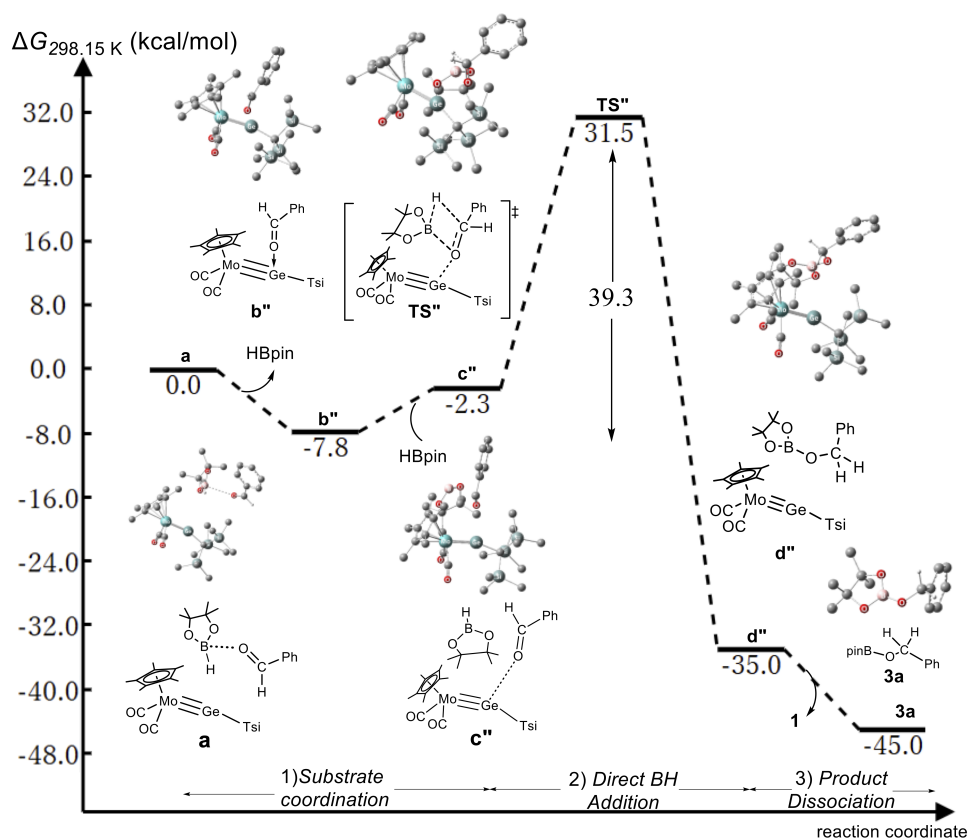


Fig. S53 Alternative pathway for hydroboration of **2a** by HBpin with **1** featuring direct addition.

Table S5 Energy and structural parameters for alternative pathway

	HBpin	2a	1	a	b''	c''	TS''	d''	3a
G [a.u.] = G_{corr} + SPE	-412.39474	-346.08004	-4031.13487	-4789.57730	-4377.19496	-4789.58097	-4789.52712	-4789.63308	-758.51421
H [a.u.] = H_{corr} + SPE	-412.35146	-346.04233	-4031.01677	-4789.42159	-4377.06251	-4789.42115	-4789.37679	-4789.48084	-758.45429
ΔG (kcal/mol)	-	-	-	-	-7.8	-2.3	31.5	-35.0	-45.0
ΔH (kcal/mol)	-	-	-	-	4.8	0.3	28.1	-37.2	-31.0
ΔS (cal/mol*K)	-	-	-	-	36.6	7.5	-9.8	-6.3	40.8
Imag. freq., cm^{-1}	-	-	-	-	-	-	-575.8	-	-
FMO Gap, eV	9.12	5.96	4.25	3.60	3.61	3.45	2.87	4.12	7.02
$d(\text{Mo-Ge})$, Å	-	-	2.29	2.30	2.28	2.31	2.31	2.31	-
$d(\text{Mo-HBpin})$, Å	-	-	-	4.85	-	5.90	4.75	4.05	-
$d(\text{Mo-Bpin})$, Å	-	-	-	5.63	-	5.87	4.81	5.26	-
$d(\text{H-B})$, Å	1.2	-	-	1.20	-	1.20	1.27	2.55	-
$d(\text{Ge-O})$, Å	-	-	-	5.94	3.90	1.21	1.27	4.59	-
θ (Mo-Ge-O)	-	-	-	120.60	83.50	93.30	97.90	97.20	-
θ (Mo-Ge-Tsi)	-	-	165.58	162.60	166.20	159.90	160.30	160.60	-
u (D)	3.0271	3.5077	4.3144	7.8766	7.2247	5.3088	7.3080	2.4609	2.7592

11. Cartesian Coordinates

1 *E*(RPW6B95) = -4790.375037640051 a.u.

Mo	0.20683452	0.59352517	0.00000000
Ge	0.11255552	-1.41171083	-1.09711900
C	-0.89531548	-0.27634783	1.35283600
O	-1.53064648	-0.70923483	2.22226700
C	-1.41388448	1.02718317	-0.99633900
O	-2.36028948	1.39172417	-1.55961900
C	1.32591852	1.72200217	1.70991200
C	0.47840952	2.64614617	1.01301900
C	0.97963252	2.76773517	-0.32743400
C	2.10899152	1.91093217	-0.45741700
C	2.32300252	1.26214217	0.80383100
C	1.23536852	1.38469917	3.16118600
H	1.82324552	2.09348517	3.76187700
H	1.61768952	0.37940217	3.36715500
H	0.20243552	1.42547017	3.52195700
C	-0.62394348	3.45356517	1.61424000
H	-1.12196348	2.91131917	2.42502600
H	-1.38900948	3.70460117	0.87177500
H	-0.24437848	4.39838017	2.03089500
C	0.46861952	3.71316917	-1.36360100
H	-0.61282148	3.86226917	-1.27792600
H	0.67233052	3.34948117	-2.37618600
H	0.94658952	4.69822017	-1.26223700
C	2.98318652	1.78644717	-1.66149700
H	3.79714652	2.52620517	-1.63329200
H	2.42179452	1.95061617	-2.58723000
H	3.44255952	0.79465217	-1.72634700
C	3.45677152	0.34892517	1.13461100
H	3.76943852	-0.23847083	0.26494500
H	3.18912252	-0.35487483	1.92959600
H	4.33253652	0.91871417	1.47972100
Si	-2.14423848	-3.53594583	-1.17865100
Si	-0.55426848	-2.69216883	-3.80540400
Si	0.91404352	-4.35016083	-1.50893600
C	-0.44301048	-3.07015083	-1.93264500
C	-2.10226748	-1.71146883	-4.21809200
H	-2.08708248	-1.47455283	-5.29118900
H	-2.11867648	-0.75702883	-3.67367000
H	-3.04072048	-2.23832983	-4.01082000
C	2.46423752	-4.08550583	-2.54175300
H	2.88182952	-3.08207083	-2.38192600
H	2.31948952	-4.22668683	-3.61897300
H	3.22442552	-4.80873883	-2.21450100
C	1.50121152	-4.15655583	0.26996400
C	2.18864352	-4.98027183	0.51011600
H	0.69603052	-4.16787783	1.01135100
H	2.06082452	-3.21979983	0.40306800
C	0.31778352	-6.10956583	-1.78360800
H	-0.02300148	-6.27132083	-2.81322100
H	-0.49725848	-6.39238983	-1.10700200
H	1.15252952	-6.79973783	-1.59763000
C	0.86556852	-1.58723683	-4.36566700
H	1.86069252	-1.98662883	-4.14454500
H	0.79219852	-0.58848583	-3.91228800
H	0.79718252	-1.45232583	-5.45466200
C	-3.02489648	-4.80134683	-2.25556100
H	-2.42229548	-5.69930583	-2.43326200
H	-3.31963948	-4.39133883	-3.22921700
H	-3.94518248	-5.11495783	-1.74300200
C	-3.26816148	-2.04296283	-0.97067000
H	-3.32832248	-1.38834783	-1.84493900
H	-2.96374848	-1.43137383	-0.11211600
H	-4.28424748	-2.40649983	-0.75927000
C	-0.53314148	-4.26877483	-4.82778700
H	-0.68239848	-4.00817383	-5.88496500
H	-1.33219648	-4.96238183	-4.54183300
H	0.42162452	-4.80346283	-4.75618000
C	-1.96397948	-4.23850583	0.55493000
H	-2.97048848	-4.44972783	0.94276600
H	-1.50823248	-3.50230983	1.23060300

H -1.38625348 -5.16789683 0.61542000

HBpin *E*(RPW6B95) = -412.553054287737 a.u.

C	1.09557110	0.78088577	0.00000000
C	0.78361508	-0.75215834	-0.06689600
H	-0.05834998	0.35449674	-3.17160823
C	-0.02594098	-1.28740538	1.09420008
H	-1.00419805	-0.80296334	1.16179409
H	-0.19057299	-2.36332545	0.96642907
H	0.50691206	-1.13635837	2.04086415
C	2.02739117	-1.59913940	-0.28587502
H	2.65407121	-1.63743140	0.61206604
H	1.72337215	-2.62086447	-0.53894104
H	2.63019321	-1.20994237	-1.11488408
C	0.00503003	1.57560883	0.70105405
H	-0.98611805	1.31848181	0.30914002
H	0.00777003	1.39987982	1.78253113
H	0.17239804	2.64381790	0.52420904
C	2.45474620	1.12855580	0.56730204
H	2.55079920	0.76038477	1.59596712
H	3.26369126	0.70356277	-0.03380000
H	2.58257921	2.21686487	0.58370304
O	1.05542110	1.15987580	-1.39323210
O	-0.00321697	-0.84937735	-1.27437909
B	0.30230805	0.23154873	-2.03759715

2a *E*(RPW6B95) = -346.160735043189 a.u.

C	0.67599068	0.99067598	0.00000000
C	-0.54606382	0.98801118	0.67405249
C	1.87348540	0.98798330	0.72119794
C	-0.57376601	0.98276689	2.06326309
C	1.84458103	0.98275486	2.10671906
C	0.62103934	0.98019998	2.77674566
H	-1.47377464	0.99002013	0.10174429
H	2.81166669	0.99009483	0.16951439
H	-1.52498541	0.98072542	2.59175750
H	2.77390686	0.98068981	2.67317133
H	0.60063674	0.97618683	3.86529906
C	0.70318183	0.99647529	-1.47499922
O	1.70752876	0.99890063	-2.14155123
H	-0.30262468	0.99864003	-1.95663071

3a *E*(PW6B95) = -758.779823114880 a.u.

C	-0.16129033	0.64516128	0.00000000
C	1.10239182	1.15475198	-0.29150004
C	-0.94374130	0.14142811	-1.04056673
C	1.58043373	1.15943794	-1.59767131
C	-0.47121418	0.15236510	-2.34775091
C	0.79281351	0.66182966	-2.63058609
H	1.71082563	1.56937150	0.51152009
H	-1.93705590	-0.24753927	-0.82162420
H	2.56754392	1.56601270	-1.81142468
H	-1.09334885	-0.23886043	-3.15112288
H	1.16178397	0.67336154	-3.65466927
C	-0.69110700	0.65770253	1.40979044
O	-2.06072542	1.00275079	1.46614473
H	-0.09140370	1.34488536	2.02228526
H	-0.60462714	-0.34155878	1.85709538
B	-2.41770742	2.23959853	1.04624165
O	-3.71762421	2.59960964	0.83706516
O	-1.52029129	3.23800250	0.77994734
C	-2.25165016	4.24428777	0.05636473
C	-3.70794730	4.01824489	0.58653848
C	-4.80144584	4.35149732	-0.40444901
C	-2.11545077	3.91188343	-1.42216915
C	-1.66370119	5.60347046	0.36204565
C	-3.95403725	4.71274182	1.91655887
H	-5.78276485	4.17454688	0.05059654
H	-4.75027480	5.40661009	-0.69971859
H	-4.73032810	3.73170554	-1.30301320
H	-2.59466410	2.95277923	-1.65223171

H	-2.56362053	4.68548970	-2.05582588
H	-1.05257113	3.82245538	-1.67481223
H	-0.65143156	5.67103525	-0.05289148
H	-2.26824789	6.39954971	-0.08925209
H	-1.59876502	5.77980357	1.43986542
H	-3.14333775	4.50099544	2.62428019
H	-4.03749288	5.79896183	1.79873407
H	-4.88906020	4.33863013	2.34807727

a $E(\text{RPW6B95}) = -4790.37503764005 \text{ a.u.}$

C	0.44289045	1.38694637	0.00000000
C	-0.48058408	1.82053510	-0.95405170
C	1.80821274	1.63455396	-0.18034596
C	-0.04692694	2.50062629	-2.08452877
C	2.23646223	2.31592457	-1.30991137
C	1.31164637	2.74804472	-2.26002696
H	-1.54134333	1.62071827	-0.80206867
H	2.51596231	1.29172323	0.57279710
H	-0.76461838	2.84003966	-2.82811539
H	3.29701597	2.51322865	-1.45461485
H	1.65392618	3.28330035	-3.14475012
C	-0.03950684	0.67155090	1.19260480
O	0.66317415	0.22706333	2.06924458
H	-1.14662195	0.55762252	1.24720692
C	4.09820263	-0.37348907	4.33679311
C	4.16176961	0.92826058	3.46304047
H	2.97833848	-1.42438049	1.29787286
C	5.47788279	1.67434148	3.52836676
H	6.31200595	1.05987672	3.17722289
H	5.42716939	2.56771201	2.89505276
H	5.68933917	1.99939350	4.55420964
C	3.00301845	1.87558804	3.73013715
H	3.10195277	2.35774805	4.70922302
H	2.99482863	2.65922146	2.96343848
H	2.04465195	1.34952183	3.68636614
H	5.45893359	-1.02746643	4.51876670
H	5.98297598	-1.12289868	3.56150514
H	6.09335976	-0.45410197	5.20399044
H	5.32068959	-2.03200753	4.93452335
C	3.40830451	-0.20551228	5.67382188
H	3.92668728	0.53976139	6.28924512
H	2.36650182	0.10336220	5.55016744
H	3.41647547	-1.15833870	6.21548834
O	3.31159633	-1.26106736	3.51805952
O	3.99130637	0.40435775	2.12786523
B	3.36886952	-0.80304037	2.24279928
Mo	4.17362362	-5.98681546	0.18846481
Ge	1.98741556	-5.32319412	0.40760867
C	3.45002474	-7.32388735	-1.01693779
O	3.14221531	-8.14633267	-1.77850508
C	3.75438324	-7.14577518	1.70379506
O	3.61450510	-7.85327373	2.61273069
C	5.91491590	-5.62580026	-1.31297176
C	6.34734668	-6.57221742	-0.31945994
C	6.38986639	-5.89099882	0.93873270
C	5.97228617	-4.54556217	0.73312404
C	5.67495227	-4.38261299	-0.66069849
C	5.84619519	-5.87926828	-2.78284983
H	6.82173276	-5.69886128	-3.25767102
H	5.11509350	-5.22551805	-3.27009332
H	5.56118658	-6.91349409	-3.00330333
C	6.81115520	-7.96715077	-0.58041157
H	6.28206971	-8.41516906	-1.42868358
H	6.64222118	-8.61313855	0.28776087
H	7.88669097	-7.99301240	-0.81076216
C	6.88363481	-6.46436925	2.22532635
H	6.70131901	-7.54236310	2.28490003
H	6.39831402	-5.99674738	3.08847717
H	7.96692826	-6.30712476	2.32852609
C	5.95101552	-3.46930733	1.76595681
H	6.95037263	-3.02617330	1.89274520
H	5.62918595	-3.84310451	2.74342835
H	5.26752815	-2.66424048	1.48276821

C	5.28651991	-3.10157813	-1.32312172
H	4.71586922	-2.45549310	-0.64787217
H	4.67164066	-3.27619012	-2.21225870
H	6.17756868	-2.54098060	-1.64276182
Si	-0.53692766	-7.12356915	0.16351843
Si	-0.35689425	-4.82145280	2.35817048
Si	-0.56973778	-4.08499137	-0.74033937
C	0.05196810	-5.34194826	0.55972042
C	-0.04404555	-6.24325608	3.54779838
H	-0.23723192	-5.89021971	4.57046809
H	1.00656214	-6.56393596	3.50634874
H	-0.67543937	-7.12299891	3.37820327
C	-0.34688969	-2.31899619	-0.14065817
H	0.70147194	-2.10475496	0.10597242
H	-0.95592913	-2.08431145	0.73911073
H	-0.64196588	-1.63444633	-0.94845376
C	0.43728726	-4.18232379	-2.32960141
H	-0.05336268	-3.57160666	-3.10113337
H	0.55432705	-5.19504072	-2.72880109
H	1.44354438	-3.76618589	-2.18045190
C	-2.39111555	-4.32848694	-1.13536344
H	-3.01498882	-4.26374692	-0.23574441
H	-2.60205658	-5.28516876	-1.62723011
H	-2.71112412	-3.53011880	-1.81974967
C	0.75846999	-3.43584273	2.96123238
H	0.62101318	-2.47544867	2.45531616
H	1.82231327	-3.70154012	2.89500635
H	0.54809435	-3.26526444	4.02702346
C	-2.30115037	-7.39162601	0.76100662
H	-3.00562828	-6.65603560	0.35672492
H	-2.38017010	-7.37308342	1.85478489
H	-2.63200954	-8.38552052	0.42780580
C	0.54787518	-8.44548049	0.94579541
H	0.80025227	-8.26904888	1.99518377
H	1.48492020	-8.57525179	0.39141387
H	0.00891427	-9.40258412	0.89155503
C	-2.14588544	-4.26409284	2.52481875
H	-2.34910855	-4.04874183	3.58338049
H	-2.86290388	-5.02562711	2.19805352
H	-2.34790642	-3.34352996	1.96370114
C	-0.47342912	-7.47964231	-1.68103218
H	-0.79864895	-8.51785029	-1.83829778
H	0.55360697	-7.40532011	-2.06124087
H	-1.11709087	-6.83655262	-2.29211830

b $E(\text{RPW6B95}) = -4377.81643318 \text{ a.u.}$

Mo	-0.40467624	0.55755395	0.00000000
Ge	-0.92114624	-1.37916205	-1.16877000
C	-1.02758024	-0.36605605	1.58375900
O	-1.32057224	-0.82800705	2.61026700
C	-2.24616924	1.11987795	-0.32398400
O	-3.32261524	1.52968595	-0.48191700
C	0.73600776	2.04157295	1.37969100
C	0.29449176	2.77903095	0.24401200
C	0.96653376	2.27244795	-0.91215600
C	1.81227476	1.19977795	-0.49010100
C	1.67034376	1.05330095	0.92450100
C	0.38048276	2.32146195	2.80185300
H	1.07372976	3.05247095	3.24329500
H	0.42343676	1.41580995	3.41594800
H	-0.63213924	2.72919795	2.88947800
C	-0.61922224	3.95917795	0.26179100
H	-1.35070524	3.89129995	1.07391700
H	-1.17589324	4.05093895	-0.67722700
H	-0.05298424	4.89159895	0.40245400
C	0.90853576	2.89867095	-2.26714200
H	-0.12095224	3.10827595	-2.58006600
H	1.37037176	2.26357095	-3.02910900
H	1.45215376	3.85532795	-2.27761300
C	2.80333476	0.45814895	-1.32747200
H	3.82750476	0.78228095	-1.09208700
H	2.65042576	0.63976295	-2.39565800
H	2.75352376	-0.62405605	-1.16236600

C	2.45420876	0.11975395	1.78703500	H	0.05781647	-2.71864262	-0.05848042
H	2.73774176	-0.78490705	1.23829400	H	-1.23687262	-2.25442951	-1.16351854
H	1.88121676	-0.19600905	2.66584200	C	-3.05838455	-0.02572596	-0.79559385
H	3.37979276	0.59229995	2.14935400	H	-2.73780235	-0.65427841	-1.63321285
Si	-2.72615224	-3.52332605	0.04341000	H	-3.26541174	0.97429793	-1.18889950
Si	-3.14024424	-2.72536105	-2.97948800	H	-3.99941645	-0.44532052	-0.41050731
Si	-0.55973724	-4.36520905	-2.11133200	C	-2.85454659	2.18025592	1.42923795
C	-1.85585824	-3.04757905	-1.61006100	H	-3.27620323	2.49923933	0.47187894
C	-4.58553724	-1.71014305	-2.33827600	H	-2.40069982	3.05936414	1.89907192
H	-5.20015524	-1.39725105	-3.19416800	H	-3.69208734	1.87153692	2.07389199
H	-4.25666224	-0.80025305	-1.81831100	C	-0.46435451	1.36937573	3.41920523
H	-5.23677124	-2.27278105	-1.65912000	H	-0.93532777	0.88512819	4.28770281
C	-0.15737224	-4.42331005	-3.95158800	H	-0.78737284	2.41478922	3.42545302
H	0.33411476	-3.51201805	-4.30296900	H	0.61850555	1.35577925	3.58587442
H	-1.02841524	-4.61484705	-4.58807200	C	0.65829685	-1.42160800	2.48071771
H	0.54158676	-5.25878405	-4.10289300	H	1.36625867	-0.79296554	3.03175893
C	1.06812076	-4.06399205	-1.21270800	H	1.24052937	-2.05236775	1.80052757
H	1.75649176	-4.89753005	-1.41220800	H	0.16760306	-2.08501736	3.20840873
H	0.95104876	-3.98176305	-0.12625000	Si	4.38933513	1.81129837	-1.70790070
H	1.55238476	-3.14586405	-1.56984600	Si	3.06116443	4.59006632	-2.36565822
C	-1.15011624	-6.11056405	-1.71817700	Si	4.38737330	4.09520534	0.46800365
H	-2.06526424	-6.35746705	-2.27145200	C	3.42214546	3.31691856	-0.99538361
H	-1.33384824	-6.29717305	-0.65458600	C	2.52176157	3.73295306	-3.95008037
H	-0.37079024	-6.81352805	-2.04488400	H	2.14520461	4.48609365	-4.65571007
C	-2.43707824	-1.72405905	-4.41009900	H	1.72399485	2.99876431	-3.78150006
H	-1.55240624	-2.17110705	-4.87499400	H	3.35563818	3.21794131	-4.44201165
H	-2.18971324	-0.70377705	-4.08563300	C	4.02295281	5.91050547	0.82218837
H	-3.21260524	-1.63488005	-5.18391100	H	3.00156883	6.06843129	1.17673305
C	-3.98399824	-4.90909705	-0.16367700	H	4.19971880	6.57231252	-0.03279333
H	-3.60464724	-5.82049405	-0.63465100	H	4.71062330	6.22456921	1.62073742
H	-4.85722124	-4.56253905	-0.73102500	C	4.02617351	3.16411949	2.06675322
H	-4.34296224	-5.17580805	0.84106200	H	4.68202218	3.54022083	2.86463237
C	-3.72833324	-2.11050805	0.79604300	H	4.19060653	2.08426358	1.97928013
H	-3.43282924	-1.10574805	0.47889000	H	2.99059768	3.31694774	2.39742959
H	-3.62098824	-2.14553305	1.88741900	C	6.25093052	4.07791265	0.18104359
H	-4.79326224	-2.23073805	0.56405000	H	6.52600659	4.68446863	-0.69119245
C	-3.83862724	-4.32909205	-3.67722000	H	6.68976086	3.08291342	0.05586826
H	-4.64698024	-4.08065605	-4.37967400	H	6.72519606	4.53765054	1.05976693
H	-4.26646224	-4.97078405	-2.89927700	C	1.69017448	5.78104376	-1.89161595
H	-3.09961224	-4.92000105	-4.22990200	H	1.92656496	6.35501531	-0.98944910
C	-1.43814524	-4.03593505	1.31426000	H	0.73740691	5.26492659	-1.72008073
H	-1.93915724	-4.21766105	2.27483000	H	1.53426601	6.49331740	-2.71416078
H	-0.70389124	-3.23677205	1.47781800	C	5.88868609	2.31302840	-2.73446530
H	-0.89522624	-4.94932905	1.04478900	H	6.60086163	2.97799583	-2.23794080
C	1.39042476	-0.24730905	-4.96310700	H	5.57891757	2.77944977	-3.67833933
C	1.25262176	0.94014395	-5.68882300	H	6.42240110	1.38786179	-2.99731489
C	2.31565576	-1.21731205	-5.36865000	C	3.38124706	0.75912587	-2.90916154
C	2.03058776	1.15568795	-6.81811700	H	2.29626253	0.81343945	-2.78427583
C	3.09346876	-0.99545805	-6.49272000	H	3.66718394	-0.29204315	-2.77960700
C	2.94925876	0.18891495	-7.21627700	H	3.60955510	1.03979508	-3.94400509
H	0.52819276	1.68561595	-5.36339700	C	4.58584428	5.60960315	-2.80262301
H	2.41321476	-2.13161305	-4.78680800	H	4.33735441	6.24803903	-3.66273593
H	1.92366476	2.07599195	-7.38811900	H	5.43837554	4.98659872	-3.09420657
H	3.81689276	-1.74256005	-6.81223500	H	4.91515633	6.27197276	-1.99420052
H	3.56218276	0.35893495	-8.09969900	C	4.96842869	0.69924029	-0.30397652
C	0.55608376	-0.45823505	-3.78367600	H	5.38735059	-0.22242524	-0.72995777
O	0.53037976	-1.49663105	-3.14701800	H	4.13818408	0.40632408	0.34909188
H	-0.08103224	0.39272095	-3.46617200	H	5.74498179	1.15944127	0.31787501
c E(RPW6B95) = -4790.37730145 a.u.				C	-0.31448269	5.72270284	2.27080798
Mo	0.16317016	0.85081584	0.00000000	C	-1.34085744	5.55175926	3.20485802
Ge	1.74452450	2.54884068	-0.29766416	C	0.15470716	7.00823042	1.97296891
C	1.59990527	-0.35224599	-0.42857432	C	-1.88737067	6.65465445	3.84642472
O	2.34860711	-1.22329161	-0.62210758	C	-0.39830582	8.10692426	2.60944918
C	-0.15340258	1.00781565	-1.91333267	C	-1.41597385	7.92930471	3.54687945
O	-0.39338561	0.99030145	-3.05209444	H	-1.70281718	4.54970816	3.42877453
C	-1.07961338	-1.00746724	0.58032842	H	0.94215032	7.12454523	1.23125427
C	-2.02259911	0.02166367	0.27880286	H	-2.68246477	6.52284427	4.57695056
C	-1.89390051	1.05146131	1.25749654	H	-0.04192593	9.10807312	2.37639092
C	-0.84614365	0.67298242	2.15488142	H	-1.84733242	8.79573694	4.04515267
C	-0.34691112	-0.59792454	1.74504986	C	0.25491915	4.55454540	1.60453447
C	-0.96456979	-2.32850616	-0.10520020	O	1.23550248	4.60723344	0.88300589
H	-1.62645076	-3.07511192	0.35809820	H	-0.23975117	3.57484906	1.76736445
				H	-1.73336412	4.41172885	-0.24507503

B	-2.12392455	4.34183932	-1.37105488
O	-1.94954582	5.33443988	-2.28015700
O	-2.82484640	3.28111909	-1.85131766
C	-3.33552404	3.65795825	-3.15112230
C	-2.35573051	4.80555253	-3.56340683
C	-2.98397237	5.91552996	-4.37684737
C	-4.75854732	4.14654527	-2.93168909
C	-3.31775023	2.45286946	-4.06668360
C	-1.09631781	4.28717265	-4.23524125
H	-2.22697857	6.66996796	-4.61923144
H	-3.38510371	5.52343103	-5.31931547
H	-3.79230126	6.41084200	-3.83099587
H	-4.77877935	5.03236831	-2.28547982
H	-5.25081959	4.39512140	-3.87844790
H	-5.33676803	3.35496230	-2.44199848
H	-4.05017577	1.71337170	-3.72230627
H	-3.59341651	2.74630477	-5.08722567
H	-2.33594265	1.97230467	-4.08676788
H	-0.63960156	3.48765813	-3.64119423
H	-1.30133185	3.89824227	-5.23866020
H	-0.37605512	5.10726994	-4.32354028

TS-1 $E(\text{RPW6B95}) = -4790.35837065341$ a.u.

Mo	1.04895106	0.40792540	0.00000000
Ge	2.60516199	-1.44108936	-0.14818171
C	2.55449078	1.44411772	0.61153254
O	3.33156502	2.23851582	0.95117260
C	0.66868983	0.31216601	1.91055452
O	0.40034466	0.38879249	3.03496420
C	0.07478546	2.44096445	-0.45986992
C	-0.99976971	1.51056073	-0.31680077
C	-0.93961700	0.59099578	-1.40709387
C	0.20015127	0.91387401	-2.19987746
C	0.83113689	2.05554870	-1.61628498
C	0.28791253	3.67034666	0.35939455
H	-0.30864679	4.50785570	-0.03036523
H	1.33704099	3.98317006	0.35391729
H	-0.00276975	3.51441737	1.40400384
C	-2.09230743	1.58279673	0.69818893
H	-1.77929387	2.15113904	1.58012387
H	-2.38400600	0.58265897	1.03236451
H	-2.97908143	2.08186789	0.28193373
C	-1.99518446	-0.39932068	-1.75410748
H	-2.59612877	-0.66209566	-0.88073991
H	-1.58092190	-1.32805687	-2.15770531
H	-2.66668566	0.01582170	-2.52003689
C	0.53495727	0.36403600	-3.54904675
H	0.28833413	1.09843417	-4.32976829
H	-0.03977423	-0.54018579	-3.77469422
H	1.59914334	0.12632864	-3.65411768
C	1.96859951	2.80876071	-2.22241183
C	2.63069823	2.14221913	-2.78661025
H	2.57529680	3.31425674	-1.46379337
H	1.60186284	3.57771605	-2.91836377
Si	5.47928236	-0.77284194	0.79933157
Si	4.50616969	-3.72573131	1.17519933
Si	4.97955353	-2.61584588	-1.73402290
C	4.42233479	-2.18573840	0.05014671
C	4.37062782	-3.26495991	2.99583730
H	4.18447824	-4.18253439	3.57166836
H	3.54203228	-2.57325939	3.19097085
H	5.28799221	-2.81348365	3.39190319
C	4.48618099	-4.33215584	-2.32775211
C	3.40248829	-4.48092238	-2.30775183
H	4.95850907	-5.14387757	-1.76291257
H	4.82183421	-4.42724077	-3.37069768
C	4.22024314	-1.41091137	-2.97436324
H	4.68620851	-1.56190470	-3.95839401
H	4.35344957	-0.35837490	-2.69925199
H	3.14532579	-1.60018122	-3.09326555
C	6.85237628	-2.55463361	-1.92638443
H	7.34912166	-3.27701482	-1.26739939
H	7.29073198	-1.56795956	-1.74214572

H	7.09538726	-2.83451426	-2.96131205
C	3.12551916	-4.95207940	0.86938023
H	3.13369347	-5.35335813	-0.14849601
H	2.15475823	-4.47566477	1.04250133
H	3.23950895	-5.79126432	1.57044418
C	7.20742392	-1.31401026	1.31752788
H	7.80161393	-1.77752592	0.52386949
H	7.17514856	-2.00009391	2.17303539
H	7.74277884	-0.41279255	1.65045441
C	4.72054424	-0.09251534	2.38975308
H	3.63098228	-0.20004703	2.45626812
H	4.94730363	0.97691060	2.47129052
H	5.15905817	-0.58985969	3.26173251
C	6.13640217	-4.65035567	0.96538558
H	6.16913121	-5.45283140	1.71646896
H	7.01754354	-4.01944684	1.12163116
H	6.23213524	-5.12664462	-0.01735793
C	5.67947611	0.61879768	-0.45439004
H	6.13275210	1.48924120	0.03829239
H	4.72195152	0.94368538	-0.87636018
H	6.33369856	0.32997443	-1.28610470
C	-0.06158918	-4.05511854	-2.00799984
C	-1.10122442	-4.00217617	-2.94942658
C	0.11884630	-5.22303846	-1.25496392
C	-1.95193626	-5.08285067	-3.11906295
C	-0.73472238	-6.30260487	-1.43097197
C	-1.77465069	-6.23597168	-2.35562612
H	-1.23214954	-3.10436401	-3.55236096
H	0.92420419	-5.25326892	-0.52887058
H	-2.75563323	-5.03094241	-3.85106093
H	-0.59078117	-7.20515578	-0.83952689
H	-2.44332434	-7.08455713	-2.48763772
C	0.79507960	-2.89905180	-1.82099911
O	1.90453755	-2.96989411	-1.19385367
H	0.61751762	-2.03500374	-2.47465532
H	-0.04601467	-1.83952329	-0.67393784
B	-0.27249111	-2.03994827	0.53675539
O	0.24075586	-3.18393910	1.10558797
O	-1.45471559	-1.66484253	1.12791755
C	-1.88706301	-2.75099732	1.96842486
C	-0.54879217	-3.51593448	2.25830069
C	-0.69515977	-5.02313163	2.33285891
C	-2.86379106	-3.57562781	1.14257099
C	-2.55765633	-2.17273922	3.19547536
C	0.19182021	-3.01274163	3.48606611
H	0.28609936	-5.48041144	2.50631480
H	-1.34989742	-5.30500351	3.16676309
H	-1.10551732	-5.43948027	1.40964213
H	-2.37397723	-3.98923662	0.25090888
H	-3.29094099	-4.40287695	1.72055000
H	-3.68469193	-2.93022449	0.80997866
H	-3.49546520	-1.68021141	2.91298753
H	-2.79469767	-2.96087085	3.92044264
H	-1.91551428	-1.42903637	3.67728931
H	0.33245604	-1.92931256	3.45656157
H	-0.33935782	-3.26988636	4.40933952
H	1.17973101	-3.48650098	3.51936434

d(from TS1) $E(\text{RPW6B95}) = -4790.42189074623$ a.u.

Mo	-0.04662005	0.01165501	0.00000000
Ge	-0.39123407	-1.87133712	-1.56823711
C	-0.74839010	-1.14767107	1.40178610
O	-1.12402413	-1.63784111	2.37943017
C	-1.79780417	0.74972206	0.34473803
O	-2.80417325	1.23836810	0.64953905
C	0.93666302	1.38127711	1.55794411
C	0.90912902	2.09791816	0.31798402
C	1.80791009	1.45459811	-0.59120004
C	2.36358013	0.32153803	0.07295001
C	1.81911909	0.27035103	1.39140910
C	0.26104498	1.78657814	2.82612220
H	0.92215802	2.41567118	3.43912425
H	-0.02163805	0.91767307	3.43084725

H	-0.65025209	2.36134818	2.62908019	O	-2.42421922	0.01504801	-2.37895117
C	0.21465697	3.39409225	0.06226600	O	-0.88627011	1.67167213	-2.55560218
H	-0.69841009	3.48702126	0.66061205	C	-1.73808417	1.79224014	-3.71675827
H	-0.06557005	3.48455626	-0.99151207	C	-3.00569426	1.01590908	-3.25531523
H	0.86575202	4.24300732	0.31684802	C	-3.78327332	0.34611404	-4.36515231
C	2.25035812	2.05161716	-1.88463513	C	-1.02388512	1.10894409	-4.86957735
H	1.39584606	2.32522118	-2.51132318	C	-1.95964218	3.25965524	-4.00964729
H	2.89059816	1.37291511	-2.45424017	C	-3.93095333	1.86893615	-2.40348218
H	2.83173016	2.96486522	-1.69281212	H	-4.68182238	-0.13171600	-3.96018028
C	3.50129821	-0.53720803	-0.37792403	H	-4.10514534	1.09260609	-5.10188737
H	4.36201727	-0.39533102	0.29067502	H	-3.19412827	-0.41649002	-4.87854035
H	3.83381023	-0.27979201	-1.38724610	H	-0.87397511	0.04601101	-4.65257933
H	3.25674819	-1.60499911	-0.36412603	H	-1.58391816	1.19878110	-5.80699444
C	2.24205012	-0.69693604	2.44737217	H	-0.03739905	1.56402013	-5.01444736
H	2.42481913	-1.69357111	2.02978815	H	-1.01728412	3.72117728	-4.32667531
H	1.48819106	-0.79887505	3.23448223	H	-2.68586224	3.38719325	-4.82185635
H	3.17421318	-0.36337102	2.92649921	H	-2.32200621	3.79795429	-3.12909723
Si	-2.10390319	-4.09036729	-0.16337101	H	-3.37587028	2.41742018	-1.63540312
Si	-2.51628722	-3.72838226	-3.23650123	H	-4.48175137	2.58944020	-3.01881022
Si	0.24897497	-4.77576033	-2.18686016	H	-4.65524638	1.22094310	-1.89808314
C	-1.25138814	-3.63082225	-1.81229013	d'(from TS2) E(RPW6B95) = -4790.42175001948 a.u.			
C	-4.17191835	-2.97340321	-2.76184420	Mo	0.97902099	1.08391607	0.00000000
H	-4.77209339	-2.85074820	-3.67441927	Ge	0.40533495	-0.79734607	-1.50506211
H	-4.05509334	-1.99116613	-2.29266017	C	0.13237092	0.06820200	1.43107110
H	-4.74402539	-3.61701025	-2.08285015	O	-0.30458011	-0.33701703	2.42221917
C	0.76982201	-4.87881234	-3.98884128	C	-0.66530713	2.04510613	0.31311502
H	0.99381603	-3.88857527	-4.39576232	O	-1.60153520	2.66595518	0.60091604
H	0.03409796	-5.37286037	-4.63362733	C	2.11673807	2.36289916	1.52934111
H	1.68959908	-5.48039538	-4.02843629	C	2.18121407	3.04438021	0.27105602
C	1.77843208	-4.16566929	-1.25778009	C	2.99749213	2.27175615	-0.61437905
H	2.56027214	-4.93687835	-1.30183409	C	3.41195716	1.09952707	0.08395101
H	1.59737107	-3.93934827	-0.20063201	C	2.85864512	1.14906407	1.39853310
H	2.18684012	-3.26849223	-1.74192213	C	1.48933802	2.88185420	2.78074820
C	-0.07879805	-6.56068348	-1.67858212	H	2.21340007	3.46115224	3.37129425
H	-0.93107511	-6.98535949	-2.22221916	H	1.12046300	2.06926014	3.41631724
H	-0.24967006	-6.70920549	-0.60759005	H	0.64110696	3.53950624	2.56202918
H	0.80796102	-7.14986948	-1.95306514	C	1.65261804	4.40887931	-0.02265800
C	-1.94705418	-2.87824120	-4.80595535	H	0.74722597	4.62479632	0.55509604
H	-1.09610612	-3.39773923	-5.25644038	H	1.40360402	4.51002531	-1.08309308
H	-1.65078716	-1.84426612	-4.61475933	H	2.39725809	5.17831637	0.22801302
H	-2.77149524	-2.88385720	-5.53244140	C	3.51048717	2.77197219	-1.92287914
C	-3.16822927	-5.64280439	-0.24801402	H	2.69681911	3.13426722	-2.55887819
H	-2.63776123	-6.54200744	-0.57780304	H	4.05779321	2.00147613	-2.47217218
H	-4.05086334	-5.50728039	-0.88462406	H	4.20391322	3.60882325	-1.75644613
H	-3.53526930	-5.83192841	0.77156206	C	4.44191224	0.10072900	-0.33584702
C	-3.29824728	-2.73306519	0.38317903	H	5.31494330	0.16601300	0.32873202
H	-3.06255726	-1.74342512	-0.02715200	H	4.79989826	0.28295101	-1.35286410
H	-3.30376028	-2.65049718	1.47630711	H	4.07656621	-0.93069408	-0.28430302
H	-4.31775535	-2.98559221	0.07070501	C	3.15621014	0.16664200	2.48295018
C	-2.86333125	-5.51640439	-3.73038327	H	3.23130615	-0.85414307	2.09125315
H	-3.67630031	-5.50525338	-4.47098232	H	2.38520509	0.16863200	3.26010724
H	-3.18845427	-6.14825046	-2.89780021	H	4.11361421	0.40512902	2.96900921
H	-2.00232719	-5.99925743	-4.20720430	Si	-1.56627320	-2.74036321	-0.03159600
C	-0.81334610	-4.42196531	1.17067308	Si	-1.92213022	-2.44633719	-3.11911522
H	-1.30452014	-4.45484431	2.15201416	Si	0.69397396	-3.77875428	-2.01260415
H	-0.03476405	-3.65468125	1.22285109	C	-0.65852013	-2.44808619	-1.68980112
H	-0.31855807	-5.38798538	1.01515307	C	-3.47403634	-1.47637312	-2.68729320
C	2.07092410	-0.95514006	-4.75265034	H	-4.05211938	-1.31933511	-3.60883826
C	3.36583120	-0.48258702	-4.97872636	H	-3.23710832	-0.49663604	-2.25973916
C	1.33924105	-1.44330309	-5.83443445	H	-4.12252938	-2.01510115	-1.98615814
C	3.91096224	-0.48308102	-6.25742344	C	1.20537700	-4.00471230	-3.80609927
C	1.88500209	-1.45098309	-7.11397149	H	1.56050502	-3.06509523	-4.23938631
C	3.17072319	-0.96775806	-7.33165654	H	0.41372094	-4.41488733	-4.44329232
H	3.95944724	-0.11729800	-4.14026830	H	2.03704606	-4.72407635	-3.82023527
H	0.33907498	-1.82706412	-5.65771941	C	2.28383208	-3.32923525	-1.09396708
H	4.92280031	-0.11280800	-6.41408446	H	2.97360513	-4.18421131	-1.13082508
H	1.30061105	-1.84015612	-7.94626459	H	2.13339907	-3.07262423	-0.03894300
H	3.59835622	-0.97526906	-8.33270262	H	2.79031412	-2.49002019	-1.58935911
C	1.48033706	-0.88797105	-3.37207024	C	0.15144593	-5.49099938	-1.44286910
O	0.47436799	-1.84064212	-3.17152623	H	-0.74402414	-5.83170243	-1.97595814
H	2.28991612	-1.01366906	-2.63913319	H	-0.03934509	-5.57482244	-0.36826303
H	1.07724403	0.12419302	-3.20556723	H	0.96223398	-6.19226444	-1.68702512
B	-1.25255013	0.54184905	-1.85725813				

C	-1.25017418	-1.72873413	-4.71372334
H	-0.45116112	-2.35009718	-5.12849237
H	-0.85334415	-0.72233406	-4.56136033
H	-2.06266823	-1.68171813	-5.45216839
C	-2.80990129	-4.15518431	-0.06894101
H	-2.39053226	-5.12338037	-0.36119803
H	-3.66717635	-3.93754130	-0.71720305
H	-3.20066732	-4.26052932	0.95391907
C	-2.59304227	-1.23170310	0.45648803
H	-2.24841125	-0.29197303	0.00799800
H	-2.58780527	-1.10598209	1.54545011
H	-3.63537735	-1.37841111	0.15145501
C	-2.48107327	-4.19733031	-3.54694426
H	-3.28976132	-4.11768131	-4.28794931
H	-2.87494829	-4.75496735	-2.69132919
H	-1.68494421	-4.79617436	-4.00446029
C	-0.33263811	-3.17978024	1.32517010
H	-0.82573314	-3.10354323	2.30314916
H	0.54150895	-2.52208119	1.35120510
H	0.02874092	-4.20922631	1.21540509
C	2.95733813	-0.26439903	-4.70424934
C	4.29106022	0.07579800	-4.94172035
C	2.18037607	-0.70944606	-5.77262443
C	4.83195026	-0.01250601	-6.21898644
C	2.72123011	-0.80502107	-7.05094949
C	4.04702721	-0.45389704	-7.28024655
H	4.91669327	0.40763302	-4.11261730
H	1.14769900	-0.98768608	-5.58625143
H	5.87421134	0.25501001	-6.38502946
H	2.10078606	-1.15863909	-7.87296454
H	4.47045524	-0.53024205	-8.28019358
C	2.38080408	-0.10035802	-3.32614724
O	1.27256301	-0.92548607	-3.10308822
H	2.09869307	0.95543406	-3.18279723
H	3.17208714	-0.30204303	-2.58993519
B	-0.16040810	1.69538011	-1.87473714
O	-1.38542319	1.29429608	-2.38598717
O	0.33436394	2.75619119	-2.60135819
C	-0.49678912	2.94335320	-3.76833127
C	-1.84620622	2.33155616	-3.29174724
C	-2.69464228	1.72799211	-4.38783532
C	0.13370592	2.15118114	-4.90013335
C	-0.54812213	4.41840431	-4.09930229
C	-2.66860328	3.30805423	-2.46732318
H	-3.64450535	1.36961809	-3.97664029
H	-2.92410329	2.48794817	-5.14515237
H	-2.19791525	0.88893305	-4.87912735
H	0.15375593	1.08326707	-4.65725633
H	-0.40838112	2.28481815	-5.84284043
H	1.16796500	2.48124217	-5.05039036
H	0.44137195	4.76165133	-4.42275432
H	-1.25357418	4.60731832	-4.91787136
H	-0.84951315	5.01536735	-3.23358523
H	-2.05736523	3.80589627	-1.70748212
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H	-3.46666534	2.76194919	-1.95267214

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Ge	-1.24242696	-1.18368616	-1.32477800
C	-1.39399096	-0.26908116	1.48257300
O	-1.81080996	-0.69204116	2.47646600
C	-2.36915996	1.52538984	0.11137900
O	-3.39465796	2.01403484	0.31837800
C	0.35215604	2.18905284	1.46009500
C	0.47065704	2.75706584	0.14998300
C	1.39061604	1.95984684	-0.59913600
C	1.78794404	0.86243584	0.21669600
C	1.15943404	1.00660784	1.49041100
C	-0.38125096	2.78362784	2.61688100
H	0.28029704	3.42731584	3.21429100
H	-0.78215896	2.01226584	3.28398600
H	-1.22389196	3.39885584	2.28330600

C	-0.09984796	4.05166484	-0.32282900
H	-1.04099696	4.29237784	0.18405900
H	-0.29335996	4.00891684	-1.39922900
H	0.59697704	4.88231584	-0.13660500
C	2.04399504	2.39208584	-1.86859300
H	1.32706104	2.51674684	-2.68414700
H	2.81192404	1.67582184	-2.17564400
H	2.54851104	3.35568284	-1.70895000
C	2.80760304	-0.17180616	-0.12868500
H	3.81924304	0.17177684	0.13388500
H	2.80730504	-0.40325116	-1.19879900
H	2.62997604	-1.10651316	0.41342000
C	1.43040604	0.15613384	2.68822600
H	1.53444504	-0.90094616	2.41971300
H	0.62845804	0.23044784	3.42901400
H	2.36352804	0.46784884	3.17874700
Si	-3.14845196	-3.18805816	0.04263900
Si	-3.56484296	-2.75759916	-3.04010300
Si	-0.91326496	-4.14140716	-1.98446200
C	-2.26640296	-2.82800316	-1.63022200
C	-5.08248696	-1.78626516	-2.50562100
H	-5.69433796	-1.58771016	-3.39680500
H	-4.81186796	-0.82048216	-2.06427400
H	-5.71185396	-2.33438916	-1.79468100
C	-0.39172096	-4.16277116	-3.78781500
H	-0.10465196	-3.17059416	-4.15059200
H	-1.17073996	-4.55345316	-4.45279900
H	0.48371504	-4.81949216	-3.88837300
C	0.66780404	-3.79641416	-1.00694400
H	1.38718604	-4.59553516	-1.23703600
H	0.51451704	-3.79115716	0.07718900
H	1.15408104	-2.84730016	-1.27129200
C	-1.44962796	-5.89097016	-1.55550400
H	-2.34439696	-6.20046416	-2.10687500
H	-1.63656196	-6.04080716	-0.48653900
H	-0.63402396	-6.56929016	-1.84391000
C	-2.99184696	-2.00802316	-4.65761000
H	-2.23579796	-2.62204816	-5.15598500
H	-2.60068396	-0.99888716	-4.51833900
H	-3.86797896	-1.96451216	-5.32048300
C	-4.37799596	-4.60982316	-0.04442500
H	-3.95957496	-5.55756516	-0.39781900
H	-5.24842396	-4.36069216	-0.66310700
H	-4.74698696	-4.77127916	0.97906000
C	-4.16817696	-1.71783816	0.64090700
H	-3.83463896	-0.74663016	0.26004300
H	-4.13542696	-1.67089216	1.73608700
H	-5.21700996	-1.84121116	0.34879300
C	-4.13116396	-4.49701316	-3.50739400
H	-4.96559896	-4.39301116	-4.21615700
H	-4.48743296	-5.10220716	-2.66855100
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C	-1.88315196	-3.65007616	1.35906800
H	-2.38040996	-3.66591616	2.33808700
H	-1.05252496	-2.93983716	1.42700300
H	-1.46204696	-4.64821716	1.18659400
C	1.11506904	-0.37856916	-4.75250600
C	2.23748304	0.39360384	-5.05147300
C	0.41783904	-0.97581816	-5.80272300
C	2.65171004	0.57094384	-6.36788300
C	0.82579404	-0.79874616	-7.11878800
C	1.94479604	-0.02308116	-7.40749600
H	2.78861004	0.87250284	-4.24527800
H	-0.47877896	-1.54654816	-5.58131300
H	3.52601004	1.18364484	-6.58134100
H	0.26095904	-1.26306516	-7.92547300
H	2.26222804	0.12033884	-8.43886200
C	0.70557904	-0.58934116	-3.32173300
O	-0.69744196	-0.64870616	-3.13737200
H	1.12416304	0.20772784	-2.69407400
H	1.15163504	-1.53535816	-2.97476700
B	-1.40216996	0.89797884	-2.42129200
O	-2.75946096	0.85179484	-2.76282400

O	-0.78872596	1.97580184	-3.05164000	H	2.74704025	4.95921084	2.07090966
C	-1.68095596	2.45313984	-4.08107600	H	1.99020524	3.57665132	2.85598593
C	-3.07767196	2.02865484	-3.52582100	H	2.50531611	4.95708607	3.82416884
C	-4.10399396	1.67271184	-4.58258500	C	-3.00299567	6.64817977	1.94726792
C	-1.35416896	1.75653884	-5.38810800	H	-2.68481748	7.53319689	1.38622824
C	-1.47994896	3.94722184	-4.23425200	H	-2.68396602	6.76932190	2.98981129
C	-3.65258996	3.07152084	-2.58140500	H	-4.10252305	6.63237462	1.94652054
H	-5.05150096	1.40335684	-4.10134700	C	-3.06063373	3.66101453	2.34259232
H	-4.29453496	2.52913284	-5.24157900	H	-2.39024902	2.79862352	2.44342250
H	-3.78364796	0.82676284	-5.19585600	H	-4.00838083	3.28366426	1.93926841
H	-1.53769596	0.68218784	-5.31152300	H	-3.25841918	4.04797268	3.34888580
H	-1.96111696	2.15617584	-6.20884900	C	0.45627544	7.30342769	2.92508315
H	-0.29781296	1.90431584	-5.63686100	H	0.87597719	7.52883868	3.91564960
H	-0.47398096	4.14566984	-4.62281500	H	-0.52837891	7.78254833	2.86798968
H	-2.20190496	4.36278984	-4.94816900	H	1.10676751	7.77811438	2.18123923
H	-1.58902396	4.47817784	-3.28484500	C	-3.19112564	4.81531087	-0.47786610
H	-2.90438196	3.39823584	-1.85171200	H	-4.28190144	4.76657729	-0.35606378
H	-4.00719196	3.95071684	-3.13201300	H	-2.87519759	3.88483170	-0.96615914
H	-4.49544796	2.64219884	-2.03091400	H	-2.97203567	5.65080847	-1.15442565
e <i>E</i> (RPW6B95) = -4790.4384812827 a.u.				C	5.12204297	4.59173406	-1.46494251
Mo	-0.25641026	0.92074591	0.00000000	C	5.28756085	4.74765497	-2.84269670
Ge	-0.03600947	3.14851808	0.54884803	C	5.59803433	5.58271123	-0.61010310
C	-2.14559058	1.30724707	0.14426189	C	5.91977583	5.87223850	-3.35624142
O	-3.30444786	1.38988883	0.13510087	C	6.23077821	6.71107239	-1.12489087
C	-0.22800908	0.53223033	1.91787117	C	6.39414503	6.86027313	-2.49681816
O	-0.24075172	0.20499767	3.02999385	H	4.91413589	3.97927284	-3.52007478
C	-0.72097239	-1.16661016	-0.85947190	H	5.46062772	5.46807724	0.46235013
C	0.65757318	-1.18997915	-0.46936755	H	6.04211607	5.98037198	-4.43268624
C	1.36503383	-0.26173424	-1.28184139	H	6.59589038	7.47985214	-0.44581423
C	0.42999439	0.34588250	-2.18335267	H	6.88790669	7.74355580	-2.89794038
C	-0.85035526	-0.22435878	-1.93724319	C	4.42507653	3.36393503	-0.94542477
C	-1.79810666	-2.06519722	-0.34887723	O	4.23438461	3.41427359	-1.12489087
H	-1.86895229	-2.98454277	-0.94863635	H	4.99555711	2.46610351	-1.22169983
H	-2.77731680	-1.57468515	-0.37761082	H	3.43681956	3.28096107	-1.42385404
H	-1.61226271	-2.36033632	0.68927433	B	4.59254537	2.38576393	1.24710937
C	1.26389329	-2.11045172	0.53675323	O	4.41920552	2.43063049	2.59950944
H	0.55504972	-2.36810053	1.33059645	O	5.15757347	1.21868213	0.80529053
H	2.14353902	-1.66320057	1.01086130	C	5.56781096	0.49717027	1.98569711
H	1.58410812	-3.04937698	0.06253458	C	4.59569642	1.07904731	3.06401559
C	2.84200610	-0.06358144	-1.28974990	C	5.14865141	1.10714327	4.47090651
H	3.27555648	-0.10241881	-0.28722387	C	7.01828321	0.86476785	2.25197957
H	3.11510691	0.90203692	-1.72271260	C	5.42631592	-0.98746406	1.73564306
H	3.33481611	-0.84257189	-1.89102575	C	3.22661228	0.41825677	3.02495506
C	0.76529225	1.30566697	-3.27643001	H	4.40219715	1.53051281	5.15246470
H	1.00227160	0.77296624	-4.20953948	H	5.38570348	0.09355990	4.81636510
H	1.63623188	1.91808767	-3.01961026	H	6.05178412	1.72135412	4.53503785
H	-0.06597483	1.98667203	-3.48644781	H	7.11566944	1.93486005	2.47162505
C	-2.08562490	0.02278965	-2.73803529	H	7.43150777	0.29852354	3.09399996
H	-2.12419553	1.05140973	-3.11242683	H	7.61477111	0.64271336	1.36009974
H	-2.99264286	-0.14776304	-2.14976208	H	6.12973113	-1.30352955	0.95676596
H	-2.12376897	-0.64969963	-3.60710995	H	5.65110390	-1.55555470	2.64640817
Si	-2.39991553	5.02255308	1.21509587	H	4.41675222	-1.24848284	1.40533172
Si	0.34763154	5.43479690	2.72805236	H	2.83103878	0.40281948	2.00086601
Si	0.17766121	6.01553141	-0.38822509	H	3.25314041	-0.60791964	3.40831806
C	-0.48915271	4.96842884	1.07417751	H	2.52686807	0.99491633	3.63867608
C	-0.60310329	4.77124051	4.20893644	b' <i>E</i> (RPW6B95) = -4377.815906865378 a.u.			
H	-0.00096941	4.96653462	5.10770698	Mo	0.72580647	1.29032256	0.00000000
H	-0.75550212	3.68588182	4.14753726	Ge	-1.46904668	1.68550559	-0.49430004
H	-1.57874649	5.24632843	4.36144962	C	0.95002849	1.37499257	-1.92948214
C	2.03215027	6.27161838	-0.25186336	O	1.20310851	1.46826457	-3.05991322
H	2.54880070	5.30831670	-0.16861689	C	0.38618845	-0.64105358	-0.13321901
H	2.34559821	6.88828081	0.59805585	O	0.28768144	-1.79090066	-0.19400001
H	2.39345305	6.76090238	-1.16708978	C	2.13888058	3.06841669	0.54824704
C	-0.04538669	5.10758441	-2.02923098	C	2.95892364	1.94321761	0.20753002
H	0.13413670	5.81586421	-2.85098655	C	2.71949062	0.91374453	1.16251808
H	-1.03908141	4.66978024	-2.17352955	C	1.75812655	1.39557957	2.10793215
H	0.69270118	4.30064449	-2.13486649	C	1.39760253	2.72548267	1.72147412
C	-0.66757111	7.68681527	-0.51467202	C	2.13518958	4.38896878	-0.14914601
H	-0.58461363	8.26665118	0.41187353	H	2.91871163	5.05321383	0.24523502
H	-1.72961058	7.60397390	-0.77490909	H	1.17550351	4.90373082	-0.02935700
H	-0.17702536	8.26208517	-1.31243591	H	2.31226659	4.27522378	-1.22440109
C	2.05136631	4.67266995	2.86447374	C	3.96543571	1.89884860	-0.89322607

H	3.66697969	2.52463265	-1.74067712	C	0.85851062	-0.17295457	-1.76356613
H	4.10504772	0.87976953	-1.26875409	O	1.13342864	0.26909646	-2.80196820
H	4.94212978	2.26156463	-0.54194704	C	0.46543759	-2.66855176	-0.88658207
C	3.42727667	-0.39706756	1.24766709	O	0.49807559	-3.69866383	-1.41872110
H	3.72804969	-0.76058558	0.25948602	C	2.47268273	0.34285246	0.69215905
H	2.79555162	-1.16494362	1.70708812	C	2.95181876	-0.94623163	0.26943402
H	4.33662473	-0.30967756	1.86005814	C	2.44122273	-1.92004370	1.18702908
C	1.33875252	0.67555052	3.34805924	C	1.65236167	-1.24759965	2.15930015
H	2.15816958	0.64783852	4.08125929	C	1.65960367	0.15159045	1.84653413
H	1.04650850	-0.36134356	3.14387323	C	2.86800476	1.65325156	0.09543601
H	0.49182846	1.17037955	3.83427828	H	3.80191883	2.02162458	0.54465204
C	0.49307446	3.63881173	2.48262318	H	2.10050671	2.41791161	0.25483102
H	-0.30440260	3.08305769	2.98863822	H	3.03309677	1.57409755	-0.98434307
H	0.01898942	4.37697578	1.82716313	C	3.92861683	-1.20006865	-0.83041906
H	1.04999350	4.18975677	3.25468223	H	3.80886883	-0.48217460	-1.64914312
Si	-4.16067188	0.38878650	-1.30658609	H	3.80163683	-2.20215672	-1.25396409
Si	-3.98666187	3.42447071	-0.33409702	H	4.96435891	-1.12050764	-0.46876303
Si	-2.74099977	2.57986465	-3.13859123	C	2.76402275	-3.37719781	1.20916709
C	-3.17412881	2.03153061	-1.35106810	H	2.96607377	-3.76549983	0.20551601
C	-3.71955284	3.13215369	1.50978911	H	1.94171169	-3.96068785	3.11834122
H	-4.27594789	3.88322275	2.08816615	H	3.65900582	-3.56272482	1.82081813
H	-2.65688877	3.24979370	1.76907313	C	1.06808963	-1.89573470	3.37003724
H	-4.04761687	2.14403362	1.84889813	H	1.86594469	-2.19904072	4.06368529
C	-1.32371567	3.82816674	-3.18740423	H	0.50094859	-2.79748677	3.11834122
H	-0.60533762	3.72317474	-2.36439417	H	0.41090258	-1.21628765	3.92070428
H	-1.69461470	4.85978182	-3.18219723	C	1.03048063	1.23024353	2.66569819
H	-0.76245263	3.68358173	-4.12026730	H	0.10406356	0.88895450	3.14103523
C	-2.18554574	1.10171955	-4.15505230	H	0.78358661	2.10693159	2.05854715
H	-2.93684979	0.30841949	-4.24103630	H	1.70737568	1.56167755	3.46707525
H	-1.26947567	0.66057652	-3.74142427	Si	-4.10296874	-2.32384973	-1.32107910
H	-1.94697772	1.44446957	-5.17145837	Si	-4.44010377	0.66404049	-0.35718103
C	-4.20686588	3.40704971	-3.97758329	Si	-2.84893365	0.07114044	-3.02555222
H	-4.45013290	4.36735378	-3.50524925	C	-3.31819568	-0.57278861	-1.27648709
H	-5.11295793	2.79185767	-3.98945029	C	-4.32986976	0.41829147	1.50562411
H	-3.93519186	3.62077173	-5.02119536	H	-5.04491082	1.08520151	2.00746414
C	-3.17611880	5.08436784	-0.68686005	H	-3.32883369	0.68986148	1.87003113
H	-3.40014782	5.47123686	-1.68808912	H	-4.54945377	-0.60512861	1.82586013
H	-2.08349673	5.03240283	-0.58000504	C	-1.74583257	1.60289655	-2.95414521
H	-3.54594483	5.82125389	0.03990600	H	-1.15959953	1.69443956	-2.03219515
C	-5.49589996	0.36024649	-2.63022819	H	-2.34160862	2.51619062	-3.06718622
H	-5.10356297	0.40729450	-3.65244926	H	-1.02903752	1.56733155	-3.78386027
H	-6.21073402	1.18289455	-2.50180318	C	-1.92130859	-1.26732965	-3.96435528
H	-6.05656103	-0.58050157	-2.53747518	H	-2.55159763	-2.13076072	-4.21023230
C	-5.01839893	0.10316648	0.34189102	H	-1.05123052	-1.63376868	-3.40267824
H	-5.73542299	0.88011653	0.62934505	H	-1.54798756	-0.85112663	-4.90998336
H	-4.29048689	-0.01868153	1.15182108	C	-4.35243876	0.60434048	-4.02386629
H	-5.57139095	-0.84416259	0.26937802	H	-4.81696280	1.49870154	-3.58884826
C	-5.82212699	3.57725473	-0.69977805	H	-5.12250784	-0.16509058	-4.13610030
H	-6.22352502	4.44629179	-0.15973901	H	-4.00630474	0.88051550	-5.03045036
H	-6.39793306	2.70025366	-0.38284703	C	-3.92712073	2.44878661	-0.65077305
H	-6.01005603	3.73657074	-1.76820113	H	-4.13488674	2.79049864	-1.67158912
C	-2.99177679	-1.07068161	-1.50016811	H	-2.86210965	2.61630563	-0.44470603
H	-3.56531483	-1.97955467	-1.73098113	H	-4.50208677	3.09058666	0.03174300
H	-2.46647076	-1.25393062	-0.55221604	C	-5.29642284	-2.51348274	-2.76264820
H	-2.23647374	-0.94547060	-2.28418517	H	-4.80609577	-2.43146874	-3.73980027
C	-2.69546977	0.16407048	4.16879130	H	-6.11445186	-1.78372769	-2.72650420
C	-2.59649877	1.40052657	4.80909435	H	-5.74464788	-3.51545381	-2.70487219
C	-3.42039182	-0.87485260	4.75904134	C	-5.05386381	-2.76010776	0.24245002
C	-3.21731881	1.60036158	6.03588741	H	-5.89635389	-2.09842871	0.47154803
C	-4.03822487	-0.67491358	5.98332344	H	-4.39112376	-2.79856076	1.11408208
C	-3.93640586	0.56206351	6.62050148	H	-5.46266784	-3.77136584	0.10151501
H	-2.03360972	2.20383163	4.33317131	C	-6.23152989	0.51273048	-0.90983307
H	-3.48329983	-1.82701566	4.23564430	H	-6.82358996	1.28502453	-0.39868103
H	-3.14294580	2.56332965	6.53692148	H	-6.68409090	-0.45659360	-0.67329305
H	-4.60328191	-1.48031864	6.44863545	H	-6.33658290	0.67873348	-1.98848014
H	-4.42366890	0.71625052	7.58180355	C	-2.77010565	-3.63679582	-1.44315511
C	-2.04405873	-0.03153053	2.86011820	H	-3.23916768	-4.62628389	-1.53743011
O	-2.10920273	-1.04919261	2.21347216	H	-2.17163360	-3.63675982	-0.52304704
H	-1.47729268	0.84575453	2.47646518	H	-2.08508560	-3.51002582	-2.28739116
				C	-2.68057664	-1.69429769	4.46439532
				C	-2.41134462	-0.54432860	5.20948437
Mo	0.66532260	-0.94758063	0.00000000	C	-3.38837869	-2.75507076	5.03914736
Ge	-1.60448356	-0.69873561	-0.34191102	C	-2.84852165	-0.44899760	6.52426345

c' E(RPW6B95) = -4790.377837223890 a.u.

C	-3.82222472	-2.65778976	6.35173844
C	-3.55376070	-1.50613767	7.09191548
H	-1.85829058	0.27390246	4.74704034
H	-3.57272270	-3.64918883	4.44659032
H	-2.64089064	0.44580647	7.10738852
H	-4.36908076	-3.48107481	6.80699852
H	-3.89668273	-1.43484567	8.12275658
C	-2.21642761	-1.76959269	3.07164622
O	-2.42523662	-2.69827876	2.32556217
H	-1.64272156	-0.88717763	2.71386120
H	-0.86540351	-4.35274088	4.56714033
C	-0.70853449	-6.55518004	1.98009414
C	-2.20071960	-6.66340904	2.44917618
C	-2.68939064	-8.07726715	2.67992020
H	-2.10628460	-8.58832516	3.45150625
H	-3.73598972	-8.05711116	3.00472722
H	-2.63432864	-8.66161118	1.75343013
C	-3.16058868	-5.90539099	1.54734911
H	-3.28054568	-6.40734602	0.58067004
H	-4.14208975	-5.85459598	2.03321715
H	-2.81410565	-4.88256591	1.37847410
C	0.15998657	-7.68758912	2.50561518
H	0.03209056	-7.81727612	3.58693326
H	-0.07246245	-8.63743016	2.01145214
H	1.21200664	-7.44849011	2.31435916
C	-0.52474248	-6.39208303	0.48836904
H	-0.93891151	-7.25527110	-0.04707300
H	-1.00542452	-5.48501996	0.11642801
H	0.54173659	-6.32367602	0.24722602
O	-0.26214947	-5.35312795	2.64781719
O	-2.17466960	-5.96807199	3.71722026
B	-1.08982553	-5.15115194	3.70572427

TS' $E(\text{RPW6B95}) = -4790.331973594826$ a.u.

Mo	0.10080645	1.22983869	0.00000000
Ge	-2.17465571	1.47523971	-0.29487802
C	0.20287246	1.88629874	-1.81565413
O	0.43308848	2.29036877	-2.88094221
C	-0.12181856	-0.57551044	-0.72671205
O	-0.11290956	-1.64029352	-1.17687208
C	1.75139958	2.74278980	0.62153405
C	2.39086162	1.56089671	0.10808001
C	2.09314160	0.48401564	0.99541607
C	1.27948554	0.98341867	2.05240815
C	1.05739452	2.37928077	1.81341513
C	1.89433558	4.11726990	0.05544700
H	2.80766165	4.60510693	0.42663103
H	1.04579353	4.75474595	0.32493102
H	1.95359859	4.09851190	-1.03838807
C	3.31835069	1.50676471	-1.05978108
H	3.04491367	2.23771176	-1.82790013
H	3.31126069	0.51801164	-1.53062411
H	4.35157276	1.72193073	-0.75069805
C	2.62142964	-0.90800346	0.90309806
H	2.84330865	-1.18854748	-0.13158401
H	1.90264159	-1.63346652	1.29825909
H	3.55100670	-1.00902547	1.48153710
C	0.91843152	0.20927062	3.27523723
H	1.79697657	0.09341261	3.92758128
H	0.55730149	-0.79413145	3.02923122
H	0.14886546	0.71164865	3.87044128
C	0.32969047	3.30871684	2.72860720
H	-0.53253059	2.81863481	3.19459223
H	-0.04363256	4.18938591	2.19671416
H	0.98635352	3.66166087	3.53747925
Si	-4.74527689	-0.02294240	-1.31492409
Si	-4.92897791	2.92122881	-0.14656001
Si	-3.45540280	2.42082478	-2.90745421
C	-3.90105284	1.69797672	-1.18382108
C	-4.77065489	2.49926478	1.68016412
H	-5.40846997	3.15979883	2.28393617
H	-3.73550082	2.65775279	2.01908014
H	-5.05170492	1.46628471	1.90661513

C	-2.28952372	3.90317688	-2.79213820
H	-1.65427767	3.91249488	-1.89865214
H	-2.85226376	4.84355495	-2.81787320
H	-1.61818767	3.89314588	-3.65985127
C	-2.61286474	1.09878168	-3.94414729
H	-3.28123879	0.27051062	-4.20778230
H	-1.74056568	0.67536865	-3.42994925
H	-2.25384771	1.54704672	-4.88053835
C	-4.96307591	3.07387183	-3.82567227
H	-5.36706396	3.96695189	-3.33168124
H	-5.77454796	2.34986377	-3.94681328
H	-4.63788488	3.38321285	-4.82959335
C	-4.30599786	4.68820194	-0.30625602
H	-4.52051988	5.13176397	-1.28575709
H	-3.22556678	4.76507795	-0.12606001
H	-4.81315790	5.30428798	0.44980403
C	-5.93225998	-0.09371841	-2.77415220
H	-5.45259594	0.05125061	-3.74848027
H	-6.73758002	0.64546365	-2.67567819
H	-6.39947999	-1.08860447	-2.78339720
C	-5.76850296	-0.49985043	0.19004001
H	-6.57732504	0.19790862	0.43270803
H	-5.14313892	-0.63821044	1.07738208
H	-6.23484702	-1.46992450	-0.03589900
C	-6.73852804	2.92857781	-0.65674405
H	-7.26231906	3.70959187	-0.08750801
H	-7.25353408	1.98184075	-0.46226503
H	-6.85752307	3.16255583	-1.72112113
C	-3.43914280	-1.36020550	-1.48159511
H	-3.92639683	-2.32798257	-1.66669312
H	-2.86354276	-1.45004350	-0.54953304
H	-2.72873975	-1.18571348	-2.29711717
C	-3.47039180	0.41309363	4.27631931
C	-3.01996477	1.50254471	5.02778236
C	-4.63066288	-0.27597342	4.64693333
C	-3.73409582	1.91111074	6.14419946
C	-5.33636994	0.13294861	5.76688042
C	-4.88981691	1.22530669	6.51035747
H	-2.11652570	2.03026375	4.72526134
H	-4.94256291	-1.13234648	4.05296729
H	-3.39467780	2.76234380	6.73014251
H	-6.23677498	-0.39817342	6.06800143
H	-5.44936293	1.54394071	7.38817854
C	-2.74009575	0.02004461	3.07779422
O	-3.22768478	-0.76106245	2.20329916
H	-1.84863868	0.61859165	2.82336120
H	-1.61909867	-1.24955949	3.66716726
C	-1.55311166	-3.85216967	1.72592912
C	-2.95182577	-4.04280469	2.40457518
C	-3.12654378	-5.35637479	3.13721122
H	-2.41044573	-5.45204781	3.95899229
H	-4.13583185	-5.41498879	3.56200525
H	-2.99723977	-6.20612783	2.45506318
C	-4.09536485	-3.82215967	1.42336611
H	-4.19448285	-4.65524774	0.71755205
H	-5.03432091	-3.72865167	1.98174014
H	-3.94384683	-2.89996361	0.85488106
C	-0.42888758	-4.44007172	2.56799819
H	-0.50991659	-4.10900969	3.61047926
H	-0.43068258	-5.53635681	2.54937618
H	0.53216149	-4.09373769	2.17077416
C	-1.47176266	-4.36325671	0.30277902
H	-1.73519268	-5.42805878	0.25893602
H	-2.13871771	-3.80340267	-0.35866703
H	-0.45328959	-4.24745970	-0.08299601
O	-1.40822765	-2.42770357	1.72797512
O	-2.95830076	-2.97933961	3.36231224
B	-2.19694271	-1.95319354	2.78407020

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Mo	0.52419356	0.62499999	0.00000000
Ge	-1.74966960	0.91859901	-0.24467302
C	0.52602257	1.29494904	-1.81410613

O	0.68455458	1.72397307	-2.88252321	C	-5.81494887	-0.08446906	-2.53684818
C	0.40893656	-1.16976114	-0.77108206	H	-5.50476485	0.21488896	-3.54589326
O	0.46152556	-2.21991721	-1.25996509	H	-6.55242796	0.64060899	-2.17562616
C	2.13651968	2.21783711	0.49907204	H	-6.32010391	-1.05660313	-2.62725419
C	2.79836773	1.00395802	0.10605401	C	-4.89594982	-1.08687613	0.21181102
C	2.51284071	0.01500795	1.09775208	H	-5.64449686	-0.50034509	0.75799505
C	1.67961965	0.60091199	2.09052215	H	-4.05650576	-1.26701815	0.89527507
C	1.43540963	1.96329109	1.71442912	H	-5.34693885	-2.06418320	-0.00896000
C	2.26213869	3.53659720	-0.18948601	C	-6.24342792	2.41239212	0.01715800
H	3.16670376	4.06671224	0.14219901	H	-6.70356093	3.07876617	0.76029105
H	1.40422563	4.18341824	0.02217400	H	-6.69420598	1.42120805	0.14416801
H	2.32781269	3.42193619	-1.27683409	H	-6.51566094	2.78626715	-0.97685707
C	3.73832080	0.85003901	-1.04307808	C	-3.17728870	-1.51289417	-2.22594816
H	3.46184578	1.49867305	-1.88123714	H	-3.66528074	-2.49751523	-2.23878516
H	3.74917180	-0.18014607	-1.41491710	H	-2.22050563	-1.63376017	-1.70270612
H	4.76629387	1.10925903	-0.75026305	H	-2.95605169	-1.24755914	-0.97646024
C	3.08421875	-1.36162115	1.15529708	C	-3.00353069	0.58287399	5.03651736
H	3.27245776	-1.76767218	0.15576101	C	-2.39246564	1.72175407	5.56545137
H	2.41205770	-2.05017420	1.67647312	C	-4.33673378	0.32633797	5.34549541
H	4.04228282	-1.35926815	1.69520912	C	-3.10005570	2.58757813	6.38905745
C	1.27694862	-0.06183306	3.36716824	C	-5.04695986	1.19451003	6.17019942
H	2.16743369	-0.32160608	3.95740228	C	-4.43352879	2.32660111	6.69398150
H	0.70369558	-0.98150612	3.20694623	H	-1.34988757	1.93400308	5.32642540
H	0.66846958	0.60677599	3.98284329	H	-4.81529382	-0.55448009	6.32486135
C	0.68483958	2.97265016	2.52064418	H	-2.61028166	3.47223720	6.79254949
H	-0.12071548	2.50851413	3.09932322	H	-6.08974093	0.98380502	6.40229847
H	0.22989654	3.73870722	1.88409613	H	-4.99094285	3.00530116	7.33709352
H	1.35070663	3.48395520	3.23151723	C	-2.21133563	-0.32550408	4.14162230
Si	-4.33754778	-0.28657907	-1.39290610	O	-3.03017969	-1.30848915	3.55644126
Si	-4.38536579	2.41258312	0.29044202	H	-1.73102760	0.26538796	3.34708424
Si	-3.13760070	2.41849012	-2.61133819	H	-1.40090757	-0.80077311	4.71343634
C	-3.46628572	1.38095505	-1.03617308	C	-0.95000654	-4.05889535	2.69348819
C	-3.99326776	1.78431407	2.01671614	C	-2.23810864	-4.29117636	1.83628113
H	-4.67478781	2.25018811	2.74208920	C	-2.76088867	-5.70969245	1.84688513
H	-2.97646069	2.08915210	2.30230916	H	-3.02923669	-6.03371450	2.85685721
H	-4.06752376	0.69933700	2.14086515	H	-3.65800374	-5.77738745	1.22104609
C	-1.84359060	3.76539822	-2.32678517	H	-2.01294762	-6.40172553	1.44127910
H	-1.14799856	3.54515820	-1.50741811	C	-2.08234062	-3.77208633	0.41762603
H	-2.31720464	4.73145029	-2.11620315	H	-1.38954257	-4.37927437	-0.17442601
H	-1.24026956	3.88201622	-3.23601823	H	-3.06062269	-3.78109032	-0.07398401
C	-2.53974665	1.32479404	-4.01567829	H	-1.71277960	-2.73955525	0.42782203
H	-3.33743371	0.67953199	-4.40454131	C	-0.93102354	-4.90236941	3.95774528
H	-1.69464960	0.69008900	-3.72365527	H	-1.88567061	-4.82899240	4.49269232
H	-2.20126163	1.96385709	-4.84270835	H	-0.73708753	-5.95779148	3.73659827
C	-4.70653081	3.27980618	-3.19573023	H	-0.13851648	-4.53767738	4.62085133
H	-5.06177984	4.03431024	-2.48336018	C	0.34945155	-4.19364735	1.93278814
H	-5.52884385	2.58291213	-3.39339224	H	0.44245356	-5.19726842	1.50031711
H	-4.48276980	3.80310622	-4.13652730	H	0.41894656	-3.45929830	1.12609208
C	-3.79824975	4.19985425	0.31300602	H	1.19635461	-4.04218435	2.61228219
H	-4.07648277	4.77929029	-0.57423704	O	-1.11584456	-2.68586525	3.10458622
H	-2.70821567	4.26140025	0.43366403	O	-3.19280170	-3.43012330	2.49004818
H	-4.25220778	4.69292528	1.18439308	B	-2.46177365	-2.43360523	3.06634622

12. References

1. T. P. Dhungana, H. Hashimoto, M. Ray and H. Tobita, *Organometallics*, 2020, **39**, 4350–4361.
2. C. S. Wei, C. A. J.-Hoyos, M. F. Videa, J. F. Hartwig and M. B. Hall, *J. Am. Chem. Soc.* 2010, **132**, 3078–3091.
3. T. Ghatak, K. Makarov, N. Fridman and M.S. Eisen, *Chem. Commun.*, 2018, **54**, 11001–11004.
4. C. P. Giarrusso, D. V. Zeil and V. L. Blair, *Dalton Trans.*, 2023, **52**, 7828–7835.
5. P. Ghosh and A. J. von Wangelin *Angew. Chem. Int. Ed.*, 2021, **60**, 16035–16043.
6. J. Bhattacharjee, D. Bockfeld and M. Tamm, *J. Org. Chem.*, 2022, **87**, 1098–1109.
7. D. Wu, R. Wang, Y. Li, R. Ganguly, H. Hirao and R. Kinjo, *Chem*, 2017, **3**, 134–151.
8. L. J. Bole, M. Uzelac, A. Hernán-Gómez, A. R. Kennedy, C. T. O'Hara and E. Hevia, *Inorg. Chem.*, 2021, **60**, 13784–13796.
9. W. Wang, X. Shen, F. Zhao, H. Jiang, W. Yao, S. A. Pullarkat, L. Xu and M. Ma, *J. Org. Chem.*, 2018, **83**, 69–74.
10. A. S. Chang, K. E. Kawamura, H. S. Henness, V. M. Salpino, J. C. Greene, L. N. Zakharov and A. K. Cook, *ACS Catal.*, 2022, **12**, 11002–11014.
11. Gaussian 16, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
12. GaussView, Version 6.1, Roy Dennington, Todd A. Keith, and John M. Millam, Semichem Inc., Shawnee Mission, KS, 2016.
13. (a) Y. Zhao and D.G. Truhlar, *J. Phys. Chem. A* 2005, **109**, 5656–5667; (b) K. Burke, J. P. Perdew, Y. Wang, in *Electronic Density Functional Theory: Recent Progress and New Directions*, Ed. J. F. Dobson, G. Vignale, M. P. Das (Plenum 1998). (c) J. P. Perdew, in *Electronic Structure of Solids '91*, Ed. P. Ziesche and H. Eschrig (Akademie Verlag, Berlin, 1991) 11. (d) J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh and C. Fiolhais, *Phys. Rev. B*, 1992, **46**. (f) J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh and C. Fiolhais, *Phys. Rev., B* 1993, **48**. (g) J. P. Perdew, K. Burke and Y. Wang, *Phys. Rev., B* 1996, **54**.
14. S. Grimme, S. Ehrlich and L. Goerigk, *J. Comp. Chem.*, 2011, **32**, 1456–1465.
15. A.V. Marenich, C.J. Cramer and D.G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378–6396.
16. F. Weignend and R. Ahlrichs *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297–3305.
17. K. Fukui, *J. Phys. Chem.*, 1970, **74**, 4161–4163.
18. R.F.W. Bader *Chem. Rev.*, 1991, **91**, 893–928.
19. A.E. Reed, R.B. Weinstock and F. Weinhold, *J. Chem. Phys.*, 1985, **83**, 735–746.
20. E. D. Glendening, C. R. Landis and F. Weinhold, *J. Comput. Chem.*, 2019, **40**, 2234–2241.
21. K.B. Wiberg, *Tetrahedron*, 1968, **24**, 1083–1096.
22. T. L. Anderson and E. E. Kwan, *PyQuiver* 2020.
23. E. P. Wigner, *J. Chem. Phys.* 1938, **6**, 219–220.
24. R. A. Angnes, *mechaSVG v0.1.1*, Zenodo 2020.