

## SUPPORTING INFORMATION

**Low Coordinate Germanium(II) and Tin(II) Hydride Complexes: Efficient Catalysts for the  
Hydroboration of Carbonyl Compounds**

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## 1. Synthetic Procedures.

**General considerations.** All manipulations were carried out using standard Schlenk and glove box techniques under an atmosphere of high purity dinitrogen. Diethyl ether and pentane were distilled over Na/K alloy (25:75), while THF, hexane and toluene were distilled over molten potassium. Dichloromethane was distilled over  $\text{CaH}_2$ .  $^1\text{H}$ ,  $^{13}\text{C}\{^1\text{H}\}$ ,  $^{29}\text{Si}\{^1\text{H}\}$ ,  $^{119}\text{Sn}\{^1\text{H}\}$  and  $^{11}\text{B}\{^1\text{H}\}$  NMR spectra were recorded on either Bruker AvanceIII 400 or Varian Inova 500 spectrometers and were referenced to the resonances of the solvent used, external  $\text{SiMe}_4$ , external  $\text{SnMe}_4$  or external  $\text{BF}_3(\text{OEt}_2)$ . Mass spectra were obtained from the EPSRC National Mass Spectrometric Service at Swansea University. IR spectra were recorded for solid samples using an Agilent Cary 630 attenuated total reflectance (ATR) spectrometer. Melting points were determined in sealed glass capillaries under dinitrogen, and are uncorrected. Microanalyses were carried out at the Science Centre, London Metropolitan University. A reproducible microanalysis could not be obtained for **4** as the compound contained hexane of crystallization which could not be completely removed by placing the sample under reduced pressure for several hours. Similarly, obtaining a suitable microanalysis of **5** was hampered by consistent contamination of the recrystallized compound by small amounts ( $< 5\%$  as determined by  $^1\text{H}$  NMR spectroscopy) of free amine,  $\text{L}^\dagger\text{H}$ . The starting materials  $\text{L}^\dagger\text{H}$ ,<sup>1</sup>  $\text{L}^\dagger(\text{H})\text{Ge}=\text{Ge}(\text{H})\text{L}^\dagger$ <sup>2</sup> and  $\text{L}^\dagger\text{Sn}(\mu\text{-H})_2\text{SnL}^\dagger$ ,<sup>2</sup> were prepared by literature procedures. Liquid aldehyde and ketone substrates were dried over activated molecular sieves. All other reagents were used as received.

**Preparation of  $\text{L}^\dagger\text{SnOBu}^\dagger$ .** To a solution of  $\text{L}^\dagger\text{H}$  (1.80 g, 2.88 mmol) in THF (70 mL) at  $-80^\circ\text{C}$  was added  $\text{Bu}^\text{n}\text{Li}$  (1.98 mL of a 1.6 M solution, 3.17 mmol) over 10 mins. The reaction mixture was then warmed to ambient temperature over 3 hrs, after which time it is added slowly, *via* cannula, to a solution of  $\text{SnBr}_2$  (0.88 g, 3.17 mmol) in THF (20 mL) at  $-80^\circ\text{C}$ . The resultant mixture was warmed to ambient temperature and stirred for 16 hr, and which, all volatiles were removed *in vacuo*. The residue was extracted into warm toluene (30 mL), and the extract filtered into a flask containing a suspension of  $\text{KOBU}^\dagger$  (323 mg, 2.88 mmol) in toluene (10 mL) at  $-80^\circ\text{C}$ . The resultant mixture was stirred for 2 hr, then warmed to ambient temperature and stirred for a further hour. The mixture was subsequently filtered, all volatiles removed *in vacuo*, and the residue dissolved in the minimum amount of hexane (*ca.* 10 mL). Storage of the solution at  $-30^\circ\text{C}$  overnight afforded pale yellow crystals of the title compound (1.35 g, 56 %). M.p.:  $164\text{--}172^\circ\text{C}$ ;  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 400 MHz, 298 K),  $\delta = 1.00$  (d,  $^3J_{\text{HH}} = 6.8$  Hz, 6H,  $\text{Ar}^\dagger\text{-CH}(\text{CH}_3)_2$ ), 1.20 (s, 9H,  $\text{OC}(\text{CH}_3)_3$ ), 1.45 (br, 18H,  $\text{SiPr}^i_3\text{-CH}(\text{CH}_3)_2$ ), 2.30 (b, 3H,  $\text{SiPr}^i_3\text{-CH}(\text{CH}_3)_2$ ), 2.55 (sept,  $^3J_{\text{HH}} = 5.2$  Hz, 1H,  $\text{Ar}^\dagger\text{-CH}(\text{CH}_3)_2$ ), 6.51 (s, 2H,  $\text{CHPh}_2$ ), 6.84–7.38 (m, 22H,

Ar-H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 75.5 MHz, 298 K),  $\delta$  = 15.4 ( $\text{SiPr}^i_3\text{-CH}(\text{CH}_3)_2$ ), 20.0 ( $\text{SiPr}^i_3\text{-CH}(\text{CH}_3)_2$ ), 24.2 ( $\text{Ar}^\dagger\text{-CH}(\text{CH}_3)_2$ ), 33.7 ( $\text{Ar}^\dagger\text{-CH}(\text{CH}_3)_2$ ), 35.5 ( $\text{OC}(\text{CH}_3)_3$ ), 52.1 ( $\text{CHPh}_2$ ), 72.0 ( $\text{OC}(\text{CH}_3)_3$ ), 126.5, 127.4, 128.7, 129.7, 130.0, 130.1, 131.4, 142.8, 144.6, 145.0, 145.4, 145.7 (Ar-C);  $^{29}\text{Si}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 80 MHz, 298 K),  $\delta$  = 6.80;  $^{119}\text{Sn}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 149 MHz, 298 K):  $\delta$  = 215; IR ( $\text{v}/\text{cm}^{-1}$ , ATR): 3061 (w), 3026 (w), 1598 (w), 1380 (m), 1355 (m), 1227 (m), 1181 (s), 1159 (m), 945 (s), 881 (s), 832 (s), 812 (m), 760 (s), 656 (s); MS/EI  $m/z$  (%): 815.2 ( $\text{M}^+$ , 1), 623.2 ( $\text{L}^{\dagger+}$ , 62), 580.1 ( $\text{L}^{\dagger+}\text{-Pr}^i$ , 100); anal. calc. for  $\text{C}_{48}\text{H}_{61}\text{NOSiSn}$ : C, 70.76 %; H, 7.55 %; N, 1.72 %; found: C, 70.76 %; H, 7.69 %; N, 1.70 %.

**Preparation of  $\text{L}^\dagger\text{GeOC}(\text{H})(\text{Pr}^i)_2$  (3).** To a solution of  $\text{L}^\dagger(\text{H})\text{Ge}=\text{Ge}(\text{H})\text{L}^\dagger$  (200 mg, 0.143 mmol) in toluene (40 mL) (i.e. a dissolved source of 0.286 mmol  $\text{L}^\dagger(\text{H})\text{Ge}$ .) was added  $\text{O}=\text{C}(\text{Pr}^i)_2$  (41  $\mu\text{L}$ , 33 mg, 0.286 mmol) and the reaction stirred at room temperature for 3 hrs. Volatiles were subsequently removed *in vacuo*, the residue extracted into hexane (20 mL), and the extract filtered and concentrated to *ca.* 10 mL. Storage at  $-30^\circ\text{C}$  for 3 days yielded large pale yellow crystals of **3** (70 mg, 30 %). M.p.:  $194\text{-}204^\circ\text{C}$ ;  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 400 MHz, 298 K),  $\delta$  = 0.70 (d,  $^3J_{\text{HH}} = 6.8$  Hz, 6H,  $\text{OC}(\text{H})\{\text{CH}(\text{CH}_3)_2\}_2$ ), 0.77 (d,  $^3J_{\text{HH}} = 6.8$  Hz, 6H,  $\text{OC}(\text{H})\{\text{CH}(\text{CH}_3)_2\}_2$ ), 0.97 (d,  $^3J_{\text{HH}} = 6.8$  Hz, 6H,  $\text{Ar}^\dagger\text{-CH}(\text{CH}_3)_2$ ), 1.36 (br, 18H,  $\text{SiPr}^i_3\text{-CH}(\text{CH}_3)_2$ ), 1.61 (virt. oct.,  $^3J_{\text{HH}} = 5.2$  Hz,  $^3J_{\text{HH}} = 5.2$  Hz, 2H,  $\text{OC}(\text{H})\{\text{CH}(\text{CH}_3)_2\}_2$ ), 2.24 (br, 3H,  $\text{SiPr}^i_3\text{-CH}(\text{CH}_3)_2$ ), 2.52 (sept,  $^3J_{\text{HH}} = 5.2$ , 1H,  $\text{Ar}^\dagger\text{-CH}(\text{CH}_3)_2$ ), 2.88 (t,  $^3J_{\text{HH}} = 5.0$  Hz, 1H,  $\text{OC}(\text{H})\{\text{CH}(\text{CH}_3)_2\}_2$ ), 6.43 (s, 2H,  $\text{CHPh}_2$ ), 6.94-7.38 (m, 22H, Ar-H);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 75.5 MHz, 298 K),  $\delta$  = 14.6 ( $\text{SiPr}^i_3\text{-CH}(\text{CH}_3)_2$ ), 19.5 ( $\text{OC}(\text{H})\{\text{CH}(\text{CH}_3)_2\}_2$ ), 19.7 ( $\text{SiPr}^i_3\text{-CH}(\text{CH}_3)_2$ ), 20.5 ( $\text{OC}(\text{H})\{\text{CH}(\text{CH}_3)_2\}_2$ ), 24.0 ( $\text{Ar}^\dagger\text{-CH}(\text{CH}_3)_2$ ), 31.3 ( $\text{OC}(\text{H})\{\text{CH}(\text{CH}_3)_2\}_2$ ), 33.7 ( $\text{Ar}^\dagger\text{-CH}(\text{CH}_3)_2$ ), 52.0 ( $\text{CHPh}_2$ ), 83.6 ( $\text{OC}(\text{H})\{\text{CH}(\text{CH}_3)_2\}_2$ ), 126.5, 127.0, 127.9, 128.1, 128.3, 128.6, 129.0, 130.2, 131.1, 142.4, 144.2, 144.6, 145.1, 145.8 (Ar-C);  $^{29}\text{Si}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 80 MHz, 298 K),  $\delta$  = 8.79; IR ( $\text{v}/\text{cm}^{-1}$ , ATR): 3060 (w), 3028 (w), 2362 (w), 1701 (w), 1653 (w), 1599 (w), 1387 (m), 1365 (s), 1228 (m), 972 (m), 880 (s), 832 (s), 756 (s), 662 (s); MS/EI  $m/z$  (%): 811.5 ( $\text{MH}^+$ , 2), 768.3 ( $\text{M}^+\text{-Pr}^i$ , 15); anal. calc. for  $\text{C}_{51}\text{H}_{67}\text{GeNOSi}$ : C, 75.55 %; H, 8.33 %; N, 1.73 %; found: C, 75.46 %; H, 8.34 %; N, 1.82 %.

**Preparation of  $\text{L}^\dagger\text{SnOC}(\text{H})(\text{Pr}^i)_2$  (4).** Note: The tin(II) alkoxides, **4** and **6**, were initially synthesised (and subsequently isolated) *via* the addition of the ketone or aldehyde to a toluene solution of  $\text{L}^\dagger\text{Sn}(\mu\text{-H})_2\text{SnL}^\dagger$ . However, greater isolated yields were obtained using the following method. To a solution of  $\text{L}^\dagger\text{SnOBu}^t$  (200 mg, 0.238 mmol) in diethyl ether (30 mL) was added neat HBpin (0.035 mL, 0.238 mmol), and the mixture stirred for 45 min at ambient temperature. To the *in situ* generated solution of

$L^{\dagger}SnH$  was then added  $O=C(Pr^i)_2$  (37  $\mu$ L, 30 mg, 0.261 mmol), and the mixture stirred for 2 hr. All volatiles are subsequently removed *in vacuo* and the residue extracted into warm hexane (10 mL), and filtered. The filtrate was concentrated to *ca.* 2 mL and stored at -30 °C for 1 week to afford **4** as colorless crystals (50 mg, 24 %). M.p.: 172-186 °C;  $^1H$  NMR ( $C_6D_6$ , 400 MHz, 298 K),  $\delta$  = 0.79 (d,  $^3J_{HH}$  = 6.8, 6H,  $OC(H)\{CH(CH_3)_2\}_2$ ), 0.87 (d,  $^3J_{HH}$  = 6.8 Hz, 6H,  $OC(H)\{CH(CH_3)_2\}_2$ ), 0.98 (d,  $^3J_{HH}$  = 6.8 Hz, 6H,  $Ar^{\dagger}-CH(CH_3)_2$ ), 1.38 (br, 18H,  $SiPr^i_3-CH(CH_3)_2$ ), 1.68 (virt. oct,  $^3J_{HH}$  = 5.2 Hz,  $^3J_{HH}$  = 5.2 Hz, 2H,  $OC(H)\{CH(CH_3)_2\}_2$ ), 2.32 (br, 3H,  $SiPr^i_3-CH(CH_3)_2$ ), 2.54 (sept,  $^3J_{HH}$  = 5.2 Hz, 1H,  $Ar^{\dagger}-CH(CH_3)_2$ ), 2.89 (t,  $^3J_{HH}$  = 5.0 Hz, 1H,  $OC(H)\{CH(CH_3)_2\}_2$ ), 6.52 (s, 2H,  $CHPh_2$ ), 6.94-7.38 (m, 22H,  $Ar-H$ );  $^{13}C\{^1H\}$  NMR ( $C_6D_6$ , 75.5 MHz, 298 K),  $\delta$  = 15.0 ( $SiPr^i_3-CH(CH_3)_2$ ), 19.6 ( $OC(H)\{CH(CH_3)_2\}_2$ ), 19.8 ( $SiPr^i_3-CH(CH_3)_2$ ), 20.9 ( $OC(H)\{CH(CH_3)_2\}_2$ ), 24.2 ( $Ar^{\dagger}-CH(CH_3)_2$ ), 32.0 ( $OC(H)\{CH(CH_3)_2\}_2$ ), 33.7 ( $Ar^{\dagger}-CH(CH_3)_2$ ), 51.9 ( $CHPh_2$ ), 83.1 ( $OC(H)\{CH(CH_3)_2\}_2$ ), 126.6, 127.6, 127.8, 128.7, 129.8, 130.0, 131.2, 143.1, 144.3, 145.3, 145.3, 145.8 ( $Ar-C$ );  $^{29}Si\{^1H\}$  NMR ( $C_6D_6$ , 80 MHz, 298 K),  $\delta$  = 7.84;  $^{119}Sn\{^1H\}$  NMR ( $C_6D_6$ , 149 MHz, 298 K):  $\delta$  = 193; IR ( $\nu/cm^{-1}$ , ATR): 3059 (w), 3025 (w), 1598 (m), 1381 (m), 1259 (m), 1014 (s), 882 (s), 746 (m), 686 (s), 657(s); MS/EI  $m/z$  (%): 857.4 ( $M^+$ , 1), 580.4 ( $L^{\dagger+}-Pr^i$ , 100).

**Preparation of  $L^{\dagger}GeOC(H)_2(PhOMe-4)$  (**5**).** This compound was prepared similarly to  $L^{\dagger}GeOC(H)(Pr^i)_2$ , but using  $L^{\dagger}(H)Ge=Ge(H)L^{\dagger}$  (250 mg, 0.179 mmol) and  $O=C(H)(PhOMe-4)$  (41  $\mu$ L, 49 mg, 0.358 mmol). The product was crystallised from a hexane solution (*ca.* 5 mL) stored at -30 °C for 4 days (185 mg, 62 %). M.p.: 63-73 °C;  $^1H$  NMR ( $C_6D_6$ , 400 MHz, 298 K),  $\delta$  = 0.99 (d,  $^3J_{HH}$  = 6.8 Hz, 6H,  $Ar^{\dagger}-CH(CH_3)_2$ ), 1.33 (d,  $^3J_{HH}$  = 7.6 Hz, 18H,  $SiPr^i_3-CH(CH_3)_2$ ), 1.99 (sept,  $^3J_{HH}$  = 7.6 Hz, 3H,  $SiPr^i_3-CH(CH_3)_2$ ), 2.53 (sept,  $^3J_{HH}$  = 6.8 Hz, 1H,  $Ar^{\dagger}-CH(CH_3)_2$ ), 3.35 (s, 3H,  $OCH_3$ ), 4.58 (s, 2H,  $OCH_2$ ), 6.37 (s, 2H,  $CHPh_2$ ), 6.82-7.39 (m, 22H,  $Ar-CH$ );  $^{13}C\{^1H\}$  NMR ( $C_6D_6$ , 75.5 MHz, 298 K),  $\delta$  = 15.2 ( $Ar^{\dagger}-CH(CH_3)_2$ ), 20.0 ( $SiPr^i_3-CH(CH_3)_2$ ), 24.1 ( $SiPr^i_3-CH(CH_3)_2$ ), 33.8 ( $Ar^{\dagger}-CH(CH_3)_2$ ), 52.3 ( $CHPh_2$ ), 54.8 ( $OCH_3$ ), 65.5 ( $OCH_2$ ), 113.8, 126.5, 127.4, 128.7, 128.9, 128.9, 130.1, 131.3, 135.1, 142.6, 144.2, 144.5, 145.0, 159.3 ( $Ar-C$ );  $^{29}Si\{^1H\}$  NMR ( $C_6D_6$ , 80 MHz, 298 K),  $\delta$  = 8.29; IR ( $\nu/cm^{-1}$ , ATR): 3060 (w), 3026 (w), 1600 (m), 1511 (m), 1448 (s), 1430 (m), 1245 (s), 1228 (m), 1038 (s), 876 (s), 828 (s), 737 (s), 655 (s); MS/EI  $m/z$  (%): 790.3 ( $M^+-Pr^i$ , 7), 623.4 ( $L^{\dagger+}$ , 61), 580.3 ( $L^{\dagger+}-Pr^i$ , 100).

**Preparation of  $L^{\dagger}SnOC(H)_2(PhOMe-4)$  (**6**).** This compound was prepared similarly to  $L^{\dagger}SnOC(H)(Pr^i)_2$ , but using  $L^{\dagger}SnOBu^t$  (200 mg, 0.238 mmol), neat HBpin (0.035 mL, 0.238 mmol) and  $O=C(H)(PhOMe-4)$  (30  $\mu$ L, 32 mg, 0.247 mmol). The compound was recrystallized from hexane

(100 mg, 47 %). M.p.: 64-74 °C;  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 400 MHz, 298 K),  $\delta$  = 0.99 (d,  $^3J_{\text{HH}}$  = 6.8 Hz, 6H,  $\text{Ar}^\dagger\text{-CH}(\text{CH}_3)_2$ ), 1.43 (d,  $^3J_{\text{HH}}$  = 7.6 Hz, 18H,  $\text{SiPr}^i_3\text{-CH}(\text{CH}_3)_2$ ), 2.17 (sept,  $^3J_{\text{HH}}$  = 5.2 Hz, 3H,  $\text{SiPr}^i_3\text{-CH}(\text{CH}_3)_2$ ), 2.54 (sept,  $^3J_{\text{HH}}$  = 5.2 Hz, 1H,  $\text{Ar}^\dagger\text{-CH}(\text{CH}_3)_2$ ), 3.37 (s, 3H,  $\text{OCH}_3$ ), 4.90 (s, 2H,  $\text{OCH}_2$ ), 6.29 (s, 2H,  $\text{CHPh}_2$ ), 6.87-7.35 (m, 22H,  $\text{Ar-CH}$ );  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 75.5 MHz, 298 K),  $\delta$  = 15.5 ( $\text{SiPr}^i_3\text{-CH}(\text{CH}_3)_2$ ), 20.0 ( $\text{SiPr}^i_3\text{-CH}(\text{CH}_3)_2$ ), 24.2 ( $\text{Ar}^\dagger\text{-CH}(\text{CH}_3)_2$ ), 33.7 ( $\text{Ar}^\dagger\text{-CH}(\text{CH}_3)_2$ ), 52.3 ( $\text{CHPh}_2$ ), 54.8 ( $\text{OCH}_3$ ), 65.5 ( $\text{OCH}_2$ ), 113.8, 126.6, 127.3, 128.5, 128.7, 129.6, 130.3, 131.5, 138.0, 142.9, 144.6, 144.8, 145.6, 159.1 ( $\text{Ar-C}$ );  $^{29}\text{Si}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 80 MHz, 298 K),  $\delta$  = 7.03;  $^{119}\text{Sn}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 149 MHz, 298 K):  $\delta$  = 193; IR,  $\nu/\text{cm}^{-1}$  (ATR): 3059 (w), 3025 (w), 1600 (m), 1360 (m), 1300 (w), 1246 (s), 878 (s), 831 (s), 759 (m), 719 (s); MS/EI  $m/z$  (%): 623.2 ( $\text{L}^{\dagger+}$ , 32); anal. calc. for  $\text{C}_{52}\text{H}_{61}\text{NO}_2\text{SiSn}$ : C, 71.07 %; H, 7.00 %; N, 1.59 %; found: C, 70.93 %; H, 6.94 %; N, 1.55 %.

## 2. Catalysis Studies

**General procedure.** To a cooled (0 °C) J. Young's NMR tube was added the required amount (typically 0.5-5 mg) of precatalyst,  $\text{L}^\dagger(\text{H})\text{Ge}=\text{Ge}(\text{H})\text{L}^\dagger$  or  $\text{L}^\dagger\text{SnOBu}^t$ , either as a crystalline solid followed by  $\text{C}_6\text{D}_6$  (0.4 mL), or as a stock solution (2.5 mg/mL in  $\text{C}_6\text{D}_6$ ). To the resultant solution was added the neat ketone or aldehyde substrate (*ca.* 0.3 mmol), and neat HBpin (using a micro-pipette). A 1:1 substrate/HBpin ratio was used in all runs, except those involving benzil and 2-cyclohexene-1-one as substrates, for which 1:2 ratios were employed. The sample volume was then made up to 0.6 mL with  $\text{C}_6\text{D}_6$ , then rapidly warmed to 20 °C and held at that temperature for the course of the reaction. The catalysed reactions were monitored by  $^1\text{H}$  NMR spectroscopy until the reaction was either complete or conversion had slowed to a negligible rate (< 5% /day).  $^{13}\text{C}\{^1\text{H}\}$  and  $^{11}\text{B}\{^1\text{H}\}$  NMR spectra were collected post reaction completion. For specific catalyst loadings and reaction times see Table 1 (aldehydes) and Table 2 (ketones) in the main text. No reaction initiation periods were observed for any of the catalytic runs. Control runs were carried out in the absence of catalyst between HBpin, and the aldehydes or ketones on a 0.3 mM scale (of substrate) in 0.6 mL  $\text{C}_6\text{D}_6$ . These either showed no reaction over the time taken for the analogous catalyzed reaction, or substrate hydroborations were less than 5% complete (for 2,2,2-trifluoroacetophenone, benzophenone, 4-methoxybenzaldehyde, and 4-bromobenzaldehyde). All of the catalysed reactions were very clean, and, at most, only traces of by-products were spectroscopically observed. The yields of the catalyzed reactions were hence determinable by a comparison of the integrations of relevant resonances for the substrate ( $^1\text{H}$  NMR), with those of the  $\text{RCH}_2\text{OBpin}$  and  $\text{R}_2\text{CHOBpin}$  resonances of the hydroborated aldehyde and ketone products, respectively. These yields were confirmed by similar comparisons

between the integrals of the relevant substrate and product resonances, and the integral of the signal for the internal standard (0.1 equiv. tetramethylsilane, TMS). Isolated yields were not determined. Turn over frequencies were determined as averages over the full observed reaction courses.

### Selected spectroscopic data for aldehyde hydroboration products

**PhCH<sub>2</sub>OBpin**: product from hydroboration of benzaldehyde. NMR data are identical to those previously reported.<sup>3</sup>

**4-BrPhCH<sub>2</sub>OBpin**: product from hydroboration of 4-bromobenzaldehyde. <sup>1</sup>H NMR (C<sub>6</sub>D<sub>6</sub>, 400 MHz, 298 K),  $\delta$  = 1.21 (s, 12H, Bpin-CH<sub>3</sub>), 4.85 (s, 2H, pinBOCH<sub>2</sub>), 7.14 (d, <sup>3</sup>J<sub>HH</sub> = 8.4 Hz, 2H, Ar-H), 7.38 (d, <sup>3</sup>J<sub>HH</sub> = 8.4 Hz, 2H, Ar-H); <sup>13</sup>C{<sup>1</sup>H} NMR (C<sub>6</sub>D<sub>6</sub>, 75.5 MHz, 298 K),  $\delta$  = 24.7 (Bpin-CH<sub>3</sub>), 66.0 (OCH<sub>2</sub>Ph), 82.9 (Bpin-C), 121.3, 128.7, 131.6, 138.9 (Ar-C); <sup>11</sup>B{<sup>1</sup>H} NMR (C<sub>6</sub>D<sub>6</sub>, 128 MHz, 298 K),  $\delta$  = 22.5.

**4-MeOPhCH<sub>2</sub>OBpin**: product from hydroboration of 4-methoxybenzaldehyde. <sup>1</sup>H NMR (C<sub>6</sub>D<sub>6</sub>, 400 MHz, 298 K),  $\delta$  = 1.17 (s, 12H, Bpin-CH<sub>3</sub>), 3.53 (s, 3H, OCH<sub>3</sub>), 4.87 (s, 2H, OCH<sub>2</sub>), 6.80 (d, <sup>3</sup>J<sub>HH</sub> = 8.4 Hz, 2H, Ar-H), 7.25 (d, <sup>3</sup>J<sub>HH</sub> = 8.4 Hz, 2H, Ar-H); <sup>13</sup>C{<sup>1</sup>H} NMR (C<sub>6</sub>D<sub>6</sub>, 75.5 MHz, 298 K),  $\delta$  = 24.7 (Bpin-CH<sub>3</sub>), 54.9 (OCH<sub>3</sub>), 66.6 (OCH<sub>2</sub>), 82.7 (Bpin-C), 114.0, 128.8, 131.8, 159.6 (Ar-C); <sup>11</sup>B{<sup>1</sup>H} NMR (C<sub>6</sub>D<sub>6</sub>, 128 MHz, 298 K),  $\delta$  = 22.5.

**Pr<sup>n</sup>OBpin**: product from hydroboration of propionaldehyde. <sup>1</sup>H NMR (C<sub>6</sub>D<sub>6</sub>, 400 MHz, 298 K),  $\delta$  = 0.96 (t, <sup>3</sup>J<sub>HH</sub> = 7.6 Hz, 3H, CH<sub>2</sub>CH<sub>3</sub>), 1.22 (s, 6H, Bpin-CH<sub>3</sub>), 1.24 (s, 6H, Bpin-CH<sub>3</sub>), 1.62 (m, 2H, CH<sub>2</sub>CH<sub>3</sub>), 3.89 (t, <sup>3</sup>J<sub>HH</sub> = 6.8 Hz, 3H, OCH<sub>2</sub>); <sup>13</sup>C{<sup>1</sup>H} NMR (C<sub>6</sub>D<sub>6</sub>, 75.5 MHz, 298 K),  $\delta$  = 10.3 (OCH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>), 24.7 (Bpin-CH<sub>3</sub>), 25.0 (OCH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>), 66.4 (OCH<sub>2</sub>), 82.3 (Bpin-C); <sup>11</sup>B{<sup>1</sup>H} NMR (C<sub>6</sub>D<sub>6</sub>, 128 MHz, 298 K),  $\delta$  = 22.2.

**Bu<sup>i</sup>OBpin**: product from hydroboration of isobutyraldehyde. NMR data are identical to those previously reported.<sup>3</sup>

**CyCH<sub>2</sub>OBpin**: product from hydroboration of cyclohexanecarboxaldehyde. <sup>1</sup>H NMR (C<sub>6</sub>D<sub>6</sub>, 400 MHz, 298 K),  $\delta$  = 0.96-2.15 (m, 11H, Cy-H), 1.28 (s, 12H, Bpin-CH<sub>3</sub>), 3.78 (d, <sup>3</sup>J<sub>HH</sub> = 6.3 Hz, 2H, OCH<sub>2</sub>);

$^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 75.5 MHz, 298 K),  $\delta$  = 24.8 (Bpin- $\text{CH}_3$ ), 26.2, 26.9, 29.75 (Cy- $\text{CH}_2$ ), 39.8 (Cy-CH), 70.5 ( $\text{OCH}_2$ ), 82.3 (Bpin-C);  $^{11}\text{B}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 128 MHz, 298 K),  $\delta$  = 22.4.

### Selected spectroscopic data for ketone hydroboration products

**( $\text{CF}_3$ )(Ph)CHOBpin**: product from hydroboration of 2,2,2-trifluoroacetophenone.  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 400 MHz, 298 K),  $\delta$  = 0.96 (s, 6H, Bpin- $\text{CH}_3$ ), 1.00 (s, 6H, Bpin- $\text{CH}_3$ ), 5.58 (q,  $^3J_{\text{HF}}$  = 9.2 Hz, 1H, OCH), 7.05 (m, 3H, Ar- $H$ ), 7.39 (m, 2H, Ar- $H$ );  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 75.5 MHz, 298 K),  $\delta$  = 24.4 (Bpin- $\text{CH}_3$ ), 24.5 (Bpin- $\text{CH}_3$ ), 74.9 (q,  $^2J_{\text{CF}}$  = 24 Hz,  $\text{OCHCF}_3$ ), 83.7 (Bpin-C), 124.4 (q,  $^1J_{\text{CF}}$  = 281 Hz,  $\text{CF}_3$ ), 129.1, 130.0, 133.9, 135.2 (Ar-C);  $^{11}\text{B}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 128 MHz, 298 K),  $\delta$  = 22.8;  $^{19}\text{F}$  NMR ( $\text{C}_6\text{D}_6$ , 282 MHz, 298 K),  $\delta$  = -77.9.

**$\text{Ph}_2\text{CHOBpin}$** : product from hydroboration of benzophenone. NMR data are identical to those previously reported.<sup>3</sup>

**(4-MeOPh)(Me)CHOBpin**: product from hydroboration of 4-methoxyacetophenone.  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 400 MHz, 298 K),  $\delta$  = 1.10 (s, 6H, Bpin- $\text{CH}_3$ ), 1.12 (s, 6H, Bpin- $\text{CH}_3$ ), 1.50 (d,  $^3J_{\text{HH}}$  = 6.3 Hz, 3H,  $\text{OCHCH}_3$ ), 3.45 (s, 3H,  $\text{OCH}_3$ ), 5.39 (q,  $^3J_{\text{HH}}$  = 6.3 Hz, 1H,  $\text{OCHCH}_3$ ), 6.81 (d,  $^3J_{\text{HH}}$  = 8.5 Hz, 2H, Ar- $H$ ), 7.32 (d,  $^3J_{\text{HH}}$  = 8.5 Hz, 2H, Ar- $H$ );  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 75.5 MHz, 298 K),  $\delta$  = 24.6 (Bpin- $\text{CH}_3$ ), 24.7 (Bpin- $\text{CH}_3$ ), 25.6 ( $\text{OCHCH}_3$ ), 54.87 ( $\text{OCH}_3$ ), 72.5 (OCH), 82.43 (Bpin-C), 113.9, 126.9, 137.3, 159.3 (Ar-C);  $^{11}\text{B}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 128 MHz, 298 K),  $\delta$  = 22.4.

**(4-EtPh)(Me)CHOBpin**: product from hydroboration of 4-ethylacetophenone.  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 400 MHz, 298 K),  $\delta$  = 1.04 (s, 6H, Bpin- $\text{CH}_3$ ), 1.06 (s, 6H, Bpin- $\text{CH}_3$ ), 1.08 (t,  $^3J_{\text{HH}}$  = 5.7 Hz, 3H,  $\text{CH}_2\text{CH}_3$ ), 1.50 (d,  $^3J_{\text{HH}}$  = 4.8 Hz, 3H,  $\text{OCHCH}_3$ ), 2.44 (q,  $^3J_{\text{HH}}$  = 5.7 Hz, 2H,  $\text{CH}_2\text{CH}_3$ ), 5.44 (q,  $^3J_{\text{HH}}$  = 4.8 Hz, 1H, OCH), 7.12 (d,  $^3J_{\text{HH}}$  = 8.5 Hz, 2H, Ar- $H$ ), 7.35 (d,  $^3J_{\text{HH}}$  = 8.5 Hz, 2H, Ar- $H$ );  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 75.5 MHz, 298 K),  $\delta$  = 15.9 ( $\text{CH}_2\text{CH}_3$ ), 24.6 (Bpin- $\text{CH}_3$ ), 25.8 ( $\text{OCHCH}_3$ ), 28.8 ( $\text{CH}_2\text{CH}_3$ ), 72.8 (OCH), 82.5 (Bpin-C), 125.8, 128.0, 142.7, 143.1 (Ar-C);  $^{11}\text{B}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 128 MHz, 298 K),  $\delta$  = 22.4.

**$\{(\text{Ph})(\text{pinB})(\text{H})\text{C}\}_2$** : product from hydroboration of benzil. NMR data are identical to those previously reported.<sup>3</sup>

**CyOBPin:** product from hydroboration of cyclohexanone.  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 400 MHz, 298 K),  $\delta$  = 1.12 (s, 12H, Bpin- $\text{CH}_3$ ), 1.19-1.93 (m, 10H, Cy- $\text{CH}_2$ ), 4.22 (m, 1H, OCH);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 75.5 MHz, 298 K),  $\delta$  = 24.1 (Cy- $\text{CH}_2$ ), 24.7 (Bpin- $\text{CH}_3$ ), 25.8, 34.7 (Cy- $\text{CH}_2$ ), 72.7 (OCH), 82.2 (Bpin-C);  $^{11}\text{B}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 128 MHz, 298 K),  $\delta$  = 24.3.

**2-MeCyOBPin:** product from hydroboration of 2-methylcyclohexanone. NMR data are identical to those previously reported.<sup>4</sup>

**(2-cyclohexenyl)OBpin:** product from hydroboration of 2-cyclohexene-1-one. NMR data are identical to those previously reported.<sup>5</sup>

**(2-adamantyl)OBpin:** product from hydroboration of 2-adamantanone.  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 400 MHz, 298 K),  $\delta$  = 1.11 (s, 12H, Bpin- $\text{CH}_3$ ), 1.45-2.42 (m, 14H, adamantyl- $H$ ), 4.48 (m, 1H, OCH);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 75.5 MHz, 298 K),  $\delta$  = 24.7 (Bpin- $\text{CH}_3$ ), 27.5, 27.9, 31.5, 34.6, 36.7, 37.9 (adamantyl-C), 77.1 (OCH), 82.2 (Bpin-C);  $^{11}\text{B}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 128 MHz, 298 K),  $\delta$  = 22.3.

**$\text{Pr}^i_2\text{CHOBpin}$ :** product from hydroboration of 2,3-dimethyl-3-pentanone.  $^1\text{H}$  NMR ( $\text{C}_6\text{D}_6$ , 400 MHz, 298 K),  $\delta$  = 0.91 (d,  $^3J_{\text{HH}} = 5.1$  Hz, 6H,  $\text{CH}(\text{CH}_3)_2$ ), 1.00 (d,  $^3J_{\text{HH}} = 5.1$  Hz, 6H,  $\text{CH}(\text{CH}_3)_2$ ), 1.15 (s, Bpin- $\text{CH}_3$ ), 1.81 (v. oct,  $^3J_{\text{HH}} = 5.1$  Hz,  $^3J_{\text{HH}} = 5.1$  Hz, 2H,  $\text{CH}(\text{CH}_3)_2$ ), 3.71 (t,  $^3J_{\text{HH}} = 5.1$  Hz, 1H, OCH);  $^{13}\text{C}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 75.5 MHz, 298 K),  $\delta$  = 17.2 ( $\text{CH}(\text{CH}_3)_2$ ), 19.7 ( $\text{CH}(\text{CH}_3)_2$ ), 24.6 (Bpin- $\text{CH}_3$ ), 30.5 ( $\text{CH}(\text{CH}_3)_2$ ), 82.1 (Bpin-C), 84.2 (OCH);  $^{11}\text{B}\{^1\text{H}\}$  NMR ( $\text{C}_6\text{D}_6$ , 128 MHz, 298 K),  $\delta$  = 22.4.



### 3. Kinetic studies

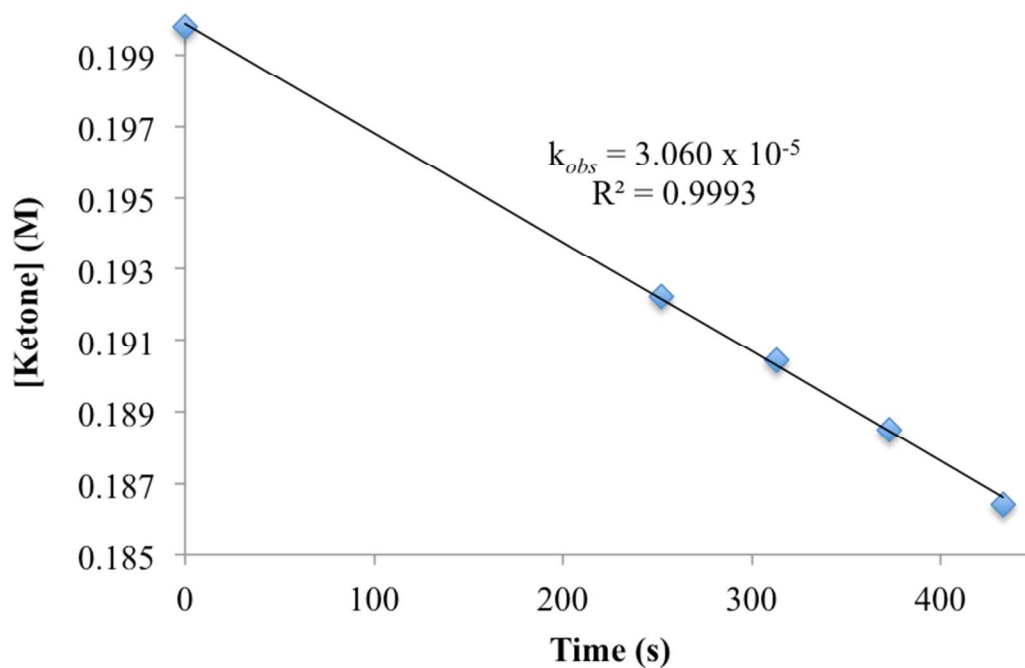
**General Method.** The order of dependence of each component of the reaction of 4-ethylacetophenone with HBpin, catalyzed by  $L^{\dagger}(H)Ge:$ , was determined by the method of initial rates. A slightly modified approach to that used by Weller et al.<sup>6</sup> was employed. Initial rate ( $k_{obs}$ ) values were determined in duplicate for three different concentrations of both  $L^{\dagger}(H)Ge:$  and HBpin, and for four concentrations of 4-ethylacetophenone. The quoted concentrations of  $L^{\dagger}(H)Ge:$  assume full dissociation of  $L^{\dagger}(H)Ge=Ge(H)L^{\dagger}$  in solution. Each  $k_{obs}$  determination experiment was run by collecting one  $^1H$  NMR spectrum per min of reaction time, from  $t = 0$  to  $t = 12$  min, followed by calculation of the consumption of 4-ethylacetophenone over this time. Ketone consumption was determined by relative integrations of ketone and product resonances, giving the percentage remaining ketone, which was multiplied by  $[ketone]_{t=0}$ . Integrations were confirmed against those of an internal TMS standard. The values of  $k_{obs}$  were calculated using approximately linear portions of each  $[ketone]$  vs. time plot, in the initial stages of each reaction run (typically within the first 7.5 min, see Figure S1 for an example). The plots of the experimentally obtained  $k_{obs}$  values vs. the respective component concentrations indicated the order of dependence of reaction in that reaction component. It was assumed that  $k_{obs}$  was 0 at zero concentration of reaction components that had an effect on the reaction rate, i.e. HBpin and  $L^{\dagger}(H)Ge:$ . The standard experimental procedure used for the determination of  $k_{obs}$  was as follows:

To a J. Youngs NMR tube, precooled by placing in a liquid  $N_2$  bath, was added  $L^{\dagger}(H)Ge:$  (from a 0.0144 M stock solution in  $C_6D_6$ ), HBpin (from a 1.453 M stock solution in  $C_6D_6$ ), and 4-ethylacetophenone (from a 1.453 M stock solution in  $C_6D_6$ , with 0.1 mole equivalents of tetramethylsilane added). The total sample volume was then made up to 0.6 mL by addition of  $C_6D_6$ , to give the component concentrations shown in Table S1. The NMR tube was then sealed, and stored in liquid nitrogen until needed. Samples were rapidly warmed to 20 °C and  $^1H$  NMR spectra collected (1 per min) over the course of the first 12 min of reaction time, as described above. The value of  $k_{obs}$  was then determined from the obtained results. Results for all reactions studied are shown in Table S1, and are represented graphically in Figures S2-S4.

**Table S1.** Initial rates for the hydroboration of 4-ethylacetophenone by HBpin, catalysed by  $L^{\dagger}(H)Ge:$ , carried out under varying concentrations of reactants and catalyst.

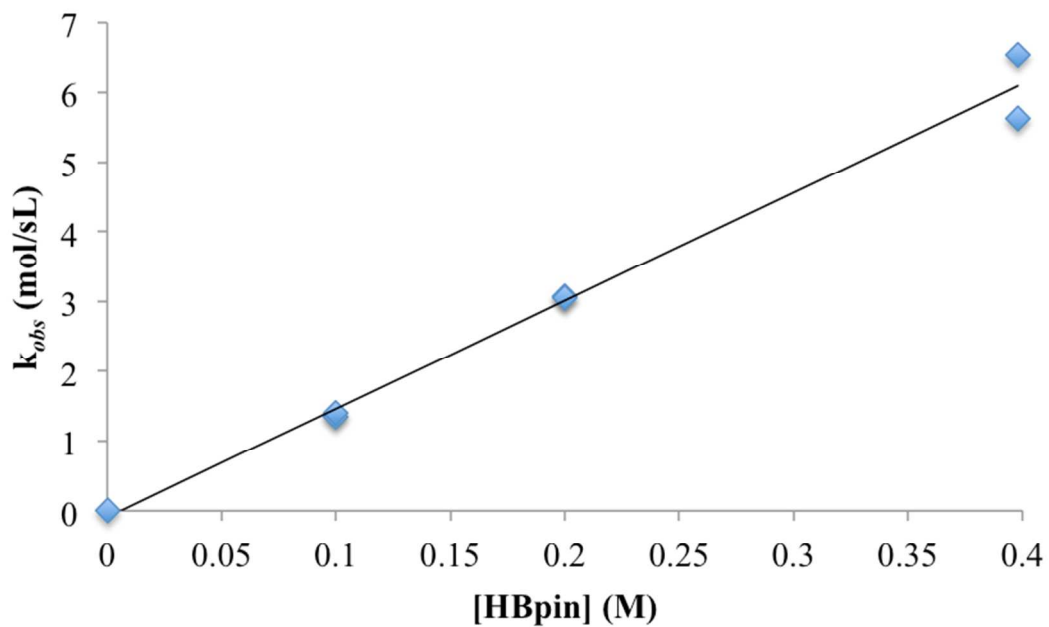
Run no.	$[L^{\dagger}(H)Ge:]$ (mM)	[HBpin] (M)	[Ketone] (M)	$k_{obs}$ ( $10^{-5}$ mol/Ls)
1	0.5978	0.1998	0.1880	1.522
2	0.5978	0.1998	0.1880	1.609
3	1.1957	0.1998	0.1880	3.063
4	1.1957	0.1998	0.1880	3.055
5	2.3913	0.1998	0.1880	5.714
6	2.3913	0.1998	0.1880	6.518
7	1.1957	0.0999	0.1880	1.337
8	1.1957	0.0999	0.1880	1.396
9	1.1957	0.3980	0.1880	5.625
10	1.1957	0.3980	0.1880	6.543
11	1.1957	0.1998	0.0469	2.803
12	1.1957	0.1998	0.0938	3.226
13	1.1957	0.1998	0.3740	2.453

A plot of runs 3,4 and 7-10 displayed in Table S1 resulted in a linear correlation between  $k_{obs}$  and [HBpin] (Figure S2). The case was similar for runs 1-6, giving a linear correlation between  $k_{obs}$  and  $[L^{\dagger}(H)Ge:]$  (Figure S3). These results suggest 1<sup>st</sup> order dependence of the reaction in both components. No significant change in  $k_{obs}$  was seen for runs 1,2 and 1-13, suggesting 0<sup>th</sup> order dependence in 4-ethylacetophenone (Figure S4). As mentioned in the main text, these results indicate that the rate determining step of the catalytic cycle is the reaction of the alkoxide intermediate,  $L^{\dagger}GeOC(H)(Me)(PhEt-4)$ , with HBpin; and therefore that the intermediate is the resting state in the cycle. The fact that the alkoxide intermediate is the resting state implies that the equilibrium between  $L^{\dagger}(H)Ge=Ge(H)L^{\dagger}$  and  $L^{\dagger}(H)Ge:$  should have little effect on the overall reaction rate, because  $L^{\dagger}(H)Ge:$  is rapidly consumed by reaction with the ketone, and is thus only present in the reaction mixture in negligible amounts throughout the cycle. In essence, the measured change in  $k_{obs}$  with change in  $[L^{\dagger}(H)Ge:]$ , is equivalent to a measure of change in  $k_{obs}$  with change in concentration of the monomeric resting state species,  $L^{\dagger}GeOC(H)(Me)(PhEt-4)$ .



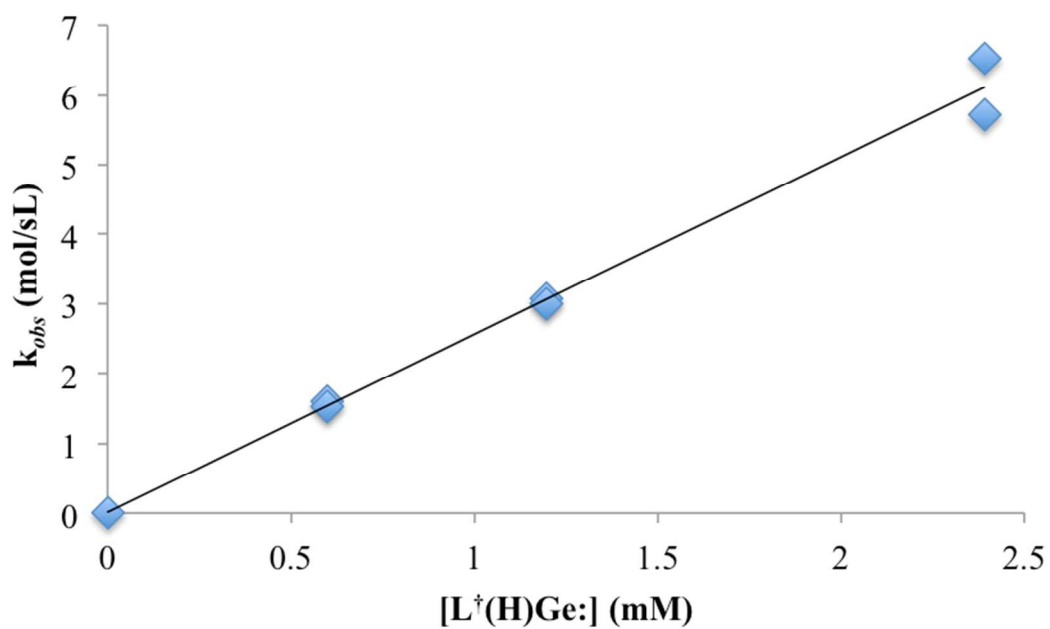
**Figure S1.** Example plot of [ketone] vs. time (including line of best fit) used for determination of  $k_{obs}$  values (Run 3, Table S1).

Order in HBpin



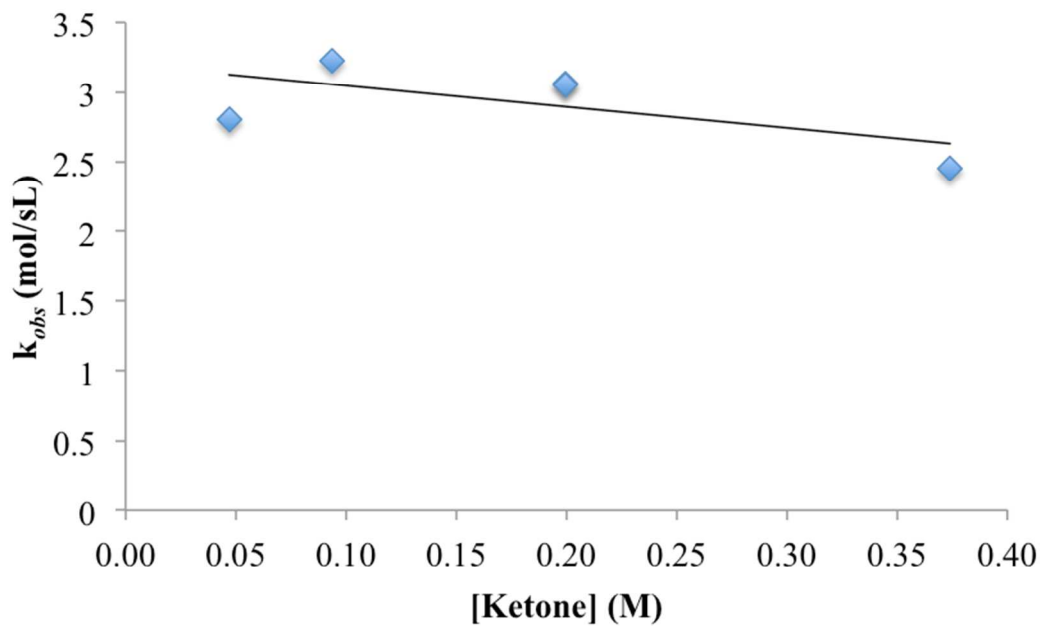
**Figure S2.** Plot of  $k_{obs}$  vs [HBpin] (including line of best fit).  $k_{obs}$  values are for runs 3,4 and 7-10 (Table S1).

Order in  $L^{\dagger}(H)Ge$ :



**Figure S3.** Plot of  $k_{obs}$  vs  $[L^{\dagger}(H)Ge:]$  (including line of best fit).  $k_{obs}$  values are for runs 1-6 (Table S1).

Order in 4-ethylacetophenone



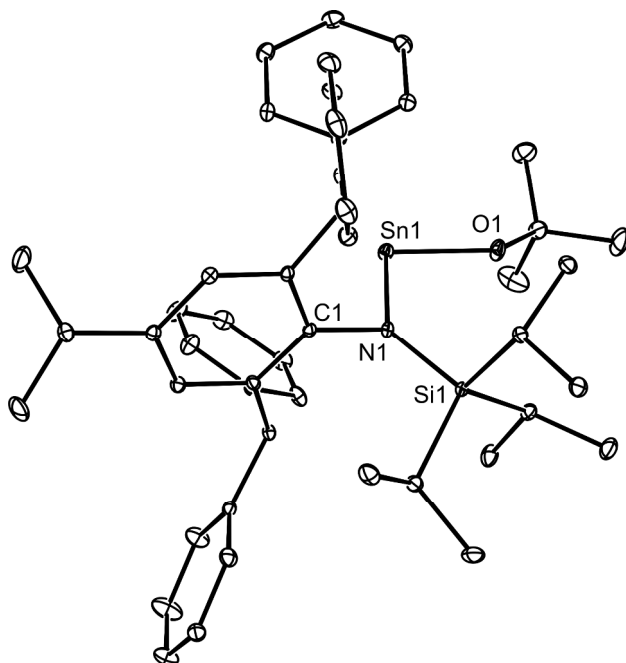
**Figure S4.** Plot of  $k_{obs}$  vs [4-ethylacetophenone] (including line of best fit).  $k_{obs}$  values are for runs 3,4 and 11-13 (Table S1).

#### 4. X-ray Crystallographic Studies

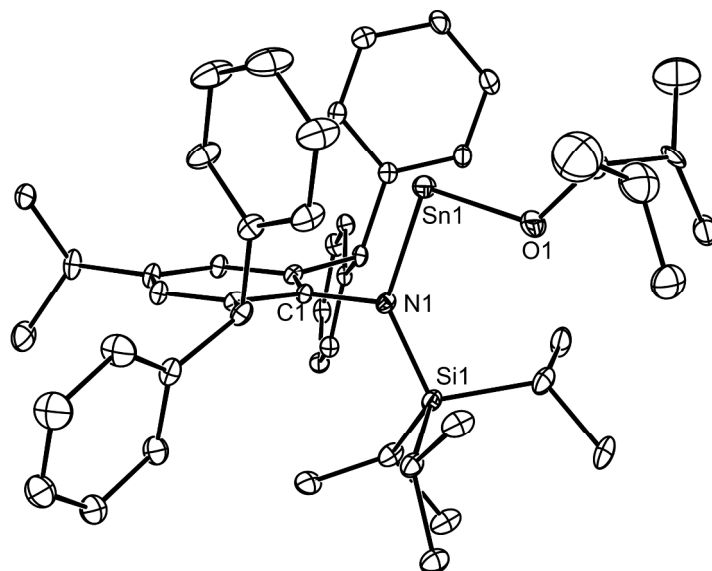
Crystals of  $L^{\dagger}SnOBu^{\dagger}$ ,  $L^{\dagger}GeOC(H)(Pr^i)_2$  **3**,  $L^{\dagger}SnOC(H)(Pr^i)_2$  **4**,  $L^{\dagger}GeOC(H)_2(PhOMe-4) \cdot (hexane)$  **5**·(hexane), and  $L^{\dagger}SnOC(H)_2(PhOMe-4) \cdot (hexane)$  **6**·(hexane), suitable for X-ray structural determination were mounted in silicone oil. Crystallographic measurements were carried out with a Bruker Apex X8 diffractometer using a graphite monochromator with Mo K $\alpha$  radiation ( $\lambda = 0.71073$  Å). All structures were solved by direct methods and refined on  $F^2$  by full matrix least squares (SHELX97)<sup>7</sup> using all unique data. All non-hydrogen atoms are anisotropic with hydrogen atoms included in calculated positions (riding model). Crystal data, details of data collections and refinements for all structures can be found in their CIF files and are summarized in Table S2.

**Table S2.** Summary of Crystallographic Data for Compounds  $L^{\dagger}SnOBu^{\dagger}$ ,  $L^{\dagger}GeOC(H)(Pr^i)_2$  **3**,  $L^{\dagger}SnOC(H)(Pr^i)_2$  **4**,  $L^{\dagger}GeOC(H)_2(PhOMe-4)$  **5**, and  $L^{\dagger}SnOC(H)_2(PhOMe-4)$  **6**.

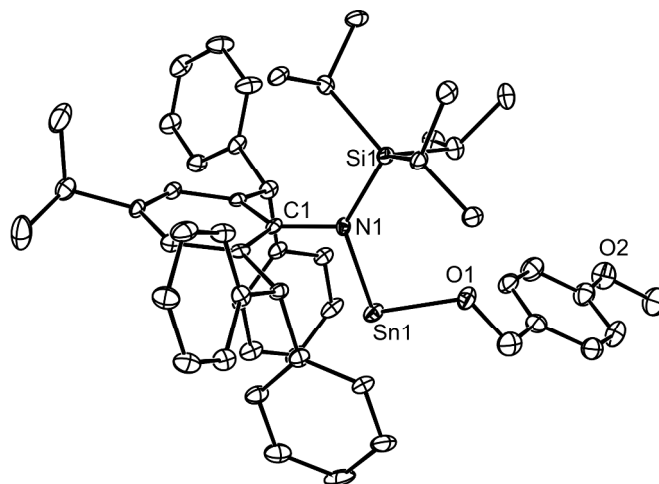
	$L^{\dagger}SnOBu^{\dagger}$	<b>3</b>	<b>4</b>	<b>5</b> ·(hexane)	<b>6</b> ·(hexane)
empirical formula	C <sub>48</sub> H <sub>61</sub> NOSiSn	C <sub>51</sub> H <sub>67</sub> GeNOSi	C <sub>51</sub> H <sub>67</sub> NOSiSn	C <sub>58</sub> H <sub>75</sub> GeNO <sub>2</sub> Si	C <sub>58</sub> H <sub>75</sub> NO <sub>2</sub> SiSn
formula weight	814.76	810.74	856.64	918.87	964.97
crystal system	triclinic	monoclinic	monoclinic	triclinic	triclinic
space group	<i>P</i> -1	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>P</i> -1	<i>P</i> -1
<i>a</i> (Å)	10.3523(5)	10.2694(7)	10.2642(14)	10.1666(4)	10.2677(11)
<i>b</i> (Å)	14.1047(7)	15.7032(12)	15.679(4)	13.8647(6)	13.9530(13)
<i>c</i> (Å)	15.5350(7)	28.1381(19)	28.312(4)	19.1051(8)	19.249(2)
$\alpha$ (deg.)	93.820(4)	90	90	95.982(2)	95.626(8)
$\beta$ (deg.)	95.712(4)	97.545(7)	98.491(13)	103.950(2)	104.476(9)
$\gamma$ (deg.)	107.061(4)	90	90	96.870(2)	97.307(8)
vol (Å <sup>3</sup> )	2146.79(18)	4498.3(6)	4506.4(14)	2569.94(18)	2624.2(5)
<i>Z</i>	2	4	4	2	2
$\rho$ (calcd) (g.cm <sup>-3</sup> )	1.260	1.197	1.263	1.187	1.221
$\mu$ (mm <sup>-1</sup> )	0.658	0.744	0.630	0.661	0.550
<i>F</i> (000)	856	1736	1808	984	1020
reflections collected	16629	22188	22935	31075	18315
unique reflections	8396	8834	8842	10057	9443
<i>R</i> <sub>int</sub>	0.0308	0.0573	0.0656	0.0380	0.0982
<i>R</i> 1 [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	0.0511	0.0615	0.0590	0.0483	0.0793
w <i>R</i> 2 (all data)	0.1458	0.1784	0.1489	0.1315	0.2053
CCDC No.	981743	981739	981740	981741	981742



**Figure. S5** Molecular structure of  $L^{\dagger}\text{SnOBu}^{\dagger}$  (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (°): Sn(1)-O(1) 2.006(3), Sn(1)-N(1) 2.107(4), Si(1)-N(1) 1.777(4), O(1)-Sn(1)-N(1) 93.82(13), C(1)-N(1)-Si(1) 118.9(3), C(1)-N(1)-Sn(1) 107.4(2), Si(1)-N(1)-Sn(1) 133.62(19), C(45)-O(1)-Sn(1) 128.3(3).



**Figure. S6** Molecular structure of  $L^{\dagger}\text{SnOC(H)(Pr)}_2$  **4** (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (°): Sn(1)-O(1) 1.998(4), Sn(1)-N(1) 2.113(3), Si(1)-N(1) 1.771(4), O(1)-Sn(1)-N(1) 96.86(14), C(45)-O(1)-Sn(1) 122.7(3), C(1)-N(1)-Si(1) 119.2(3), C(1)-N(1)-Sn(1) 107.1(2), Si(1)-N(1)-Sn(1) 133.6(2).



**Figure. S7** Molecular structure of  $L^{\dagger}\text{SnOC(H)}_2(\text{PhOMe-4})$  **6** (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (°): Sn(1)-O(1) 2.020(5), Sn(1)-N(1) 2.096(6), Si(1)-N(1) 1.783(6), O(1)-Sn(1)-N(1) 94.2(2), C(45)-O(1)-Sn(1) 116.7(5), C(1)-N(1)-Si(1) 116.9(4), C(1)-N(1)-Sn(1) 110.3(4), Si(1)-N(1)-Sn(1) 132.8(3).

## 5. Computational Studies

Geometry optimizations without symmetry constraints were carried out with the Gaussian 03<sup>8</sup> optimiser<sup>9</sup> in conjunction with Turbomole 6.2<sup>10</sup> energies and gradients at the BP86<sup>11</sup> level of theory using the basis sets def-2-TZVPP.<sup>12</sup> Stationary points were characterized by calculating the Hessian matrix analytically. Improved single-point energies were calculated with inclusion of dispersion interactions using the model D3 which was introduced by Grimme.<sup>13</sup> For the BP86 calculations the resolution of the identity method<sup>14</sup> was applied.

**Table S3.** Cartesian coordinates and total energies [hartrees] of the optimized geometries of the calculated molecules and transition states at BP86+D(BJ)/def2-TZVPP.

<b>1Sn</b>			
100			
-2268.352346389			
H	-1.0677995	3.9755325	-9.1236359
H	-1.5878970	6.2766458	-8.1193916
C	-0.8718152	3.5957736	-8.1110167
H	-1.1083297	2.5233619	-8.0935266
H	0.2042495	3.7060155	-7.9150189
H	-2.7662857	4.2264048	-7.3146404
C	-1.3919661	5.8683521	-7.1177943

C	-1.7007762	4.3630617	-7.0687846
H	-0.3361937	6.0573308	-6.8766291
H	-2.0043941	6.4199040	-6.3925356
H	4.9891517	6.4379370	-5.5958136
H	4.5783640	4.1734825	-6.5522160
C	-1.4938141	3.8112569	-5.6720878
H	0.6356816	4.1613518	-5.6447154
C	4.2746665	5.7641379	-5.1231644
C	4.0433003	4.4953113	-5.6584501
H	-3.5519439	3.2521645	-5.3852239
C	-0.2247225	3.7982924	-5.0818259
H	1.1967408	-1.1894650	-5.1351131
C	-2.5573108	3.2853710	-4.9373624
H	3.7719524	7.1429919	-3.5366538
H	-7.8153210	1.7240372	-4.8425678
H	0.5578150	1.2051430	-5.0482307
H	-8.3680276	4.1159525	-4.4184016
C	3.5911784	6.1591970	-3.9702237
H	2.9649965	2.6367180	-5.4647743
C	3.1312126	3.6306331	-5.0492469
H	-2.6009792	0.5635569	-4.9207619
H	-2.3682332	-1.9086252	-4.9317564
C	-7.0917989	2.3741890	-4.3501157
C	-7.4022824	3.7131112	-4.1135161
C	1.6143467	-0.5463049	-4.3605902
C	1.2618256	0.8038598	-4.3201773
C	2.6789645	5.2930873	-3.3665346
C	2.4304748	4.0217598	-3.9009703
H	-5.6199428	0.8090421	-4.1439939
H	-6.6949966	5.5841930	-3.2910960
C	-6.4638021	4.5358301	-3.4810006
C	-5.8526072	1.8571019	-3.9574186
C	-2.9091973	-0.0178963	-4.0524963
C	-2.7707855	-1.4062850	-4.0522859
C	-0.0162175	3.3198202	-3.7884800
H	2.7312006	-2.1375923	-3.4166812
C	-2.3901937	2.8209400	-3.6282226
H	2.1497680	5.6068587	-2.4658080
C	2.4741684	-1.0788363	-3.3986773
C	-5.2297993	4.0185289	-3.0935485
C	-4.9079997	2.6716725	-3.3253995
C	1.7765211	1.6494185	-3.3278683
C	1.3937613	3.1236870	-3.2479215
H	-4.4935476	4.6681356	-2.6184373
C	-1.1194253	2.8854842	-3.0068976
H	-2.0910813	5.3183619	-2.9738571
C	-3.5442877	2.1653243	-2.8852761
C	-3.4125391	0.6509197	-2.9278827



H	-2.9917731	-3.2324260	-2.9171161
C	-3.1211911	-2.1505890	-2.9230822
H	-1.4218405	6.9401219	-2.7285893
C	3.0007177	-0.2447317	-2.4087727
C	2.6628772	1.1102784	-2.3830265
H	1.3720830	3.3765333	-2.1794793
C	-1.7684660	6.0333561	-2.2081790
H	3.6755997	-0.6484431	-1.6539733
H	-3.4299316	2.4369356	-1.8277022
H	-2.6510026	6.3185510	-1.6178075
H	3.0908368	1.7623349	-1.6210691
C	-3.7846775	-0.1087988	-1.8054605
C	-3.6333303	-1.4990308	-1.7986313
H	0.1746540	5.1949628	-1.9998097
N	-0.9545481	2.5126300	-1.6401405
Sn	-0.6096164	0.4209861	-1.3167134
C	-0.6474852	5.4675695	-1.3199144
H	-4.1935112	0.4007163	-0.9321659
H	-3.9093479	-2.0687756	-0.9115307
H	-3.5054244	3.9885342	-0.7182181
H	0.1639921	7.4565891	-0.9480195
Si	-1.1000912	3.8262327	-0.4405401
C	-0.1126624	6.5564302	-0.3756014
H	1.7033464	2.6443695	-0.2654966
C	-2.8984643	3.9381200	0.2022062
H	-3.0489176	1.7549930	0.4236603
H	-0.8634770	6.8644745	0.3651955
H	-0.8007253	0.6082954	0.4961128
H	-3.0249717	6.1218614	0.4607871
H	0.7778353	6.2298909	0.1767924
H	1.9145254	4.3391873	0.2089981
C	1.5522230	3.3592678	0.5533724
C	-3.3114963	2.6729705	0.9668373
H	-4.3957797	2.6587796	1.1602188
C	-3.2426376	5.1988385	1.0126645
H	-4.3151309	5.2115310	1.2642180
C	0.0826680	3.3998569	0.9921746
H	-0.2056454	2.3613014	1.2340786
H	2.2025405	3.0458870	1.3854920
H	-2.8022264	2.6150735	1.9394032
H	-2.6881690	5.2435799	1.9586896
H	0.0905405	5.2989659	2.1154062
C	-0.0891344	4.2274221	2.2751138
H	-1.0947913	4.1202840	2.6999891
H	0.6255424	3.8891835	3.0423483

**2Sn**

122

-2618.948562764

H	-2.2490882	-0.2741043	-5.3044440
H	-0.7585135	0.6763189	-5.3940188
H	1.4335180	0.2638342	-4.9528451
H	2.9921879	1.0563739	-4.6707044
C	-1.6076491	0.4248430	-4.7441779
H	1.5139514	2.0238458	-4.7779362
H	-1.2188886	-2.2521547	-4.2101022
C	1.9238041	1.0767234	-4.4023658
H	-2.1850603	1.3435398	-4.5856950
H	0.3897906	-1.5115904	-4.2855597
H	6.7895490	-3.8156032	-2.0595106
H	6.1874235	-1.4326226	-2.4919047
H	-7.8664213	0.3744662	-1.5620597
C	-0.5218628	-1.5870032	-3.6763456
H	-0.9170265	3.1412365	-4.3835946
H	-8.1165418	-1.1342779	-0.6517744
H	-7.1788401	0.1864581	0.0724004
C	5.4864396	-2.0901085	-1.9769892
C	5.8252122	-3.4252520	-1.7344570
C	-1.1515524	-0.2113755	-3.4230003
C	-7.3953960	-0.3348317	-0.8682611
H	0.5837020	3.6915815	-3.6229211
H	-0.2463117	-2.0804479	-2.7369498
C	-0.4919183	3.5518856	-3.4582880
C	1.7543557	0.9387295	-2.8799163
H	2.1574013	-0.0493889	-2.6034994
H	-0.9327351	4.5509372	-3.3122570
H	-2.0591776	-0.3780100	-2.8120163
H	4.0097709	-0.5439528	-1.7287010
H	3.6477386	1.9507167	-2.4773178
C	4.2550552	-1.5916923	-1.5565485
H	5.1715491	-5.2914296	-0.8686736
C	4.9189775	-4.2497332	-1.0683081
H	-6.8107447	-3.8291421	-1.7899104
H	-5.5884589	0.9285874	-2.5503154
H	-6.5439814	-4.2504745	-0.0797371
H	-0.0000216	-3.4896455	-1.4333533
Si	-0.0637724	0.8837826	-2.2975141
H	2.2418219	3.0170520	-2.3785969
C	2.5960470	2.0011199	-2.1512593
H	-2.8663979	2.3456795	-2.8129417
C	-6.0575421	-4.1572798	-1.0589475
H	-6.3406464	-1.4527319	-2.3905069
C	3.6826086	-3.7471710	-0.6499696
H	1.4268501	-1.6453751	-1.4264684

C	3.3315772	-2.4138788	-0.8897091
C	-6.1034713	-0.8934903	-1.4726547
C	-0.7785351	2.6574311	-2.2416364
H	-5.7062416	-5.1514421	-1.3674171
C	-5.1242053	0.2379479	-1.8336952
H	-1.5282910	-4.9584896	-0.1464933
H	-4.8567308	0.8035590	-0.9312873
C	0.1069773	-3.5626455	-0.3510683
C	-2.2819393	2.6349385	-1.9285558
H	2.9840690	-4.4011459	-0.1294335
H	2.5789986	1.8767205	-1.0619711
C	1.9752663	-1.8463993	-0.4934515
H	-2.6431968	3.6227379	-1.6041454
H	-0.2641398	3.1263466	-1.3862225
C	-0.7428330	-4.4093883	0.3729470
O	-5.3319074	-1.5539168	0.6988761
C	-5.4099799	-1.8391233	-0.4887199
H	-4.1952832	-0.1442217	-2.2751007
N	-0.1292169	0.1360391	-0.6928124
C	-4.8719040	-3.1732466	-1.0035749
H	-2.5287045	1.9119076	-1.1384726
C	1.1104495	-2.8240462	0.2931965
H	-4.1675324	-3.5157384	-0.2305162
C	2.0444003	-0.5289029	0.2663208
H	-4.8182715	-2.7779549	-3.1617401
H	-3.7696973	-4.0981560	-2.6222263
C	0.9425831	0.3601075	0.2123538
Sn	-1.7756747	-1.0362510	0.0144936
C	-4.1495015	-3.1027863	-2.3529728
H	1.2900740	4.0302059	0.0119928
C	-0.5804530	-4.5451252	1.7511683
H	3.9805712	-0.9248585	1.1119297
C	3.1266526	-0.2450233	1.1056369
H	-1.2464518	-5.1922602	2.3211086
H	1.6860790	6.4223500	0.5195511
H	-0.8238048	2.2976059	0.2600351
C	1.2731230	-2.9872071	1.6754503
C	0.7725701	4.5003497	0.8492254
C	0.9256572	1.4616725	1.1050973
H	-3.2943068	-2.4156615	-2.3114468
H	5.3094894	2.4933269	1.3181910
C	0.4444594	-3.8449124	2.3954926
C	1.0039211	5.8425911	1.1418792
H	2.0364150	-2.4064147	2.1918572
C	-0.3474805	2.2822424	1.2478173
C	3.1529093	0.8857144	1.9247529
H	-3.0022937	1.8517287	0.8320939
C	2.0259371	1.7141495	1.9254321

C	-0.1007778	3.7301421	1.6351952
H	5.0846552	0.3854569	2.6374383
H	0.5788883	-3.9472068	3.4722011
C	5.0158543	2.5184582	2.3759373
C	4.3545119	1.1956426	2.7959256
C	0.3676996	6.4428402	2.2338620
C	-2.6559624	1.3645770	1.7446256
H	4.3220991	3.3606980	2.5103534
H	1.9971649	2.5898206	2.5758503
H	0.5501971	7.4918116	2.4670112
C	-1.3226300	1.5399121	2.1503309
H	5.9120577	2.7194397	2.9799766
C	-0.7318591	4.3397177	2.7240834
H	-4.5598783	0.4184829	2.1411036
C	-0.4987447	5.6863802	3.0227210
C	-3.5470251	0.5919220	2.5022013
H	-1.4111401	3.7565260	3.3450537
C	-0.9134442	0.9687084	3.3617363
H	0.1232451	1.0780242	3.6785561
C	3.9847179	1.2133188	4.2875881
H	3.5304904	0.2614031	4.5936574
H	-0.9982711	6.1425449	3.8778051
H	3.2635044	2.0145857	4.5035074
H	4.8735808	1.3880127	4.9100980
C	-3.1158121	0.0138067	3.6958259
C	-1.8044400	0.2246271	4.1335118
H	-3.7981246	-0.6036632	4.2789288
H	-1.4643492	-0.2230563	5.0675052
H	-1.0195759	-1.3044709	1.5936223

**3Sn**

122

-2618.998536343

H	-2.6657989	0.1482442	-5.1756862
H	-1.2335006	1.1888446	-5.2190027
H	0.9938289	0.8685841	-4.8662131
H	2.4409345	1.8569521	-4.5873851
C	-2.0367456	0.8181055	-4.5676790
H	0.8373201	2.6046523	-4.5621560
H	-1.4907110	-1.8503800	-4.3820512
C	1.3950822	1.7024228	-4.2756861
H	-2.6583271	1.6774148	-4.2864417
H	0.1062631	-1.0884157	-4.2957320
H	6.6579198	-3.3398201	-3.1466130
H	5.2730230	-1.6291322	-4.3191828
H	-4.9068405	-3.1093686	-3.5077963
C	-0.8294685	-1.2477177	-3.7387623
H	-1.7598558	3.5123617	-3.7461646

H	-5.0371411	-1.3518735	-3.2924102
H	-3.4875719	-2.1574876	-3.0197821
C	4.9244031	-2.0697716	-3.3849577
C	5.7002061	-3.0293254	-2.7291364
C	-1.5070273	0.0686835	-3.3366046
C	-4.5726144	-2.2600863	-2.8951937
H	-0.1887394	4.0484370	-3.1343005
H	-0.5908879	-1.8561980	-2.8568724
C	-1.2214898	3.8221112	-2.8409585
C	1.3198202	1.4346052	-2.7638755
H	1.8676389	0.4989952	-2.5725114
H	-1.6793172	4.7636107	-2.4974988
H	-2.3814165	-0.1954688	-2.7178096
H	3.0959478	-0.9286665	-3.3672728
H	3.0932051	2.6364663	-2.3544537
C	3.6975732	-1.6766957	-2.8493932
H	5.8269968	-4.3507149	-1.0255961
C	5.2339039	-3.5946267	-1.5405944
H	-6.5707025	-0.1423311	-2.2705452
H	-4.4964143	-4.6487970	-1.5949766
H	-5.0337458	0.7573625	-2.2180585
H	0.3284789	-3.6602515	-2.1855546
Si	-0.4533090	1.0850657	-2.1262328
H	1.5770068	3.5142373	-2.1056994
C	2.0606181	2.5346397	-1.9844257
H	-3.3978633	2.3219140	-2.1241370
C	-5.9317949	0.4971746	-1.6450943
H	-6.0033064	-2.6495070	-1.3288836
C	4.0040882	-3.1996277	-1.0090959
H	1.2697480	-1.4447249	-1.9175404
C	3.2240554	-2.2297978	-1.6518978
C	-4.9133399	-2.5081379	-1.4212109
C	-1.2979352	2.7555211	-1.7359736
H	-6.4896992	1.4230168	-1.4461289
C	-4.2322412	-3.7988291	-0.9500844
H	-1.0014292	-5.4253466	-1.0597502
H	-3.1358371	-3.6934865	-0.9831448
C	0.3622097	-3.7560351	-1.1001322
C	-2.7483070	2.5648089	-1.2718368
H	3.6406515	-3.6546955	-0.0876806
H	2.1164857	2.3180800	-0.9110479
C	1.9047556	-1.7470404	-1.0734092
H	-3.1458921	3.4815393	-0.8081621
H	-0.7163590	3.1504114	-0.8847924
C	-0.3789507	-4.7557045	-0.4667752
O	-3.2771790	-0.7653268	-0.8759893
C	-4.5214558	-1.3321002	-0.4861549
H	-4.5103351	-4.0515478	0.0825718

N	-0.3041524	0.1017116	-0.6517603
C	-5.5602626	-0.1980183	-0.3339077
H	-2.8580754	1.7344174	-0.5623116
C	1.1490700	-2.8621356	-0.3574542
H	-5.0457281	0.5458423	0.2981337
C	2.0378271	-0.5404236	-0.1528425
H	-7.3826030	-1.3984072	-0.1722473
H	-7.4755529	0.1720766	0.6398198
C	0.8906738	0.2524153	0.1089515
H	-4.4340483	-1.7719635	0.5343031
Sn	-1.6507640	-1.2867625	0.2548082
C	-6.8069264	-0.6716852	0.4194794
H	0.7777734	4.0833750	0.5035836
C	-0.3269314	-4.8925834	0.9232557
H	4.1148895	-0.8770478	0.2829987
C	3.2317710	-0.2847724	0.5274237
H	-0.9126825	-5.6656742	1.4195657
H	1.2514241	6.2886149	1.5301482
H	-0.8883018	2.1100794	0.7080080
C	1.2027215	-3.0180728	1.0349999
C	0.5276696	4.2606704	1.5505633
C	0.9590966	1.1889745	1.1728825
H	-6.5431706	-1.1528934	1.3729820
H	5.2080398	2.5914811	0.8458998
C	0.4770792	-4.0293008	1.6691699
C	0.8031684	5.4967425	2.1305805
H	1.7970169	-2.3214040	1.6252239
C	-0.3140217	1.8941857	1.6180827
C	3.3249035	0.6982861	1.5159477
H	-3.0225707	1.7674482	1.6383880
C	2.1619034	1.3999219	1.8487090
C	-0.0500538	3.2249115	2.3020997
H	5.3844421	0.2880303	1.7976449
H	0.5245944	-4.1279256	2.7535725
C	5.1150827	2.4177347	1.9259581
C	4.6393416	0.9844965	2.2148580
C	0.5075234	5.7203389	3.4798521
C	-2.5878197	1.0218109	2.3041788
H	4.4003355	3.1528249	2.3226308
H	2.1875023	2.1474785	2.6425088
H	0.7233077	6.6863938	3.9359886
C	-1.1900191	0.9531108	2.4315442
H	6.0913834	2.6090167	2.3934951
C	-0.3431719	3.4581349	3.6491835
H	-4.4963675	0.1897541	2.8652055
C	-0.0656474	4.6977271	4.2353709
C	-3.4160733	0.1353800	2.9976074
H	-0.7930055	2.6656802	4.2468200

C	-0.6432963	-0.0106850	3.2920620
H	0.4398813	-0.0839415	3.3851101
C	4.5465625	0.7280869	3.7272801
H	4.2314528	-0.3033285	3.9353036
H	-0.3001937	4.8609658	5.2875198
H	3.8172803	1.4040066	4.1961608
H	5.5180113	0.8962507	4.2130157
C	-2.8572109	-0.8255476	3.8446155
C	-1.4700916	-0.8877678	3.9972941
H	-3.4999461	-1.5258440	4.3771397
H	-1.0272640	-1.6365206	4.6538531

**4Sn**

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-3031.074269646

Sn	-0.5619902	-1.7633968	0.4998115
N	0.6580437	-0.2106140	-0.3963606
Si	0.1692174	1.2820252	-1.2891328
C	2.0563339	-0.4443843	-0.2297525
C	2.7452168	0.0111530	0.9388067
C	4.1381058	-0.1377337	1.0455521
C	4.9021040	-0.7447066	0.0325355
C	4.2132121	-1.2614062	-1.0781900
C	2.8177449	-1.1494802	-1.2148377
O	-2.2637278	-0.6249321	0.2826297
C	-3.6592494	-0.8220025	0.3865611
C	-4.1153860	-1.3060077	1.7951860
C	-3.6482514	-2.7052307	2.2203334
C	2.0830974	-1.8600580	-2.3543172
C	2.9275713	-2.0794095	-3.6066676
C	2.9729894	-1.0851481	-4.6068222
C	3.7720716	-1.2465777	-5.7496310
C	4.5414439	-2.4111862	-5.9143333
C	4.4976144	-3.4131352	-4.9305312
C	3.6944193	-3.2492944	-3.7896174
C	6.4195275	-0.8363769	0.1374740
C	7.0616451	0.5656489	0.1040857
C	1.9447531	0.5815330	2.1100864
C	2.7412518	1.5756249	2.9547864
C	3.0727331	2.8296705	2.3945965
C	3.8273186	3.7649496	3.1162660
C	4.2680329	3.4636520	4.4180353
C	3.9443119	2.2216274	4.9852023
C	3.1857534	1.2853616	4.2590236
C	-0.2451538	2.7036955	-0.0500972
C	-0.3091836	4.1110716	-0.6764172
C	-1.3937173	0.8748565	-2.3353255
C	-2.0111718	2.0526406	-3.1109582

C	1.7009184	1.7956313	-2.3611628
C	1.3583687	2.5548544	-3.6572960
C	-4.2134356	-1.5872435	-0.8611282
C	-3.5424567	-2.9248902	-1.1971766
C	-5.7419283	-1.7392995	-0.8022475
C	-1.4995559	2.4151290	0.7941289
C	1.4360378	-3.1615909	-1.8669143
C	0.3082478	-3.6712371	-2.5491246
C	-0.3257928	-4.8472238	-2.1185062
C	0.1706155	-5.5500818	-1.0059715
C	1.3078473	-5.0697918	-0.3370192
C	1.9311828	-3.8824317	-0.7596016
C	1.3177812	-0.5444325	2.9344546
C	0.0702934	-0.3380584	3.5666373
C	-0.5318291	-1.3556671	4.3268377
C	0.1073926	-2.5986053	4.4721657
C	1.3548563	-2.8116453	3.8612305
C	1.9537737	-1.7950430	3.0986713
C	6.8640113	-1.6261026	1.3842900
C	-1.2363211	-0.3584986	-3.2383732
C	2.8082963	2.5254350	-1.5748958
C	-3.7003579	-0.2555116	2.8412636
B	-4.6929162	3.3012747	1.7807418
O	-5.0095974	4.5781758	1.4015431
C	-5.3993454	4.5102795	-0.0113758
C	-4.1565636	4.8993186	-0.8239243
O	-5.0281947	2.3325709	0.8692522
C	-5.8035571	2.9823043	-0.1874745
C	-5.4028890	2.3630588	-1.5245228
C	-7.2795784	2.6976063	0.1188858
C	-6.5331922	5.5048601	-0.2513892
H	-5.7290559	1.3054388	-1.5638612
H	-5.8766658	2.9020315	-2.3692769
H	-4.3085677	2.3777846	-1.6621339
H	-7.4251674	1.6013106	0.1802270
H	-7.5797695	3.1358955	1.0908427
H	-7.9458493	3.0952498	-0.6716008
H	-4.3625231	4.9209554	-1.9116020
H	-3.8200322	5.9058415	-0.5084489
H	-3.3248863	4.1944784	-0.6342978
H	-6.9092908	5.4228885	-1.2910895
H	-7.3754566	5.3410842	0.4454562
H	-6.1628812	6.5376058	-0.0992739
H	-4.1696897	3.0477202	2.8404402
H	-2.9750149	1.7475196	-3.5756846
H	-1.3636000	2.4182348	-3.9319852
H	0.6962134	1.9683021	-4.3260343
H	2.2840697	2.7818268	-4.2318113



H	0.8551045	3.5248276	-3.4614422
H	-2.1910825	-0.6018728	-3.7557181
H	-2.2268038	2.9195239	-2.4574205
H	-0.4670809	-0.2168780	-4.0287702
H	5.1672117	-2.5405551	-6.8107580
H	3.7896562	-0.4588420	-6.5186437
H	-4.0153896	-2.9452424	3.2400855
H	-1.1325531	4.2049363	-1.4115963
H	-4.0030834	-3.5040278	1.5407795
H	-2.5380772	-2.7682364	2.2662906
H	0.6253504	4.3890966	-1.2029370
H	-0.9525202	-1.2556509	-2.6533738
H	2.1373324	0.8214970	-2.6664973
H	-0.4898013	4.8816109	0.1057801
H	-2.1042788	0.5896871	-1.5283409
H	2.3719770	-0.1705596	-4.4869262
H	3.6923423	2.7089089	-2.2242544
H	5.0893151	-4.3335804	-5.0536177
H	-3.7819128	-3.7203882	-0.4633509
H	-4.1013417	-0.5003194	3.8458472
H	-2.4364980	-2.8358344	-1.2456610
H	-0.0720397	-3.1351801	-3.4323042
H	2.4736508	3.5160782	-1.2017330
H	-2.4179045	2.3723050	0.1724503
H	-5.2269374	-1.3146244	1.7578807
H	1.2422946	-1.2022265	-2.6460708
H	-3.8695006	-3.2838209	-2.1948362
H	-1.2157362	-5.2140724	-2.6522481
H	-2.5977278	-0.1987975	2.9087614
H	3.6538952	-4.0439000	-3.0288818
H	3.1622743	1.9383559	-0.7055498
H	-1.6590921	3.2042239	1.5614815
H	0.6331334	2.7023501	0.6366794
H	-4.0588647	0.7447059	2.5399523
H	-1.4544159	1.4341711	1.3052458
H	-3.9767118	-0.9014361	-1.7067953
H	-6.0443160	-2.5072154	-0.0594166
H	-6.1527458	-2.0520580	-1.7841078
H	-4.1131816	0.1940425	0.3029650
H	2.7461656	3.0629195	1.3695046
H	4.7835765	-1.7716887	-1.8698238
H	-0.3289696	-6.4689874	-0.6632868
H	4.0735343	4.7364079	2.6602198
H	1.0941577	1.1412328	1.6724967
H	-6.2362380	-0.7874520	-0.5149758
H	6.7630784	1.1198818	-0.8084034
H	2.8047243	-3.4956675	-0.2140291
H	-0.4327845	0.6349606	3.4507370

H	6.7747442	-1.3924638	-0.7581765
H	1.7075001	-5.6141455	0.5323832
H	6.7437319	1.1689316	0.9801819
H	4.6355953	0.2520582	1.9469706
H	4.8601847	4.1968902	4.9868678
H	8.1694443	0.4986928	0.1239811
H	-1.5127004	-1.1804884	4.7929110
H	2.9355128	0.3151461	4.7134779
H	2.9203848	-1.9736436	2.6049878
H	6.4153016	-2.6402287	1.3990148
H	4.2825703	1.9749231	6.0036528
H	6.5581904	-1.1087925	2.3177554
H	7.9680148	-1.7364420	1.4127395
H	-0.3683167	-3.3995508	5.0581958
H	1.8630178	-3.7822206	3.9692903

**5Sn**

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-3031.086160897

Sn	-0.9314253	-0.8298544	0.4093573
N	0.6363539	0.3348609	-0.5046730
Si	0.4914822	1.7096698	-1.6160560
C	1.9543538	-0.0448210	-0.1226695
C	2.5528394	0.4861486	1.0507290
C	3.8944817	0.2287771	1.3342704
C	4.6826253	-0.5704736	0.4996199
C	4.0595136	-1.1829218	-0.5904595
C	2.7130280	-0.9637686	-0.8927581
O	-3.2845165	-0.4859837	-0.3917565
C	-4.4916893	-1.0189013	-0.9719628
C	-5.0120423	-2.2560291	-0.1914061
C	-3.9014026	-3.0341232	0.5206947
C	1.9975113	-1.8118625	-1.9326442
C	2.9164757	-2.4210775	-2.9771136
C	3.1852925	-1.7218080	-4.1609557
C	4.0552177	-2.2430785	-5.1195448
C	4.6709112	-3.4794005	-4.9083890
C	4.4025988	-4.1900734	-3.7364218
C	3.5294634	-3.6657877	-2.7811204
C	6.1548345	-0.7887724	0.7862186
C	6.9350957	0.5329074	0.6961802
C	1.6799490	1.2352589	2.0473107
C	2.4703487	2.1426948	2.9744870
C	3.0845269	3.2834862	2.4351556
C	3.8418627	4.1347534	3.2366966
C	4.0009027	3.8582907	4.5989596
C	3.3938877	2.7276232	5.1453086
C	2.6329647	1.8760030	4.3376161

C	0.4480938	3.3625144	-0.6607928
C	0.5513964	4.6245916	-1.5329518
C	-1.1156149	1.3672008	-2.5724084
C	-1.7317819	2.5680253	-3.3026610
C	2.0406951	1.7380719	-2.7424031
C	1.8263328	2.4273341	-4.1004480
C	-4.2659656	-1.2391730	-2.4773933
C	-3.3161264	-2.3946766	-2.7836417
C	-5.5987372	-1.3986286	-3.2157342
C	-0.7520956	3.4667025	0.2837677
C	1.1517203	-2.8748561	-1.2365579
C	0.0595189	-3.4359231	-1.9140967
C	-0.7436297	-4.3994366	-1.3029419
C	-0.4635824	-4.8252577	-0.0016238
C	0.6308939	-4.2871851	0.6756523
C	1.4314784	-3.3190891	0.0635540
C	0.7807301	0.2512128	2.7861327
C	-0.5203312	0.6330295	3.1564133
C	-1.3898849	-0.2743159	3.7691732
C	-0.9548638	-1.5702145	4.0588350
C	0.3501625	-1.9497195	3.7344421
C	1.2057837	-1.0525410	3.0918344
C	6.3727224	-1.4669025	2.1482315
C	-0.9623985	0.1616060	-3.5116480
C	3.2934469	2.3037100	-2.0505099
C	-6.1010590	-1.8546988	0.8108114
B	-3.3521553	0.7563993	0.3861091
O	-3.7547970	1.9457404	-0.3161975
C	-4.7815200	2.6145428	0.4501984
C	-6.1401989	2.2653274	-0.1685323
O	-4.0943525	0.6838528	1.6197322
C	-4.5996273	2.0056413	1.8945058
C	-5.8907820	1.8757923	2.6961520
C	-3.5571942	2.7678691	2.7214906
C	-4.5631827	4.1225944	0.3641270
H	-5.6712125	1.4379092	3.6789724
H	-6.3529057	2.8595920	2.8581930
H	-6.6131737	1.2271686	2.1893685
H	-3.3392286	2.1965426	3.6330552
H	-2.6258443	2.8965898	2.1584033
H	-3.9185988	3.7603698	3.0207233
H	-6.9547080	2.8466230	0.2846804
H	-6.1064173	2.4932279	-1.2416171
H	-6.3722041	1.2001332	-0.0493306
H	-5.2970105	4.6608049	0.9804420
H	-3.5573690	4.4046626	0.6913932
H	-4.6874206	4.4516186	-0.6761153
H	-2.0323467	0.8690131	0.6739395

H	-2.6559560	2.2649754	-3.8195763
H	-1.0554582	2.9905377	-4.0590113
H	1.0047282	1.9806068	-4.6745731
H	2.7381701	2.3548334	-4.7152240
H	1.5998291	3.4960809	-3.9870842
H	-1.9141395	-0.0660726	-4.0150704
H	-2.0032993	3.3667252	-2.6022616
H	-0.2150452	0.3382811	-4.2981623
H	5.3487924	-3.8899162	-5.6566179
H	4.2484365	-1.6846088	-6.0356344
H	-4.3034659	-3.9668985	0.9409638
H	-0.3099737	4.7255148	-2.2058025
H	-3.0720331	-3.2952752	-0.1473537
H	-3.4874198	-2.4435942	1.3488784
H	1.4575203	4.6354042	-2.1510710
H	-0.6601563	-0.7425005	-2.9659023
H	2.2487869	0.6763436	-2.9461227
H	0.5752556	5.5253304	-0.8987639
H	-1.8406331	1.0816279	-1.7907158
H	2.7054399	-0.7574752	-4.3328841
H	4.1719592	2.2013805	-2.7070333
H	4.8707448	-5.1598690	-3.5661915
H	-3.7615333	-3.3614084	-2.5069013
H	-6.4815442	-2.7312422	1.3548044
H	-2.3726938	-2.2877073	-2.2361049
H	-0.1585339	-3.1101283	-2.9318862
H	3.1811728	3.3738462	-1.8259115
H	-1.7008052	3.4734125	-0.2681752
H	-5.4706101	-2.9290894	-0.9351269
H	1.2896923	-1.1578751	-2.4605315
H	-3.0771381	-2.4334091	-3.8553835
H	-1.5964958	-4.8116266	-1.8409233
H	-5.6940416	-1.1394918	1.5385177
H	3.3136072	-4.2312561	-1.8744010
H	3.5234478	1.7873775	-1.1107687
H	-0.7014086	4.3830953	0.8936222
H	1.3651354	3.3242617	-0.0450116
H	-6.9527689	-1.3794358	0.3029651
H	-0.8066376	2.6091790	0.9659677
H	-3.7964364	-0.3051024	-2.8253355
H	-6.1231898	-2.3162427	-2.9108537
H	-5.4362187	-1.4595790	-4.3006288
H	-5.2505251	-0.2261916	-0.8935850
H	2.9745705	3.4934030	1.3702178
H	4.6374190	-1.8605029	-1.2204250
H	-1.0993211	-5.5671947	0.4802650
H	4.3101508	5.0165766	2.7990179
H	1.0070063	1.8780209	1.4649659

H	-6.2674118	-0.5484500	-3.0208473
H	6.7999986	1.0038788	-0.2862442
H	2.2730959	-2.8885516	0.6039856
H	-0.8635680	1.6424541	2.9336758
H	6.5384297	-1.4648488	0.0052113
H	0.8587187	-4.6116487	1.6906926
H	6.5865719	1.2436589	1.4589434
H	4.3310977	0.6756348	2.2281005
H	4.5929279	4.5227646	5.2281159
H	8.0096828	0.3656560	0.8560583
H	-2.4147021	0.0250727	3.9823240
H	2.1602249	0.9964298	4.7739729
H	2.2093290	-1.3632312	2.8031471
H	5.8368025	-2.4240007	2.2038867
H	3.5096508	2.5035906	6.2059786
H	6.0094187	-0.8292544	2.9667396
H	7.4406050	-1.6591488	2.3232399
H	-1.6342392	-2.2829707	4.5250161
H	0.6969216	-2.9578919	3.9602634

**6Sn**

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-3031.085377999

Sn	-0.9268931	-0.5178801	0.2048117
N	0.7955768	0.4700066	-0.6617740
Si	0.8131137	1.8033946	-1.8416828
C	2.0764641	0.0372207	-0.2126540
C	2.6548437	0.5874502	0.9604065
C	3.9598399	0.2544951	1.3264537
C	4.7327117	-0.6296365	0.5678303
C	4.1292454	-1.2361312	-0.5363377
C	2.8161988	-0.9460395	-0.9178259
O	-4.4007719	-0.9710988	0.5403531
C	-5.1657110	-1.5794003	-0.5319896
C	-5.3004822	-3.0855639	-0.2284292
C	-4.0268933	-3.7138038	0.3507251
C	2.1163987	-1.7602314	-1.9949776
C	3.0578787	-2.3935927	-3.0050599
C	3.3755780	-1.7123316	-4.1872317
C	4.2643713	-2.2590772	-5.1141834
C	4.8500710	-3.5041268	-4.8727337
C	4.5311779	-4.1985946	-3.7034372
C	3.6390904	-3.6490823	-2.7807559
C	6.1705644	-0.9324035	0.9404837
C	7.0435021	0.3290861	0.8388256
C	1.7998197	1.4608366	1.8654179
C	2.6110406	2.4284025	2.7106924
C	3.3742267	3.4119277	2.0610265

C	4.1381976	4.3212910	2.7888076
C	4.1566995	4.2621213	4.1867385
C	3.4042616	3.2875974	4.8418212
C	2.6361191	2.3772794	4.1078288
C	0.6930912	3.4880913	-0.9439884
C	0.9593472	4.7323093	-1.8064133
C	-0.6896186	1.5213544	-2.9828292
C	-1.0959018	2.7108688	-3.8650242
C	2.4802271	1.7532783	-2.7865827
C	2.4232376	2.3740758	-4.1921286
C	-4.5815846	-1.1887423	-1.9045974
C	-3.2938334	-1.9089185	-2.2958920
C	-5.6454390	-1.3628524	-2.9955496
C	-0.6218248	3.6380434	-0.1725472
C	1.1977085	-2.8005002	-1.3608889
C	0.1347855	-3.3228006	-2.1117559
C	-0.7174655	-4.2841947	-1.5692916
C	-0.5191489	-4.7422358	-0.2637951
C	0.5394793	-4.2340815	0.4889179
C	1.3905906	-3.2701178	-0.0554758
C	0.8483071	0.5889711	2.6713403
C	-0.4598703	1.0354452	2.9268306
C	-1.3782024	0.2262971	3.6047329
C	-0.9883154	-1.0356133	4.0575040
C	0.3179968	-1.4782652	3.8349782
C	1.2256415	-0.6773732	3.1407696
C	6.2734813	-1.5640108	2.3377902
C	-0.5607226	0.2353786	-3.8114980
C	3.6652154	2.3323836	-1.9948792
C	-6.4790609	-3.3219378	0.7256182
B	-4.7647261	0.2700671	0.9639993
O	-5.7211210	1.0626557	0.3446239
C	-6.0151175	2.1540603	1.2704128
C	-7.2400785	1.7285747	2.0818342
O	-4.2296692	0.8390715	2.1086861
C	-4.6995065	2.2248052	2.1347907
C	-4.9124379	2.6365976	3.5842913
C	-3.6128214	3.0781155	1.4864052
C	-6.3143206	3.4074829	0.4616213
H	-3.9484640	2.6575364	4.1090709
H	-5.3466809	3.6441388	3.6393415
H	-5.5740083	1.9391691	4.1090874
H	-2.6826157	2.9595267	2.0537305
H	-3.4172626	2.7540089	0.4570949
H	-3.8775934	4.1429309	1.4854795
H	-7.5711711	2.5245986	2.7610660
H	-8.0609907	1.4994782	1.3910610
H	-7.0287986	0.8288766	2.6741342

H	-6.4576459	4.2716602	1.1245865
H	-5.5038456	3.6324203	-0.2395583
H	-7.2373090	3.2636017	-0.1143102
H	-2.0407330	0.8021758	-0.4096736
H	-1.9830916	2.4546972	-4.4662487
H	-0.3036111	3.0061808	-4.5658940
H	1.6729095	1.8928969	-4.8328220
H	3.3994421	2.2740036	-4.6936115
H	2.1863015	3.4465299	-4.1606756
H	-1.4643168	0.0691384	-4.4198190
H	-1.3532424	3.5936343	-3.2661746
H	0.2918424	0.2684669	-4.5055904
H	5.5428681	-3.9345815	-5.5957433
H	4.4952152	-1.7135411	-6.0294506
H	-4.1751329	-4.7933760	0.4941005
H	0.1917675	4.8662720	-2.5796742
H	-3.1513483	-3.5761459	-0.2903779
H	-3.7885792	-3.2683470	1.3243473
H	1.9314639	4.6907742	-2.3129586
H	-0.4316872	-0.6467965	-3.1707359
H	2.6929198	0.6812538	-2.9143456
H	0.9527775	5.6401202	-1.1818813
H	-1.5088100	1.3583551	-2.2593728
H	2.9177263	-0.7424235	-4.3849309
H	4.5994405	2.2122391	-2.5658249
H	4.9741551	-5.1760274	-3.5106150
H	-3.4695896	-2.9759337	-2.4924158
H	-6.6004720	-4.3906482	0.9502520
H	-2.5295328	-1.8514145	-1.5077755
H	-0.0178916	-2.9732505	-3.1338617
H	3.5411252	3.4077158	-1.8032362
H	-1.4707689	3.7663743	-0.8596439
H	-5.5328668	-3.5797154	-1.1869940
H	1.4627584	-1.0724833	-2.5479294
H	-2.8664334	-1.4675802	-3.2048722
H	-1.5420186	-4.6747987	-2.1653583
H	-6.3085115	-2.7982499	1.6777043
H	3.3803198	-4.2029639	-1.8781050
H	3.8036505	1.8319675	-1.0294922
H	-0.6005722	4.5149093	0.4940567
H	1.5113188	3.4383417	-0.2041519
H	-7.4229661	-2.9537899	0.2998553
H	-0.8454543	2.7513642	0.4339058
H	-4.3569231	-0.1130113	-1.8217868
H	-5.9336257	-2.4186477	-3.1092802
H	-5.2635808	-1.0210189	-3.9670417
H	-6.1758769	-1.1404740	-0.5016004
H	3.3798924	3.4477921	0.9708009

H	4.6975937	-1.9639033	-1.1171122
H	-1.1918644	-5.4848435	0.1637670
H	4.7237968	5.0773624	2.2652949
H	1.1605289	2.0667690	1.2092140
H	-6.5519670	-0.7866824	-2.7650289
H	6.9913212	0.7633890	-0.1681525
H	2.2020597	-2.8600732	0.5440610
H	-0.7580281	2.0237668	2.5743029
H	6.5455454	-1.6656505	0.2082882
H	0.6976985	-4.5778291	1.5110217
H	6.7055322	1.0951478	1.5512522
H	4.3824429	0.7169552	2.2193681
H	4.7552541	4.9714733	4.7581537
H	8.0946776	0.0988089	1.0635217
H	-2.4047956	0.5631287	3.7323172
H	2.0508587	1.6194152	4.6280261
H	2.2309624	-1.0421003	2.9328411
H	5.6700111	-2.4793455	2.4033646
H	3.4123667	3.2308816	5.9306222
H	5.9148370	-0.8685352	3.1099553
H	7.3154632	-1.8198608	2.5763928
H	-1.7061777	-1.6766447	4.5681137
H	0.6258781	-2.4644493	4.1826092

**TS2-3Sn**

122

-2618.942343016

Sn	-1.4956310	-1.1895540	0.4150122
N	-0.3261717	0.3294042	-0.6209717
Si	-0.6493342	1.2790665	-2.0713930
C	-0.3461840	2.0834746	1.6976238
C	0.8945045	0.5858384	0.0677883
C	5.4663493	-2.8333513	-1.9166389
C	2.0973339	-0.0862865	-0.2785624
C	0.9493323	1.5217040	1.1347207
C	2.1716474	1.8578097	1.7188416
C	3.3729490	1.2816018	1.2952795
C	3.3061784	0.2917129	0.3117528
C	4.2447329	-2.5633080	-1.2951859
C	3.3399673	-1.6549437	-1.8589257
C	3.6810120	-1.0352380	-3.0689108
C	4.8987089	-1.3034067	-3.6942017
C	5.7993627	-2.2028008	-3.1169946
C	2.0237402	-1.3049565	-1.1875855
C	-1.5487113	0.1062776	-3.2724394
C	-0.6403974	-0.9697637	-3.8826278
C	1.0083069	1.9092381	-2.7936054
C	1.6365840	3.0690447	-2.0031366



C	-1.7214947	2.7985183	-1.6148799
C	-3.0812824	2.4084695	-1.0199246
C	1.4275276	-2.4795266	-0.4175558
C	0.6324302	-3.4208838	-1.0863165
C	0.0166846	-4.4632343	-0.3913614
C	0.2091027	-4.5965481	0.9859406
C	1.0256038	-3.6845483	1.6579782
C	1.6231552	-2.6306690	0.9631665
O	-2.9423241	-2.4522303	-1.2442293
C	-4.0181096	-1.8945319	-0.8632624
C	-4.6830210	-0.8611328	-1.7869154
C	-5.8761448	-0.1245083	-1.1818989
C	-0.1672034	3.4493889	2.3401235
C	0.1716739	4.5375507	1.5207304
C	0.3707162	5.8057127	2.0617881
C	0.2379141	6.0094590	3.4396130
C	-0.0961291	4.9343557	4.2630686
C	-0.2982516	3.6628781	3.7159731
C	-1.0166848	1.0701682	2.6165087
C	-2.4149741	1.0717043	2.7439599
C	-3.0606022	0.1403624	3.5582852
C	-2.3157174	-0.8039515	4.2701416
C	-0.9225427	-0.8031216	4.1687240
C	-0.2788008	0.1235709	3.3457506
C	4.6989737	1.7003732	1.8984265
C	4.7476941	1.4201225	3.4088332
C	-2.3941700	0.7930511	-4.3540517
C	0.9352493	2.2673701	-4.2879483
C	-1.8945019	3.8723976	-2.7000563
C	-4.8815635	-2.5905325	0.1989018
C	-4.0569341	-3.2736093	1.2889702
C	-5.7795451	-3.6249267	-0.5156386
C	-5.0181754	-1.5082390	-3.1443249
C	4.9973413	3.1789730	1.6009597
H	-2.8983364	0.0431471	-4.9837106
H	-1.7838572	1.4188463	-5.0196973
H	0.5827851	1.4322450	-4.9059991
H	1.9302210	2.5587283	-4.6613492
H	0.2626917	3.1162109	-4.4723828
H	-1.2274472	-1.6561250	-4.5127971
H	-3.1726924	1.4360545	-3.9228787
H	0.1571611	-0.5491292	-4.5108131
H	6.7504421	-2.4164054	-3.6046311
H	5.1430058	-0.8131423	-4.6368545
H	-6.3772476	-4.1705404	0.2274259
H	-2.4391637	3.4897485	-3.5732884
H	-6.4721725	-3.1572290	-1.2255335
H	-5.1643986	-4.3516992	-1.0630305

H	-0.9324807	4.2612621	-3.0563755
H	-0.1694636	-1.5766442	-3.1016236
H	1.6931971	1.0514501	-2.6934145
H	-2.4686686	4.7273615	-2.3078446
H	-2.2366579	-0.4473206	-2.6127385
H	2.9804278	-0.3343866	-3.5250132
H	2.6086932	3.3486050	-2.4393165
H	6.1577666	-3.5435766	-1.4624741
H	-5.8440782	-2.2269116	-3.0650418
H	-4.7137766	-3.8563526	1.9492236
H	-4.1414880	-2.0337392	-3.5418787
H	0.4721612	-3.3205448	-2.1595511
H	1.0019324	3.9669191	-2.0328029
H	-3.7663687	2.0576208	-1.8051782
H	-5.5287644	-1.8338485	0.6633707
H	1.3068577	-1.0672282	-1.9838317
H	-5.3152493	-0.7320368	-3.8621334
H	-0.6305704	-5.1579295	-0.9252685
H	-3.3133274	-3.9524637	0.8511545
H	3.9855967	-3.0692998	-0.3651727
H	1.8085832	2.8126629	-0.9515331
H	-3.5670316	3.2696458	-0.5339365
H	-1.1313346	3.2656764	-0.8064719
H	-3.5273580	-2.5416039	1.9132492
H	-3.0022709	1.6003270	-0.2783464
H	-3.9048906	-0.1148873	-1.9854261
H	-6.7328923	-0.7909338	-1.0107213
H	-6.2102284	0.6702080	-1.8628867
H	-3.3050691	-0.5585438	0.2773154
H	0.2977317	4.3782490	0.4490830
H	4.2235202	-0.2098442	-0.0006691
H	-0.2801876	-5.4024691	1.5323352
H	0.6325944	6.6380857	1.4082250
H	-1.0314433	2.2116032	0.8488503
H	-5.6040317	0.3442421	-0.2263879
H	4.9901190	3.3721743	0.5203181
H	2.2232331	-1.8961395	1.4993959
H	-2.9972675	1.8000260	2.1791289
H	5.4797332	1.0914376	1.4147926
H	1.1815977	-3.7794618	2.7326267
H	4.2407841	3.8298200	2.0620587
H	2.1784538	2.6030245	2.5151956
H	0.3943644	7.0004905	3.8654003
H	5.9801916	3.4687135	1.9988900
H	-4.1483599	0.1414849	3.6233127
H	-0.5603355	2.8290245	4.3667494
H	0.8057854	0.1056016	3.2456589
H	4.5607338	0.3586952	3.6204547

H	-0.2009520	5.0813513	5.3383022
H	3.9871183	2.0084469	3.9416784
H	5.7292908	1.6869449	3.8251814
H	-2.8197978	-1.5392596	4.8968050
H	-0.3341029	-1.5380768	4.7174586

**TS4-5Sn**

144

-3031.063501684

Sn	-1.4100365	-1.4596019	0.2607882
N	0.0525339	-0.1835769	-0.6808201
Si	0.0210759	1.2731085	-1.7165933
C	1.3692150	-0.6646166	-0.3809066
C	2.0735346	-0.2170528	0.7693162
C	3.4026950	-0.5905072	0.9700791
C	4.0820396	-1.4110096	0.0650290
C	3.3578337	-1.9259038	-1.0109666
C	2.0151546	-1.6041983	-1.2285709
O	-3.3078925	-0.8150577	-0.4076324
C	-4.4336890	-1.6619480	-0.6788470
C	-4.6650147	-2.8366669	0.3130365
C	-3.7951992	-4.0925553	0.1635627
C	1.2072369	-2.3612695	-2.2743375
C	1.9832107	-2.7335847	-3.5264043
C	1.8790440	-1.9481778	-4.6812999
C	2.6036510	-2.2642029	-5.8323961
C	3.4417467	-3.3808447	-5.8482230
C	3.5346834	-4.1870838	-4.7106482
C	2.8058478	-3.8694319	-3.5640381
C	5.5481133	-1.7433258	0.2566415
C	6.4142529	-0.4764058	0.1640928
C	1.3391651	0.5821878	1.8345055
C	2.2579947	1.4549654	2.6754741
C	3.0096011	2.4564011	2.0395887
C	3.8625445	3.2825816	2.7675679
C	3.9851019	3.1202447	4.1518948
C	3.2463464	2.1264901	4.7931674
C	2.3885390	1.3001784	4.0591458
C	0.2085015	2.8573173	-0.6618961
C	0.4255170	4.1496647	-1.4676740
C	-1.6185923	1.1799005	-2.6669076
C	-2.0824212	2.5103865	-3.2750421
C	1.5549100	1.2102552	-2.8707861
C	1.3840134	1.9635156	-4.2009660
C	-4.4699030	-2.0003664	-2.1881940
C	-3.2919150	-2.8243426	-2.7073372
C	-5.8073881	-2.6275577	-2.5940661
C	-0.8935369	3.0725133	0.3783608

C	0.5450338	-3.5976088	-1.6589095
C	-0.3184061	-4.3676495	-2.4541195
C	-0.9434490	-5.5022894	-1.9425552
C	-0.7164366	-5.8942362	-0.6190691
C	0.1413502	-5.1411709	0.1806754
C	0.7684932	-4.0020748	-0.3356625
C	0.4545297	-0.3425414	2.6589641
C	-0.7976814	0.1096215	3.1044773
C	-1.6640015	-0.7411349	3.7966288
C	-1.2789563	-2.0554463	4.0720599
C	-0.0207939	-2.5058526	3.6637449
C	0.8362649	-1.6582867	2.9594168
C	5.7928076	-2.4852580	1.5801069
C	-1.6280635	0.0617414	-3.7175642
C	2.8740590	1.6324807	-2.2006380
C	-4.6280679	-2.3440764	1.7653516
B	-3.7785802	1.0176976	0.6118204
O	-3.7989576	2.0188694	-0.3562862
C	-5.1866194	2.3253994	-0.6684520
C	-5.5714591	1.5794509	-1.9460238
O	-5.0540455	0.7709347	1.1250373
C	-5.9430808	1.8064144	0.6142191
C	-7.3091653	1.1893274	0.3433694
C	-6.0505254	2.8668982	1.7135325
C	-5.2907362	3.8281521	-0.9066191
H	-7.7456294	0.8333140	1.2853551
H	-7.9932001	1.9315760	-0.0907270
H	-7.2373745	0.3380900	-0.3426523
H	-6.4119978	2.3875217	2.6319303
H	-5.0701975	3.3125837	1.9241835
H	-6.7500744	3.6679937	1.4411219
H	-6.5813634	1.8522302	-2.2794221
H	-4.8618501	1.8455502	-2.7384050
H	-5.5315457	0.4952536	-1.8060914
H	-6.3362269	4.1276795	-1.0633287
H	-4.8828358	4.3983659	-0.0654563
H	-4.7231074	4.0938190	-1.8076633
H	-2.7874488	0.8333017	1.2609533
H	-3.0140318	2.3670296	-3.8467144
H	-1.3447540	2.9369281	-3.9692071
H	0.5081053	1.6275789	-4.7694638
H	2.2700537	1.8141295	-4.8390194
H	1.2758217	3.0462023	-4.0493127
H	-2.6443706	-0.0881839	-4.1153496
H	-2.2888116	3.2543177	-2.4960463
H	-0.9773400	0.2888044	-4.5735116
H	4.0076118	-3.6304502	-6.7456640
H	2.5054089	-1.6399512	-6.7206592

H	-4.0105630	-4.7873126	0.9884308
H	-0.4672594	4.4203000	-2.0458928
H	-3.9776897	-4.6275016	-0.7741796
H	-2.7180751	-3.8770627	0.2113788
H	1.2650593	4.0766336	-2.1695406
H	-1.3012237	-0.8984907	-3.2997761
H	1.6658587	0.1438459	-3.1164833
H	0.6385602	4.9894083	-0.7869481
H	-2.3548193	0.9044346	-1.8947894
H	1.2130198	-1.0855775	-4.6837172
H	3.7170863	1.4753787	-2.8920646
H	4.1709269	-5.0723869	-4.7188846
H	-3.4096576	-3.8961684	-2.5164319
H	-5.0030996	-3.1266442	2.4400208
H	-2.3441251	-2.5139174	-2.2457433
H	-0.4918971	-4.0706916	-3.4888759
H	2.8708059	2.6987672	-1.9338654
H	-1.8424764	3.3500475	-0.0957494
H	-5.7045817	-3.1461167	0.1086194
H	0.3903987	-1.6935113	-2.5850217
H	-3.1727800	-2.6900893	-3.7909215
H	-1.6141454	-6.0822273	-2.5765731
H	-3.6002445	-2.1120809	2.0811531
H	2.8581485	-4.5201927	-2.6906893
H	3.0859001	1.0601113	-1.2904792
H	-0.6158022	3.8689874	1.0870928
H	1.1522127	2.6659402	-0.1209469
H	-5.2227003	-1.4340292	1.9008161
H	-1.1027882	2.1647111	0.9577568
H	-4.3997327	-1.0138775	-2.6738367
H	-5.9191787	-3.6395332	-2.1789076
H	-5.8850606	-2.7099410	-3.6870026
H	-5.3105347	-1.0133478	-0.5003743
H	2.9351778	2.5735270	0.9578407
H	3.8559985	-2.6048369	-1.7035644
H	-1.2100350	-6.7784765	-0.2167428
H	4.4361003	4.0544737	2.2539834
H	0.6508833	1.2563141	1.3091419
H	-6.6568511	-2.0241369	-2.2418691
H	6.2579561	0.0381551	-0.7929667
H	1.4408379	-3.4236884	0.2955905
H	-1.1014796	1.1332127	2.8870359
H	5.8372416	-2.4148334	-0.5678593
H	0.3237218	-5.4322467	1.2150275
H	6.1601089	0.2287067	0.9683613
H	3.9204794	-0.2087074	1.8505191
H	4.6531243	3.7646679	4.7231873
H	7.4814608	-0.7232242	0.2555479

H	-2.6461883	-0.3800121	4.0994963
H	1.8150099	0.5273696	4.5700051
H	1.8024193	-2.0233912	2.6121432
H	5.1926742	-3.4034109	1.6358827
H	3.3346086	1.9890291	5.8711273
H	5.5239548	-1.8543562	2.4393011
H	6.8521302	-2.7585065	1.6850894
H	-1.9590118	-2.7261582	4.5961558
H	0.2877386	-3.5290133	3.8781917

**Ketone (iPr)<sub>2</sub>CO**

22

-350.5816941027

O	0.1136393	0.9514727	0.3465927
C	0.2435483	0.5927679	1.5072057
C	1.5804967	0.0735428	2.0291348
C	-0.9439261	0.6566675	2.4763463
C	1.4580373	-1.3830167	2.5046203
H	2.2635461	0.1141492	1.1681331
C	2.1233415	0.9831299	3.1432375
C	-1.4211840	2.1114274	2.6004775
C	-2.0672371	-0.2562698	1.9614618
H	-0.6201790	0.3007438	3.4659763
H	-2.9416466	-0.1965169	2.6236782
H	-2.3691202	0.0553822	0.9532632
H	-1.7474453	-1.3059254	1.9130271
H	-2.2967936	2.1713057	3.2610750
H	-0.6378252	2.7616292	3.0127798
H	-1.7005485	2.4984897	1.6121200
H	3.1114816	0.6294420	3.4681505
H	2.2309542	2.0201278	2.7991948
H	1.4646527	0.9797480	4.0230755
H	2.4403333	-1.7570322	2.8243921
H	0.7754251	-1.4714776	3.3615057
H	1.0904031	-2.0382036	1.7040379

**HBPIn**

22

-412.0686946972

B	0.3081600	1.1812010	-0.6581625
O	0.0073690	0.0432731	0.0504316
C	1.1548300	-0.2231547	0.9305429
C	1.8391000	1.1908862	1.0357234
O	1.4365642	1.8336995	-0.2240616
C	2.0191919	-1.2601471	0.2118329
C	0.6362070	-0.7825207	2.2473369
C	3.3591939	1.1630345	1.1014530

C	1.2702759	2.0543884	2.1626250
H	3.7445607	2.1889811	1.1539101
H	3.6964023	0.6259575	1.9986830
H	3.7926691	0.6796055	0.2197631
H	1.6427730	3.0795806	2.0464786
H	0.1738478	2.0828562	2.1274040
H	1.5797854	1.6826753	3.1479471
H	2.8715551	-1.5697535	0.8303367
H	1.4073122	-2.1449977	-0.0024180
H	2.4005343	-0.8692654	-0.7399570
H	1.4628848	-0.9283979	2.9563133
H	-0.1047143	-0.1183855	2.7045262
H	0.1618941	-1.7563647	2.0727124
H	-0.3541808	1.5697601	-1.5721564

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