Electronic Supplementary Information for the paper

Entitled

Hydroboration of Carbonyls and Imines by an Iminophosphonamido Tin(II) Precatalyst

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Contents

S1. NMR charts of tin(II) chloride **1**

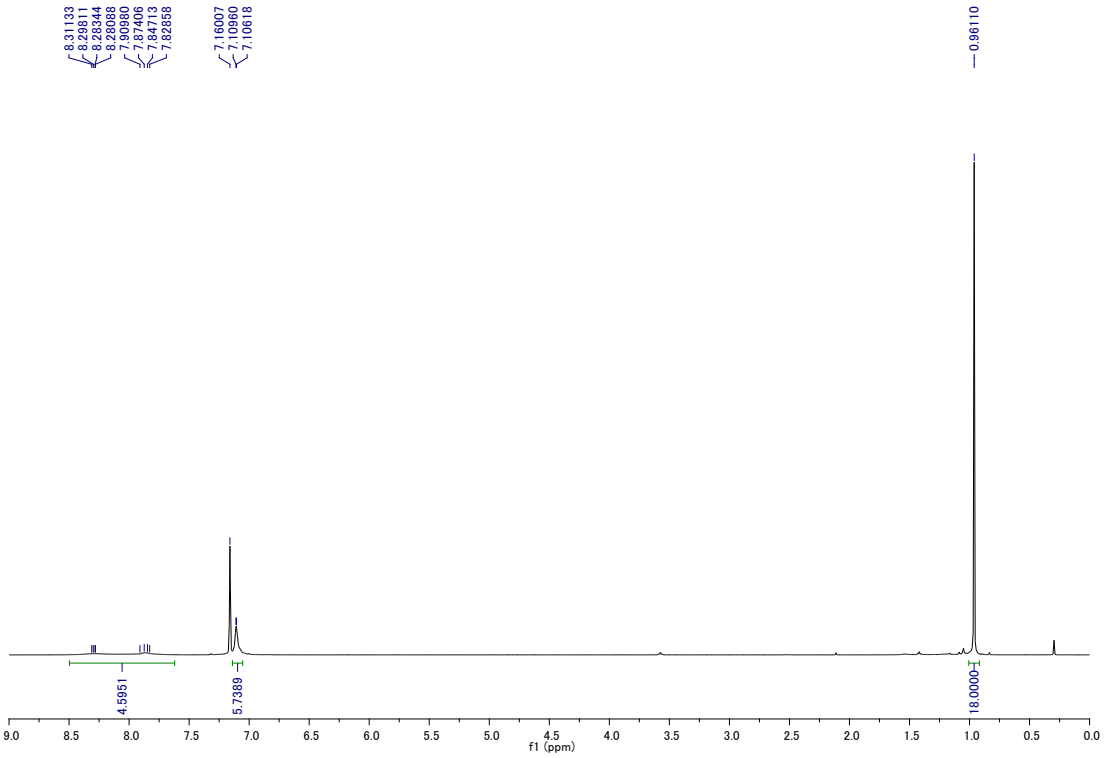


Figure S1. ^{1}H NMR spectra of **1** (500 MHz, 25 °C, C_6D_6).

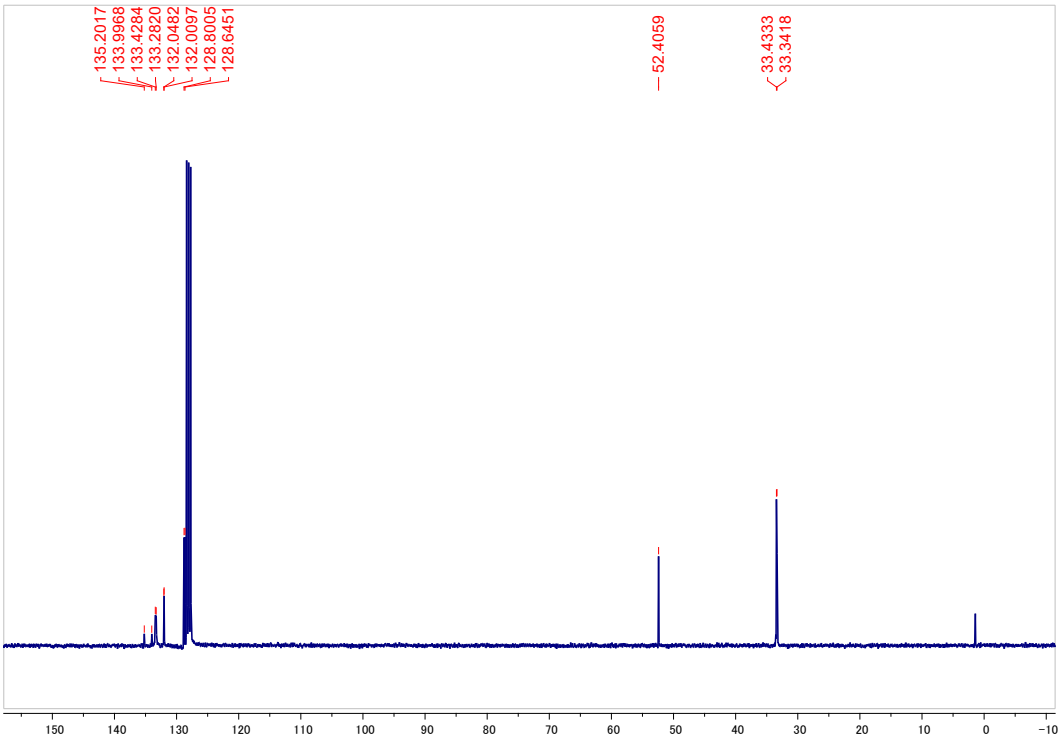


Figure S2. ^{13}C{^{1}H} NMR spectra of **1** (75 MHz, 25 °C, C_6D_6).

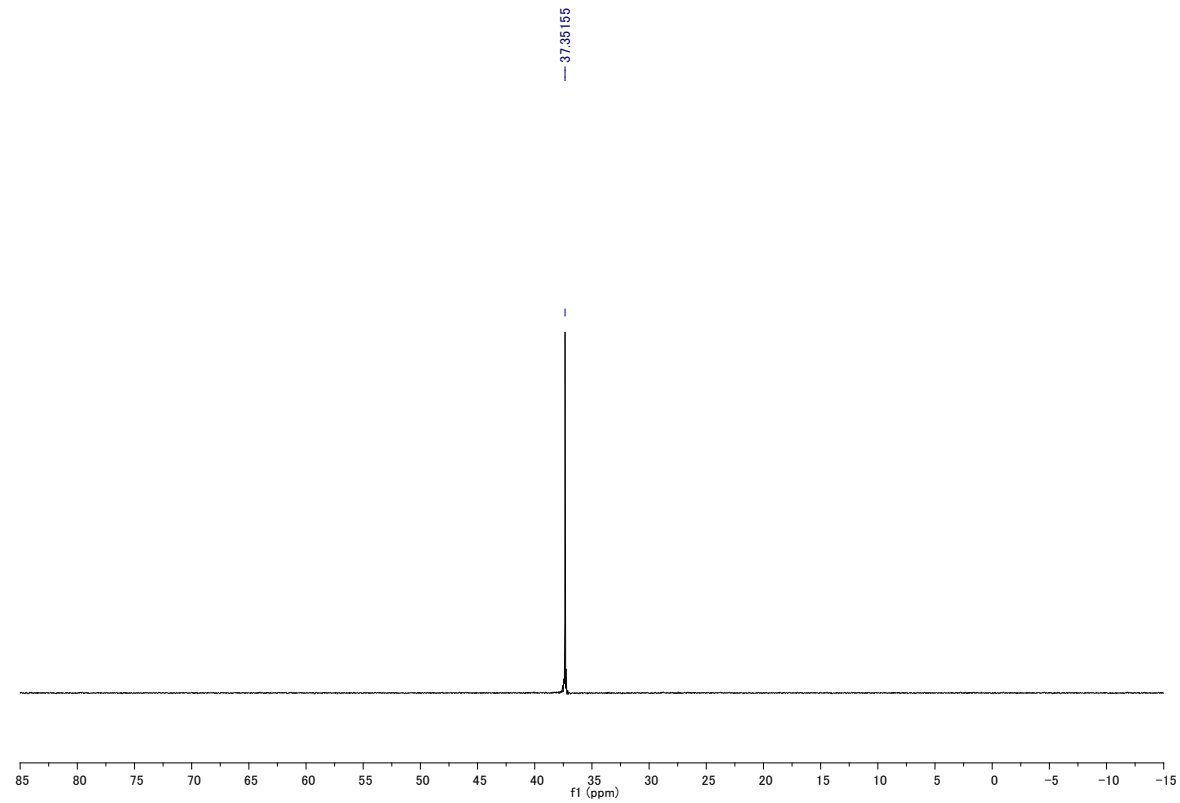


Figure S3. $^{31}P\{^{1}H\}$ NMR spectra of **1** (202 MHz, 25 °C, C_6D_6).

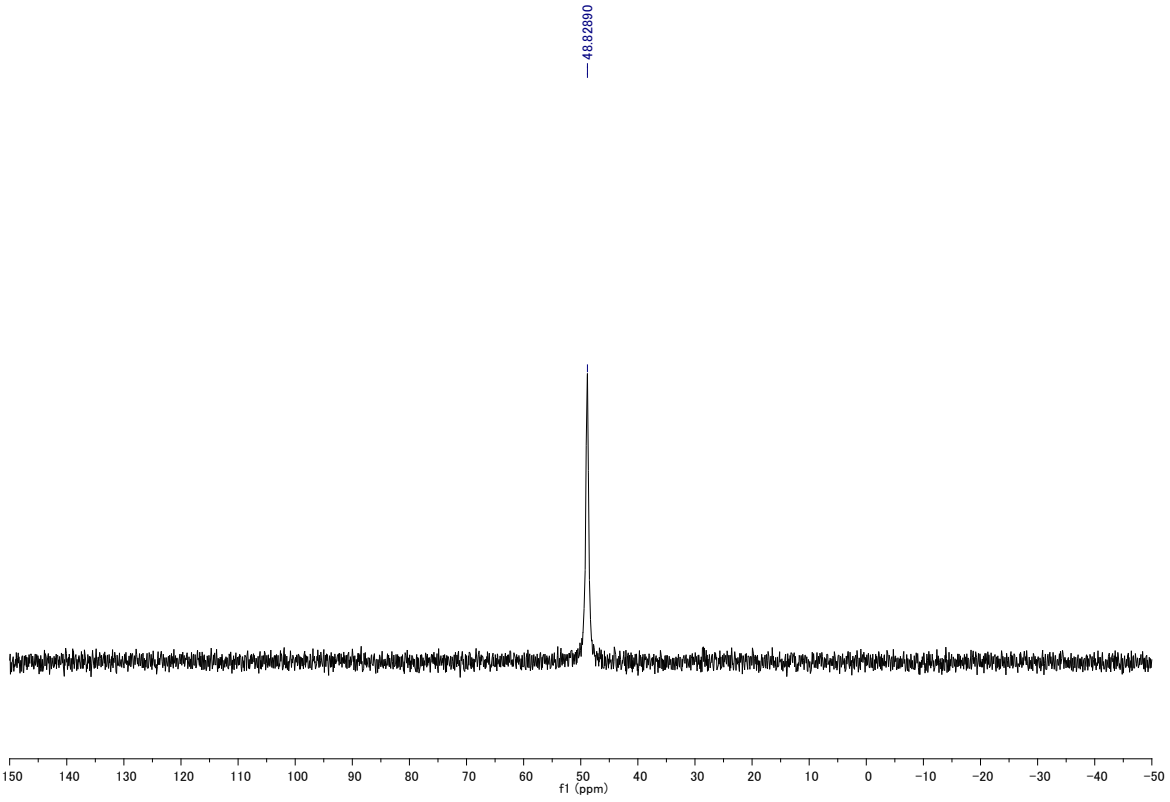
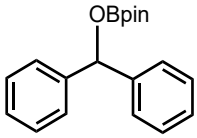


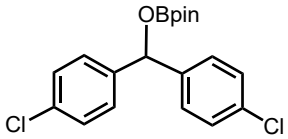
Figure S4. $^{119}Sn\{^{1}H\}$ NMR spectra of **1** (187 MHz, 25 °C, C_6D_6).

S2. Spectroscopic data of hydroboration products



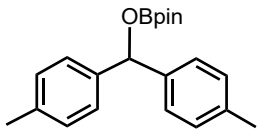
3a

^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 0.98 (s, 12H, BpinCH_3), 6.41 (s, 1H, C<u>H</u>-OBpin), 6.99−7.02 (m, 2H, Ar), 7.08−7.11 (m, 4H, Ar), 7.43−7.44 (d, J_{H-H} = 7.0 Hz, 4H, Ar). ^{13}C{^{1}H} NMR (126 MHz, 25 ˚C, C_6D_6): δ 24.6 (BpinCH_3), 78.5 (<u>C</u>H-OBpin), 82.8 (<u>C</u>-(CH_3)$_2$), 127.0 (Ar(CH)), 127.6 (Ar(CH)), 128.6 (Ar(CH)), 143.9(Ar(C)). ^{11}B{^{1}H} NMR (96.3 MHz, 25 ˚C, C_6D_6): δ 22.7.



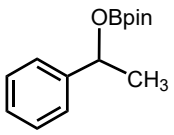
3b

^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 0.97 (s, 6H, BpinCH_3), 1.01 (s, 6H, BpinCH_3), 6.12 (s, 1H, C<u>H</u>-OBpin), 7.05−7.06 (m, 8H, Ar). ^{11}B{^{1}H} NMR (96.3 MHz, 25 ˚C, C_6D_6): δ 21.9.



3c

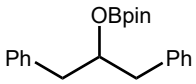
^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 1.01 (s, 12H, BpinCH_3), 2.05 (s, 6H, CH_3), 6.45 (s, 1H, C<u>H</u>-OBpin), 6.94 (d, J_{H-H} = 7.8 Hz, 4H, Ar), 7.40 (d, J_{H-H} = 8.1 Hz, 4H, Ar). ^{11}B{^{1}H} NMR (160 MHz, 25 ˚C, C_6D_6): δ 21.7.



3d

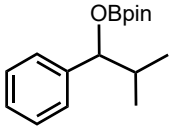
^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 0.99 (s, 6H, BpinCH_3), 1.01 (s, 6H, BpinCH_3), 1.46 (d,

$J_{H–H}$ = 6.5 Hz, 1H, CH_3), 5.41 (q, $J_{H–H}$ = 6.5 Hz, 1H, C<u>H</u>-OBpin), 7.03–7.07 (m, 1H, Ar), 7.11–7.16 (m, 2H, Ar), 7.37 (d, $J_{H–H}$ = 7.9 Hz, 2H, Ar). $^{11}B\{^1H\}$ NMR (160 MHz, 25 ˚C, C_6D_6): δ 22.6.



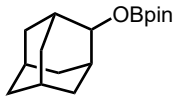
3e

^1H NMR (400 MHz, 25 ˚C, C_6D_6): δ 0.84 (s, 6H, BpinCH_3), 1.01 (s, 6H, BpinCH_3), 2.67–2.77 (m, 4H, CH_2), 4.58–4.64 (m, 1H, C<u>H</u>-OBpin), 6.96–7.18 (m, 10H, Ar). $^{11}B\{^1H\}$ NMR (160 MHz, 25 ˚C, C_6D_6): δ 21.8.



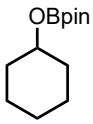
3f

^1H NMR (500 MHz, 25 ˚C, C_6D_6): δ 0.85 (d, $J_{H–H}$ = 6.8 Hz, 6H, CH_3), 0.98 (s, 12H, BpinCH_3), 1.94–2.00 (m, 1H, CH), 5.04 (d, $J_{H–H}$ = 6.2 Hz, 1H, C<u>H</u>-OBpin), 7.06–7.16 (m, 3H, Ar), 7.36 (d, $J_{H–H}$ = 8.2 Hz, 2H, Ar). $^{11}B\{^1H\}$ NMR (160 MHz, 25 ˚C, C_6D_6): δ 21.9.



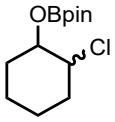
3g

^1H NMR (500 MHz, 25 ˚C, C_6D_6): δ 1.07 (s, 12H, BpinCH_3), 1.43–1.45 (m, 2H, CH_2), 1.57–1.62 (m, 5H, CH_2 and CH), 1.68–1.71 (m, 3H, CH_2 and CH), 2.06 (br, 2H, CH), 2.35–2.37 (m, 2H, CH_2), 4.45 (br, 1H, C<u>H</u>-OBpin). $^{13}C\{^1H\}$ NMR (126 MHz, 25 ˚C, C_6D_6): δ 24.8 (BpinCH_3), 27.5 (CH), 28.0 (CH), 31.5 (CH_2), 34.6 (CH), 36.7 (CH_2), 37.9 (CH_2) 77.1 (<u>C</u>H-OBpin), 82.2 (<u>C</u>-$(CH_3)_2$). $^{11}B\{^1H\}$ NMR (160 MHz, 25 ˚C, C_6D_6): δ 22.4.



3h

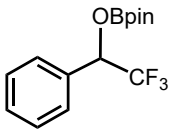
^{1}H NMR (400 MHz, 25 ˚C, C_6D_6): δ 1.07 (s, 12H, BpinCH$_3$), 1.11–1.17 (m, 3H, CH$_2$), 1.26–1.30 (m, 1H, CH$_2$), 1.44–1.52 (m, 2H, CH$_2$), 1.59–1.64 (m, 2H, CH$_2$), 1.87–1.92 (m, 2H, CH$_2$) 4.18–4.25 (m, 1H, C<u>H</u>-OBpin). ^{13}C{^{1}H} NMR (126 MHz, 25 ˚C, C_6D_6): δ 24.1 (CH$_{2Cy}$), 24.6 (BpinCH$_3$), 24.7 (CH$_3$), 25.8 (CH$_{2Cy}$), 34.8 (CH$_{2Cy}$), 72.8 (<u>C</u>H-OBpin), 82.2 (<u>C</u>-(CH$_3$)$_2$), 82.9 (<u>C</u>-(CH$_3$)$_2$). ^{11}B{^{1}H} NMR (160 MHz, 25 ˚C, C_6D_6): δ 22.4.



3i

cis-**3i**: ^{1}H NMR (400 MHz, 25 ˚C, C_6D_6): δ 0.86–1.15 (overlapped, 16H, BpinCH$_3$ and CH$_2$), 1.20–1.30 (m, 1H, CH$_2$), 1.38–1.57 (m, 2H, CH$_2$), 1.80–2.04 (m, 1H, CH$_2$), 3.83–3.86 (m, 1H, C<u>H</u>-Cl), 4.38–4.40(m, 1H, C<u>H</u>-OBpin). ^{13}C{^{1}H} NMR (100 MHz, 25 ˚C, C_6D_6): δ 20.5 (CH$_{2Cy}$), 23.8 (CH$_{2Cy}$), 24.6 (BpinCH$_3$), 24.8 (CH$_3$), 31.4 (CH$_{2Cy}$), 31.6 (CH$_{2Cy}$), 63.0 (<u>C</u>-Cl), 73.0 (<u>C</u>H-OBpin), 82.6 (<u>C</u>-(CH$_3$)$_2$). ^{11}B{^{1}H} NMR (160 MHz, 25 ˚C, C_6D_6): δ 22.5.

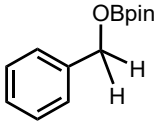
trans-**3i**: ^{1}H NMR (400 MHz, 25 ˚C, C_6D_6): δ 0.86–1.15 (overlapped, 14H, BpinCH$_3$ and CH$_2$), 1.20–1.30 (m, 1H, CH$_2$), 1.38–1.57 (m, 1H, CH$_2$), 1.80–2.04 (m, 2H, CH$_2$), 3.62–3.68 (m, 1H, C<u>H</u>-Cl), 4.14–4.20 (m, 1H, C<u>H</u>-OBpin). ^{13}C{^{1}H} NMR (100 MHz, 25 ˚C, C_6D_6): δ 23.6 (CH$_{2Cy}$), 24.7 (BpinCH$_3$), 33.59 (CH$_{2Cy}$), 35.0 (CH$_{2Cy}$), 64.4 (<u>C</u>-Cl), 77.2 (OCH), 82.7 (<u>C</u>-(CH$_3$)$_2$), 83.0 (<u>C</u>-(CH$_3$)$_2$).



3j

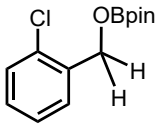
^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 0.93 (s, 6H, BpinCH$_3$), 0.97 (s, 6H, BpinCH$_3$), 5.57 (q,

J_{H-F} = 6.4 Hz, 1H, C<u>H</u>-OBpin), 7.01−7.02 (m, 3H, Ar), 7.38−7.39 (m, 2H, Ar). $^{13}C\{^1H\}$ NMR (126 MHz, 25 ˚C, C_6D_6): δ 24.3 ($BpinCH_3$), 24.5 ($BpinCH_3$), 74.9 (q, J_{C-F} = 32.4 Hz, <u>C</u>H-OBpin), 83.8 (<u>C</u>-$(CH_3)_2$) 124.6 (q, J_{C-F} = 281.7 Hz, CF_3), 127.9 (Ar(CH)), 128.7 (Ar(CH)), 129.6 (Ar(CH)), 133.9 (Ar(C)). $^{11}B\{^1H\}$ NMR (96.3 MHz, 25 ˚C, C_6D_6): δ = 22.9. $^{19}F\{^1H\}$ NMR (470 MHz, 25 ˚C, C_6D_6): δ −79.0.



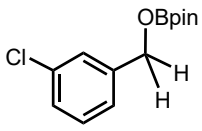
5a

^1H NMR (500 MHz, 25 ˚C, C_6D_6): δ 1.04 (s, 12H, $BpinCH_3$), 4.95 (s, 2H, C<u>H</u>$_2$-OBpin), 7.05 (t, J_{H-H} = 7.4 Hz, 1H, Ar), 7.13 (t, J_{H-H} = 7.5 Hz, 2H, Ar), 7.31 (d, J_{H-H} = 7.3 Hz, 2H, Ar). $^{13}C\{^1H\}$ NMR (126 MHz, 25 ˚C, C_6D_6): δ 24.7 ($BpinCH_3$), 67.0 (<u>C</u>H_2-OBpin), 82.8 (<u>C</u>-$(CH_3)_2$), 127.0 (Ar(CH)), 127.6 (Ar(CH)), 128.6 (Ar(CH)), 140.1 (Ar(C)). $^{11}B\{^1H\}$ NMR (96.3 MHz, 25 ˚C, C_6D_6): δ 22.9.



5b

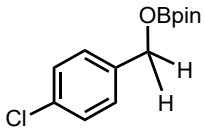
^1H NMR (300 MHz, 25 ˚C, C_6D_6): δ 1.04 (s, 12H, $BpinCH_3$), 5.15 (s, 2H, C<u>H</u>$_2$-OBpin), 6.74−6.79 (m, 1H, Ar), 6.89−6.94 (m, 1H, Ar), 7.07 (d, J_{H-H} = 7.7 Hz, 1H, Ar), 7.56 (d, J_{H-H} = 7.4 Hz, 1H, Ar). $^{13}C\{^1H\}$ NMR (126 MHz, 25 ˚C, C_6D_6): δ 24.6 ($BpinCH_3$), 64.4 (<u>C</u>H_2-OBpin), 83.0 (<u>C</u>-$(CH_3)_2$), 127.0 (Ar(CH)), 128.0 (Ar(CH)), 128.5 (Ar(CH)), 129.3 (Ar(CH)), 132.2 (Ar(C)), 137.6 (Ar(<u>C</u>Cl)). $^{11}B\{^1H\}$ NMR (96.3 MHz, 25 ˚C, C_6D_6): δ 22.8.



5c

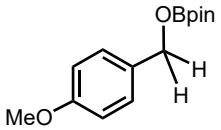
^1H NMR (400 MHz, 25 ˚C, C_6D_6): δ 1.03 (s, 12H, $BpinCH_3$), 4.74 (s, 2H, C<u>H</u>$_2$-OBpin),

6.78–6.83 (m, 1H, Ar), 6.99–7.02 (m, 2H, Ar), 7.31 (s, 1H, Ar). $^{13}C\{^{1}H\}$ NMR (101 MHz, 25 ˚C, C_6D_6): δ 24.7 ($BpinCH_3$), 66.1 ($\underline{C}H_2$-OBpin), 82.9 ($\underline{C}$-$(CH_3)_2$), 124.9 (Ar(CH)), 127.2 (Ar(CH)), 127.6 (Ar(CH)), 129.9 (Ar(CH)), 134.6 (Ar($\underline{C}$)), 142.1 (Ar($\underline{C}$Cl)). $^{11}B\{^{1}H\}$ NMR (160 MHz, 25 ˚C, C_6D_6): δ 22.8.



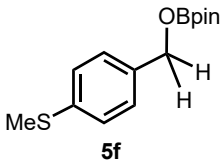
5d

^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 1.03 (s, 12H, $BpinCH_3$), 4.76 (s, 1H, $C\underline{H_2}$-OBpin), 7.00 (d, $J_{H–H}$ = 8.0 Hz, 2H, Ar), 7.06 (d, $J_{H–H}$ = 8.0 Hz, 2H, Ar). $^{13}C\{^{1}H\}$ NMR (101 MHz, 25 ˚C, C_6D_6): δ 24.7 (CH_3), 66.1 ($\underline{C}H_2$-OBpin), 82.9 ($\underline{C}$-$(CH_3)_2$), 128.4 (Ar(CH)), 128.2 (Ar(CH)), 133.4 (Ar($\underline{C}$)), 138.4 (Ar($\underline{C}$Cl)). $^{11}B\{^{1}H\}$ NMR (160 MHz, 25 ˚C, C_6D_6): δ 22.8.



5e

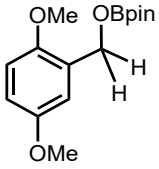
^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 1.05 (s, 12H, $BpinCH_3$), 3.29 (s, 3H, OCH_3), 4.93 (s, 2H, $C\underline{H_2}$-OBpin), 6.75(d, $J_{H–H}$ = 7.6 Hz, 2H, Ar), 7.26 (d, $J_{H–H}$ = 6 Hz, 2H, Ar). ^{13}C NMR (126 MHz, 25 ˚C, C_6D_6): δ 24.7 ($BpinCH_3$), 54.8 (OCH_3), 66.8 ($\underline{C}H_2$-OBpin), 82.7 ($\underline{C}$-$(CH_3)_2$), 114.1 (Ar(CH)), 128.9 (Ar(CH)), 132.2 (Ar($\underline{C}$)), 159.7 (Ar($\underline{C}OCH_3$)). $^{11}B\{^{1}H\}$ NMR (160 MHz, 25 ˚C, C_6D_6): δ 22.8.



5f

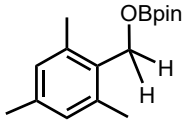
^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 1.05 (s, 12H, $BpinCH_3$), 1.99 (s, 3H, SCH_3), 4.88 (s, 2H, $C\underline{H_2}$-OBpin), 7.07 (d, $J_{H–H}$ = 8.4 Hz, 2H, Ar), 7.17 (d, $J_{H–H}$ = 8.5 Hz, 2H, Ar). ^{13}C NMR (126

MHz, 25 ˚C, C_6D_6): δ 15.5 (SCH_3), 24.7 ($BpinCH_3$), 68.3 ($\underline{C}H_2$-OBpin), 82.8 ($\underline{C}$-$(CH_3)_2$), 126.9 (Ar(CH)), 127.8 (Ar(CH)), 136.8 (Ar($\underline{C}$)), 138.2 (Ar($\underline{C}SCH_3$)). $^{11}B\{^1H\}$ NMR (160 MHz, 25 ˚C, C_6D_6): δ 22.8.



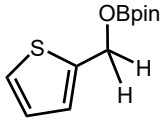
5g

^1H NMR (400 MHz, 25 ˚C, C_6D_6): δ 1.04 (s, 12H, $BpinCH_3$), 3.29 (s, 3H, OCH_3), 3.39 (s, 3H, OCH_3), 5.28 (s, 2H, $C\underline{H_2}$-OBpin), 6.46 (d, $J_{H–H}$ = 8.8 Hz, 1H, Ar), 6.72 (dd, $J_{H–H}$ = 8.8 and 3.1 Hz, 1H, Ar), 7.38 (d, $J_{H–H}$ = 3.1 Hz, 1H, Ar). ^{13}C NMR (101 MHz, 25 ˚C, C_6D_6): δ 24.7 ($BpinCH_3$), 55.3 (OCH_3), 55.3 (OCH_3), 62.8 ($\underline{C}H_2$-OBpin), 82.7 ($\underline{C}$-$(CH_3)_2$), 111.5 (Ar(CH)), 113.2 (Ar(CH)), 113.3 (Ar(CH)), 129.6 (Ar($\underline{C}$)), 150.9 (Ar($\underline{C}OCH_3$)), 154.6 (AR($\underline{C}OCH_3$). $^{11}B\{^1H\}$ NMR (160 MHz, 25 ˚C, C_6D_6): δ 22.8.



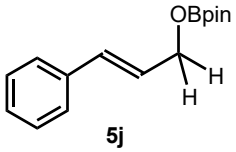
5h

^1H NMR (400 MHz, 25 ˚C, C_6D_6): δ 1.04 (s, 12H, $BpinCH_3$), 2.11 (s, 3H, $ArCH_3$), 2.37 (s, 6H, $ArCH_3$), 5.02 (s, 2H, $C\underline{H_2}$-OBpin), 6.72 (s, 2H, Ar). $^{13}C\{^1H\}$ NMR (126 MHz, 25 ˚C, C_6D_6): δ 19.7 ($ArCH_3$), 21.1 ($ArCH_3$), 24.7 ($Bpin\underline{C}H_3$), 61.5 ($\underline{C}H_2$-OBpin), 82.6 ($\underline{C}$-$(CH_3)_2$), 129.4 (Ar(CH)), 132.9 (Ar($\underline{C}$)), 137.4 (Ar($\underline{C}CH_3$)), 137.8 (Ar($\underline{C}CH_3$)). $^{11}B\{^1H\}$ NMR (160 MHz, 25 ˚C, C_6D_6): δ 22.6.



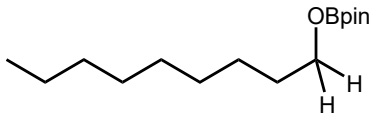
5i

^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 1.03 (s, 12H, BpinCH_3), 5.00 (s, 2H, CH_2-OBpin), 6.67 (dd, $J_{H–H}$ = 5.0 and 3.5 Hz 1H, Ar), 6.82−6.83 (m, 1H, Ar), 6.85 (dd, $J_{H–H}$ = 5.1 and 1.2 Hz 1H, Ar). ^{13}C{^{1}H} NMR (126 MHz, 25 ˚C, C_6D_6): δ 24.7 (BpinCH$_3$), 61.8 (CH$_2$-OBpin), 82.9 (C-(CH$_3$)$_2$), 125.7 (Ar(CH)), 126.1(Ar(CH)), 126.8 (Ar(CH)), 142.8 (Ar(C)). ^{11}B{^{1}H} NMR (160 MHz, 25 ˚C, C_6D_6): δ 22.8.



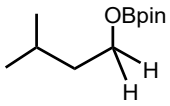
5j

^{1}H NMR (400 MHz, 25 ˚C, C_6D_6): δ 1.06 (s, 12H, BpinCH_3), 4.54 (d, $J_{H–H}$ = 5.2 Hz, 2H, CH_2-OBpin), 6.17 (dt, $J_{H–H}$ = 15.9 and 5.3 Hz, 1H, CH-CH$_2$), 6.61 (d, $J_{H–H}$ = 15.9 Hz, 1H, Ar-CH), 7.02 (m, 2H, Ar), 7.08 (t, $J_{H–H}$ = 7.4 Hz, 2H, Ar), 7.18 (d, $J_{H–H}$ = 7.5 Hz, 1H, Ar). ^{13}C{^{1}H} NMR (101 MHz, 25 ˚C, C_6D_6): δ 24.7 (BpinCH$_3$), 65.5 (CH$_2$-OBpin), 82.7 (C-(CH$_3$)$_2$), 126.8 (Ar(CH)), 127.5 (Ar-CH=CHCH$_2$), 127.7 (Ar(CH)), 128.8 (Ar(CH)), 130.9 (Ar-CH=CHCH$_2$), 137.4 (Ar(C)). ^{11}B{^{1}H} NMR (96.3 MHz, 25 ˚C, C_6D_6): δ 22.8.



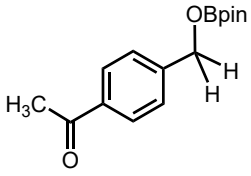
5k

^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 0.89 (t, $J_{H–H}$ = 6.8 Hz, 3H, CH$_3$), 1.08 (s, 12H, BpinCH$_3$), 1.20−1.30 (m, 10H, CH$_2$), 1.54−1.59 (m, 4H, CH$_2$), 3.95 (t, $J_{H–H}$ = 6.3 Hz, 2H, CH$_2$-OBpin). ^{13}C{^{1}H} NMR (101 MHz, 25 ˚C, C_6D_6): δ 14.4 (CH$_3$), 23.1 (CH$_2$), 24.8 (BpinCH$_3$), 26.1 (CH$_2$), 29.7 (CH$_2$), 29.8 (CH$_2$), 30.0 (CH$_2$), 32.1 (CH$_2$), 32.3 (CH$_2$), 65.2 (CH$_2$-OBPin), 82.4 (C-(CH$_3$)$_2$). ^{11}B{^{1}H} NMR (160 MHz, 25 ˚C, C_6D_6): δ 22.6.



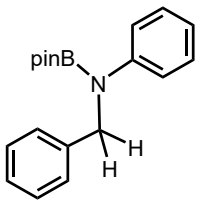
5i

^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 0.82 (d, $J_{H–H}$ = 6.7 Hz, 6H, CH_3), 1.06 (s, 12H, BpinCH_3), 1.45 (q, $J_{H–H}$ = 6.7 Hz, 2H, CH_2), 1.69 (sept, $J_{H–H}$ = 6.7 Hz, 1H, CH), 3.98 (t, $J_{H–H}$ = 6.6 Hz, 2H, C$\underline{H_2}$-OBpin). ^{13}C{^{1}H} NMR (126 MHz, 25 ˚C, C_6D_6): δ 22.7 (CH_3), 24.8 (Bpin$\underline{C}H_3$), 40.8 (CH_2), 63.4 ($\underline{C}H_2$-OBPin), 82.4 ($\underline{C}$-$(CH_3)_2$). ^{11}B{^{1}H} NMR (160 MHz, 25 ˚C, C_6D_6): δ 22.5.



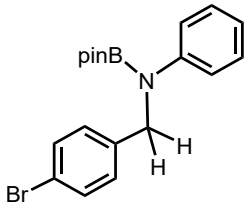
5m

^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 1.05 (s, 12H, BpinCH_3), 2.09 (s, 2H, CH_3), 4.88 (s, 2H, C$\underline{H_2}$-OBpin), 7.21 (d, $J_{H–H}$ = 8.4 Hz, 2H, Ar), 7.74 (d, $J_{H–H}$ = 8.4 Hz, 2H, Ar). ^{13}C{^{1}H} NMR (126 MHz, 25 ˚C, C_6D_6): δ 24.7 (BpinCH_3), 26.2 (CH_3), 66.3 ($\underline{C}H_2$-OBpin), 83.0 ($\underline{C}$-$(CH_3)_2$), 126.5 (Ar(CH)), 128.7 (Ar(CH)), 136.8 (Ar($\underline{C}$)), 144.8 (Ar($\underline{C}$CO)), 196.3 (C=O). ^{11}B{^{1}H} NMR (96.3 MHz, 25 ˚C, C_6D_6): δ 22.8.



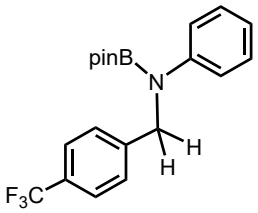
9a

^{1}H NMR (400 MHz, 25 ˚C, C_6D_6): δ 1.01 (s, 12H, BpinCH_3), 3.94 (s, 2H, C$\underline{H_2}$-NBpin), 6.45 (d, $J_{H–H}$ = 7.7 Hz, 2H, Ar), 6.71 (t, $J_{H–H}$ = 7.3 Hz, 1H, Ar), 7.02–7.21 (m, 7H, Ar). ^{11}B{^{1}H} NMR (160 MHz, 25 ˚C, C_6D_6): δ 21.8.



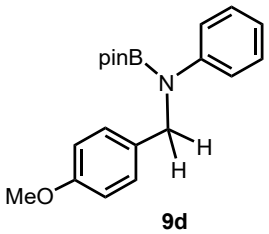
9b

^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 1.03 (s, 12H, BpinCH_3), 3.78 (d, $J_{H–H}$ = 4.9 Hz, 1H, C$\underline{H_2}$-NBpin), 6.41 (d, $J_{H–H}$ = 7.7 Hz, 2H, Ar), 6.71 (t, $J_{H–H}$ = 7.3 Hz, 1H, Ar), 6.80 (d, $J_{H–H}$ = 8.4 Hz, 2H, Ar_{Br}), 7.04–7.26 (m, 4H, Ar). ^{11}B{^{1}H} NMR (160 MHz, 25 ˚C, C_6D_6): δ 21.8.



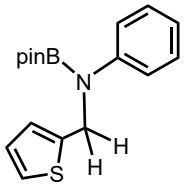
9c

^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 1.01 (s, 12H, BpinCH_3), 3.87 (br, 2H, C$\underline{H_2}$-NBpin), 6.43 (dd, $J_{H–H}$ = 8.6 and 1.0 Hz, 2H, Ar), 6.71 (tt, $J_{H–H}$ = 7.4 and 1.0 Hz, 1H, Ar), 7.00 (d, $J_{H–H}$ = 7.9 Hz, 2H, Ar), 7.06–7.21 (m, 2H, Ar), 7.32 (d, $J_{H–H}$ = 8.1 Hz, 2H, Ar). ^{13}C{^{1}H} NMR (101 MHz, 25 ˚C, C_6D_6): δ = 24.6 (BpinCH_3), 47.5 ($\underline{C}H_2$-NBpin), 83.0 ($\underline{C}$-$(CH_3)_2$), 113.2 (Ar(CH)), 118.0 (Ar(CH)), 125.6 (q, $J_{C–F}$ = 3.6 Hz, Ar(CH)), 127.6 (Ar(CH)), 129.5 (Ar(CH)), 144.8 (Ar($\underline{C}CH_2$)), 148.2 (Ar($\underline{C}$N)). ^{11}B{^{1}H} NMR (96.3 MHz, 25 ˚C, C_6D_6): δ 21.8. ^{19}F{^{1}H} NMR (470 MHz, 25 ˚C, C_6D_6): δ –63.5.



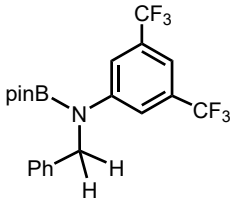
9d

^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 1.01 (s, 12H, BpinCH_3), 3.32–3.33 (m, 3H, CH_3O), 3.93–3.94 (m, 2H, C$\underline{H_2}$-NBpin), 6.73–6.76 (m, 2H, Ar), 6.73–6.76 (m, 2H, Ar), 7.12–7.15 (m, 1H, Ar), 7.20–7.21 (m, 4H, Ar).



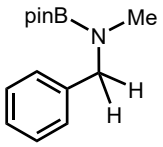
9e

^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 1.01 (s, 12H, $BpinCH_3$), 4.04 (s, 1H, C$\underline{H_2}$-NBpin), 4.05 (s, 1H, C$\underline{H_2}$-NBpin), 6.43 (d, J_{HH} = 7.7 Hz, 1H, Ar), 6.72–6.73 (m, 1H, Ar), 6.99-7.02 (m, 1H, Ar), 7.08–7.14 (m, 5H, Ar).



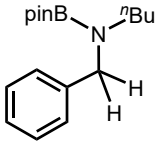
9f

^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 1.01 (s, 12H, $BpinCH_3$), 4.00–4.04 (m, 2H, C$\underline{H_2}$-NBpin), 6.60–6.67 (m, 2H, Ar), 7.00–7.03 (m, 2H, Ar), 7.08–7.21 (m, 1H, Ar), 7.30–7.31 (m, 2H, Ar), 7.62 (br, 1H, Ar), 7.71 (br, 2H, Ar).



9g

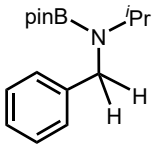
^{1}H NMR (500 MHz, 25 ˚C, C_6D_6): δ 1.15 (s, 12H, $BpinCH_3$), 2.59 (s, 3H, CH_3), 4.15 (s, 2H, C$\underline{H_2}$-NBpin), 7.09–7.13 (m, 1H, Ar), 7.19 (t, J_{HH} = 7.6 Hz, 2H, Ar), 7.27 (d, J_{HH} = 7.1 Hz, 2H, Ar).



9h

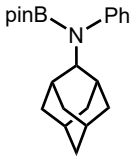
^{1}H NMR (400 MHz, 25 ˚C, C_6D_6): δ 0.83–0.85 (m, 3H, CH_3), 1.15 (s, 12H, $BpinCH_3$),

1.32–1.43 (m, 4H, CH_2), 2.99 (t, J_{HH} = 7.0j Hz, 2H, CH_2), 4.23 (s, 2H, C$\underline{H_2}$-NBpin), 7.20 (d, J_{HH} = 7.5 Hz, 3H, Ar), 7.31 (t, J_{HH} = 7.1 Hz, 2H, Ar).



9i

^{1}H NMR (400 MHz, 25 ˚C, C_6D_6): δ 0.94 (d, $J_{H–H}$ = 6.2 Hz, 6H, CH_3), 1.02 (s, 12H, BpinCH_3), 2.64 (sept, $J_{H–H}$ = 6.2 Hz, 1H, CH), 3.62 (s, 2H, C$\underline{H_2}$-NBpin), 7.09–7.21 (m, 3H, Ar), 7.29–7.30 (m, 2H, Ar).



9j

^{1}H NMR (400 MHz, 25 ˚C, C_6D_6): δ 1.06 (s, 12H, BpinCH_3), 1.36 (br, 1H, CH), 1.39 (br, 1H, CH_2), 1.50–1.92 (m, 12H, CH_2 and CH_3), 3.41–3.42 (s, 1H, C$\underline{H_2}$-NBpin), 6.54–6.56 (m, 2H, Ar), 6.72–6.76 (m, 1H, Ar), 7.18–7.21 (m, 2H, Ar).

S3. NMR charts of Hydroboration products

(a) ketones

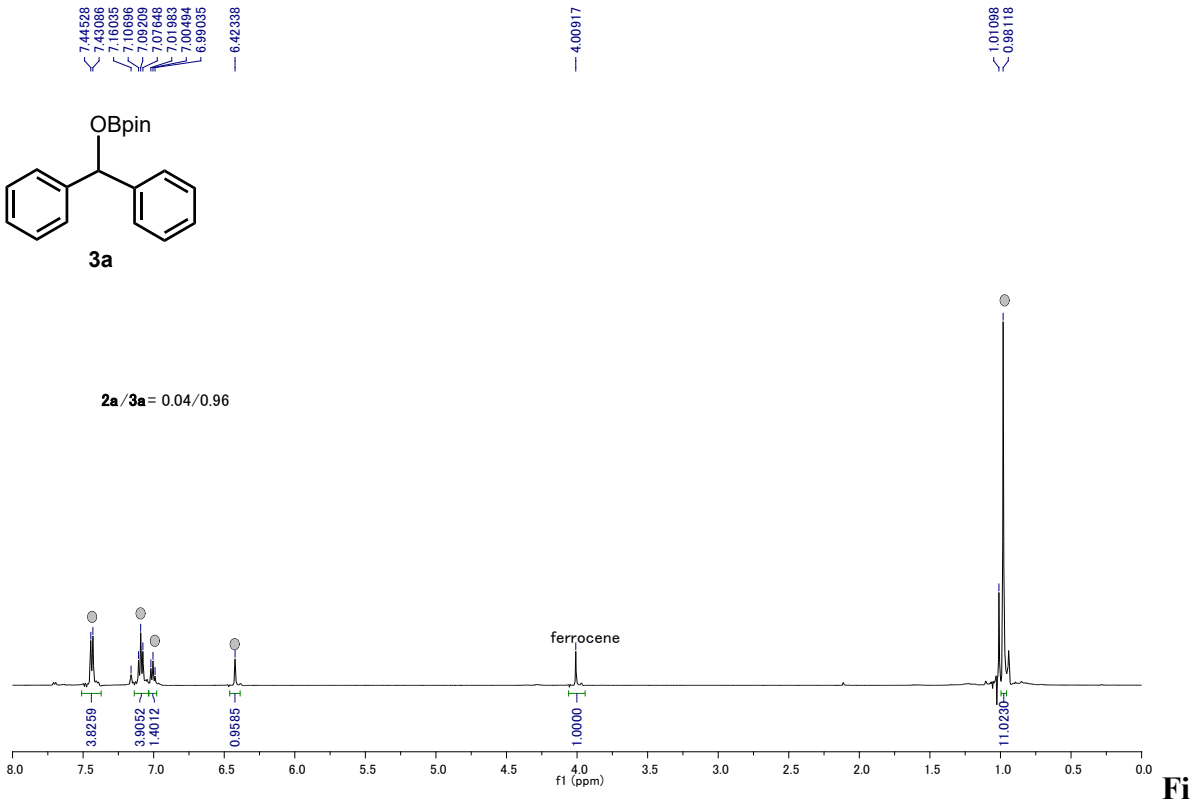


Figure S5. ^{1}H NMR spectra of **3a** (500 MHz, 25 °C, C_6D_6).

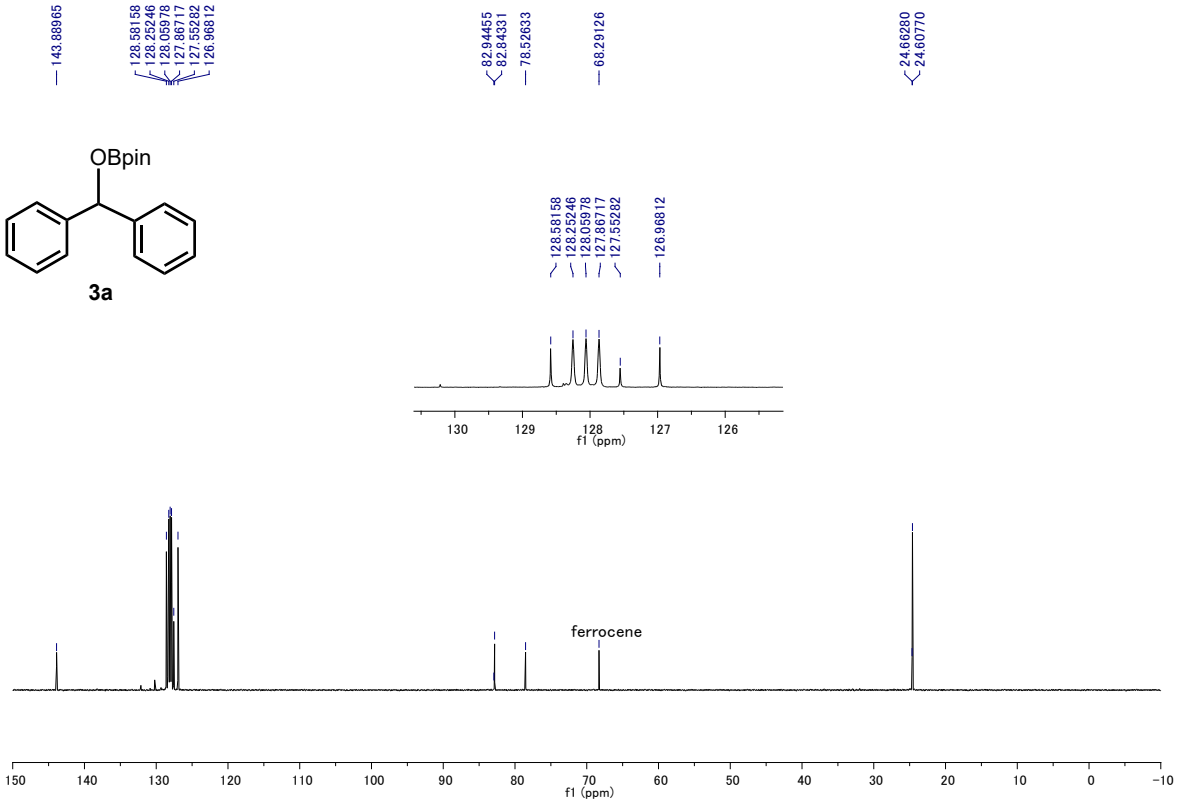


Figure S6. $^{13}C\{^{1}H\}$ NMR spectra of **3a** (126 MHz, 25 °C, C_6D_6).

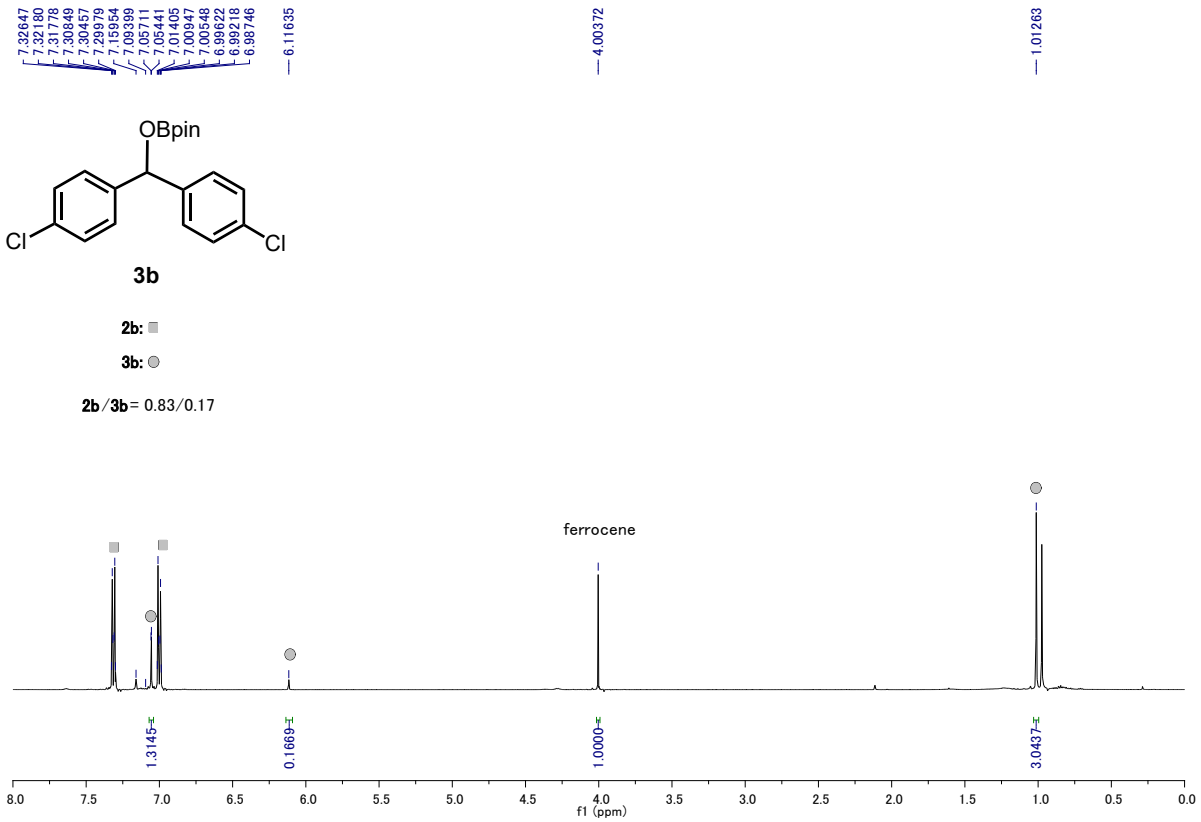


Figure S7. ^{1}H NMR spectra of **3b** (500 MHz, 25 °C, C_6D_6).

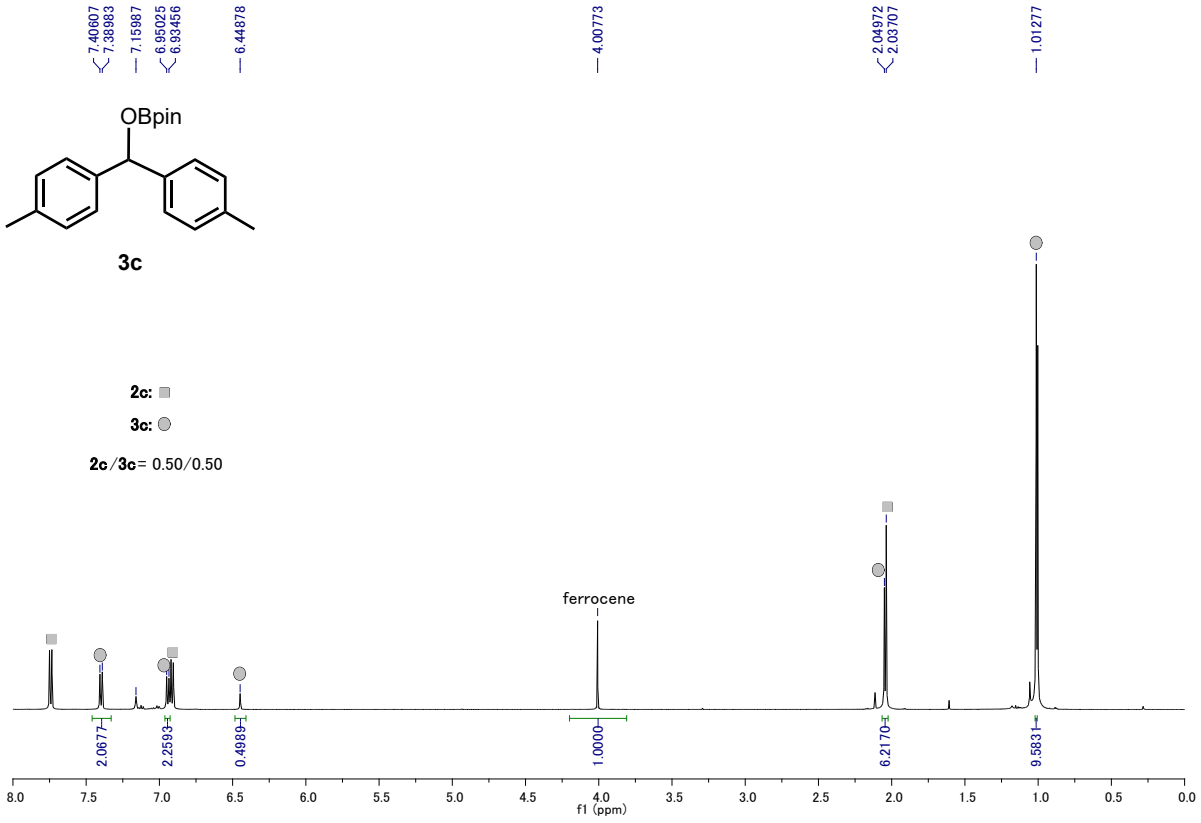


Figure S8. ^{1}H NMR spectra of **3c** (500 MHz, 25 °C, C_6D_6).

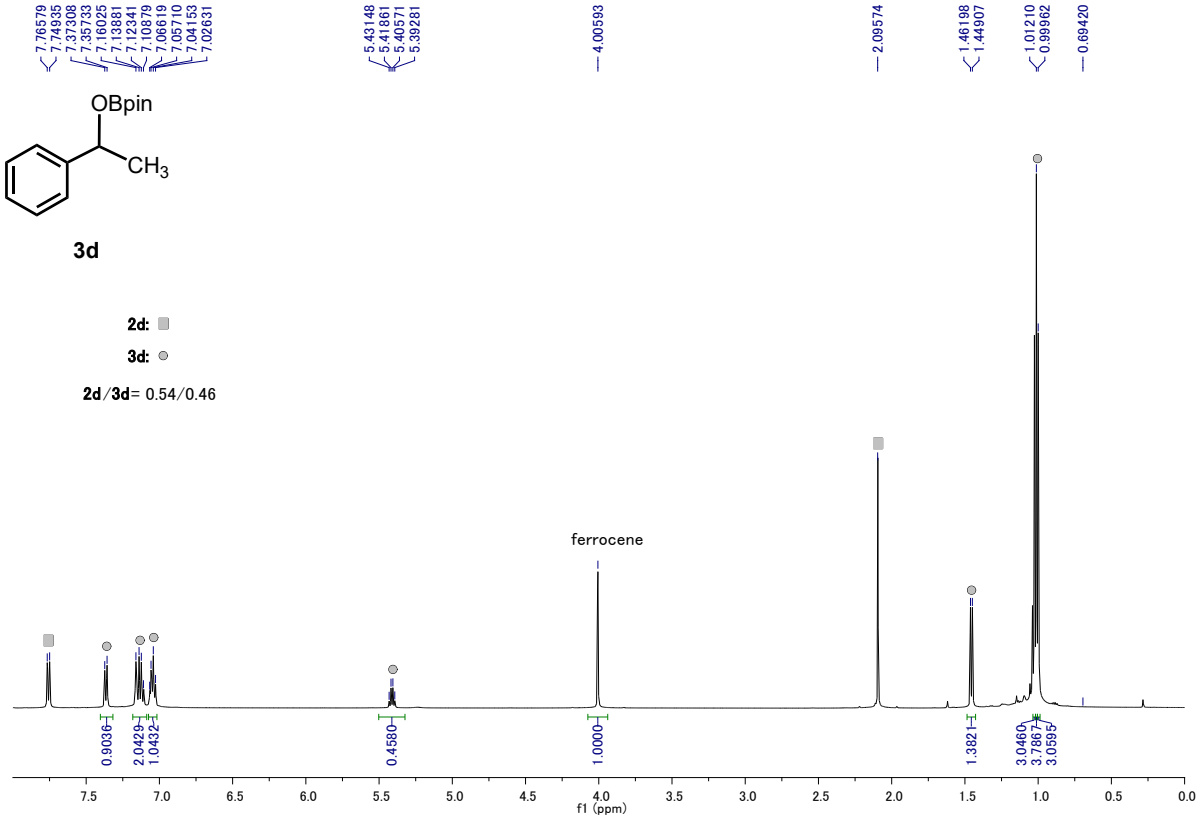


Figure S9. ^{1}H NMR spectra of **3d** (500 MHz, 25 °C, C_6D_6).

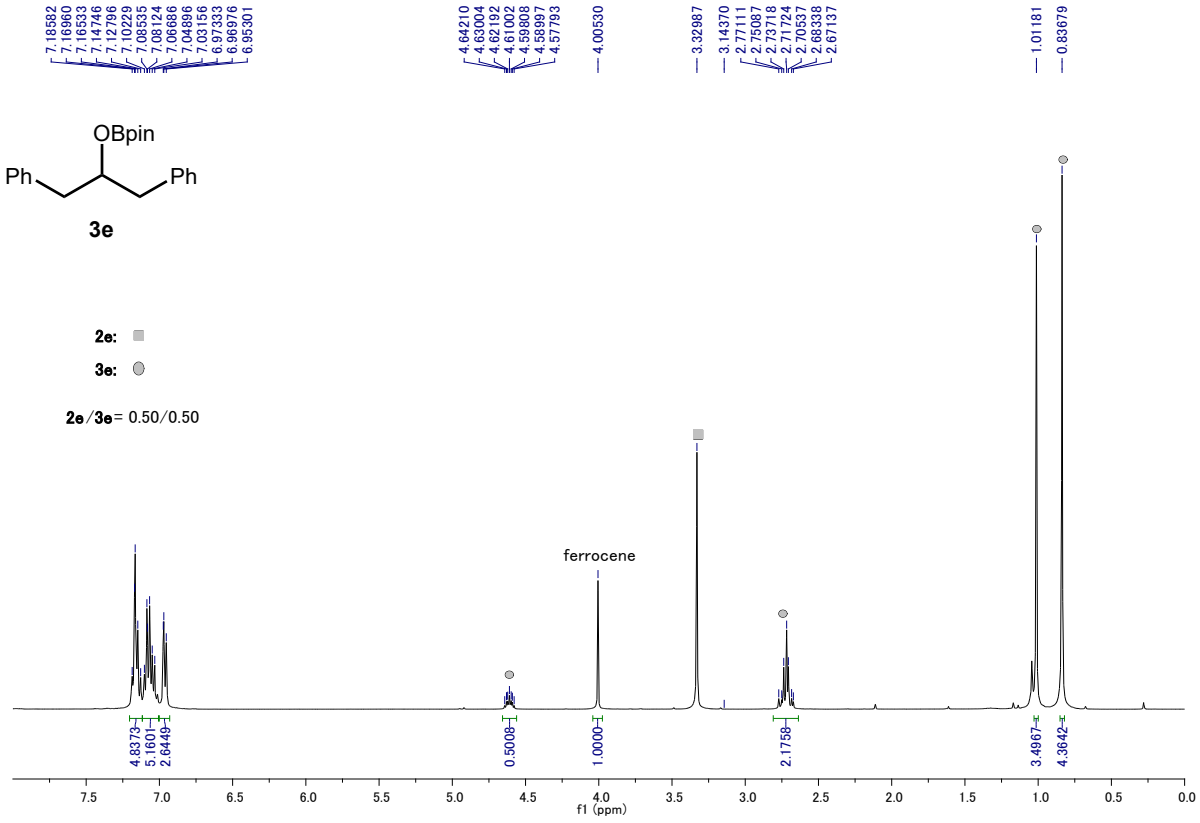


Figure S10. ^{1}H NMR spectra of **3e** (400 MHz, 25 °C, C_6D_6).

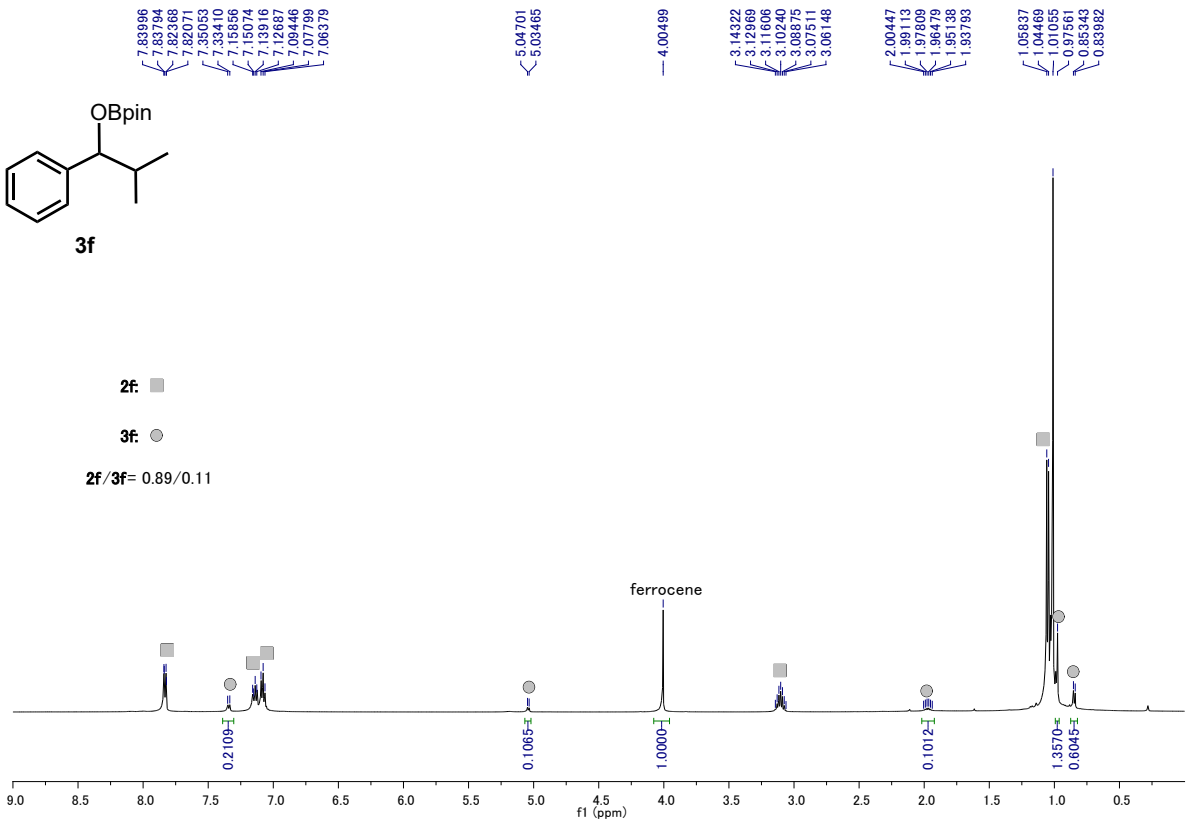


Figure S11. ^{1}H NMR spectra of **3f** (500 MHz, 25 °C, C_6D_6).

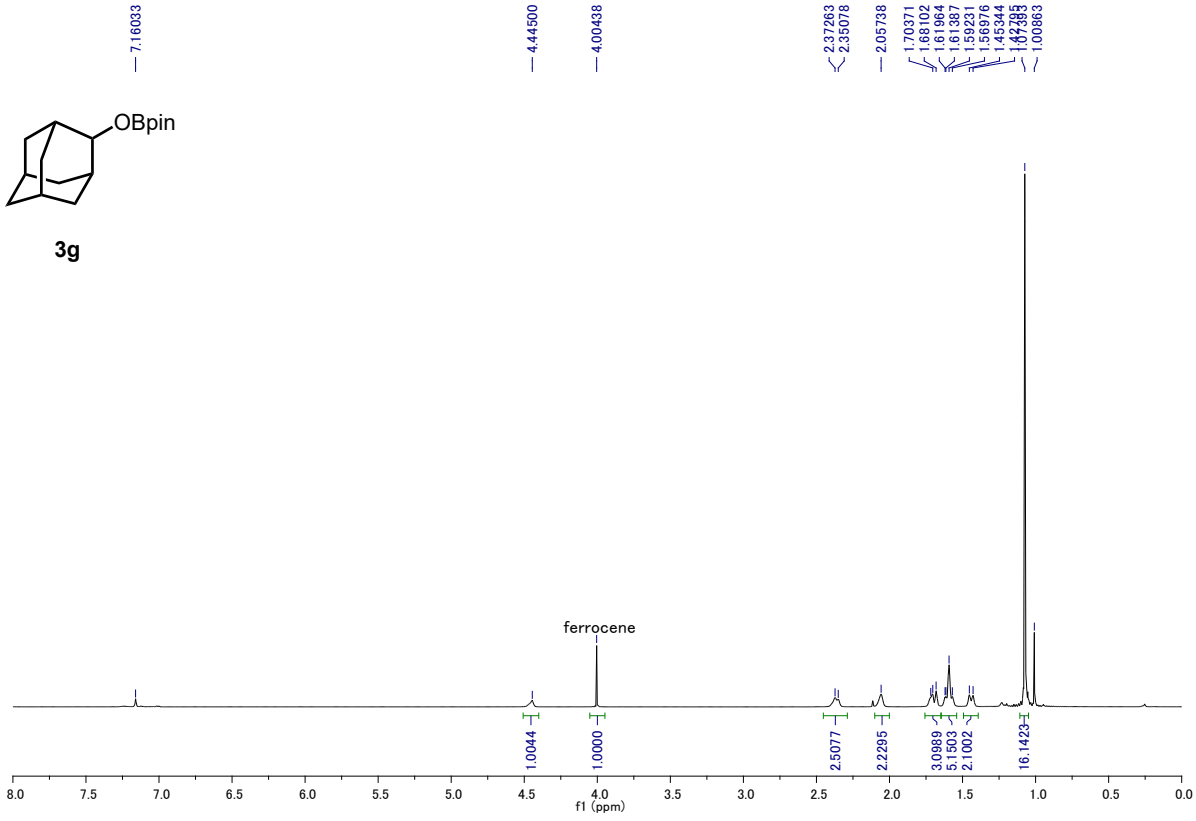


Figure S12. ^{1}H NMR spectra of **3g** (500 MHz, 25 °C, C_6D_6).

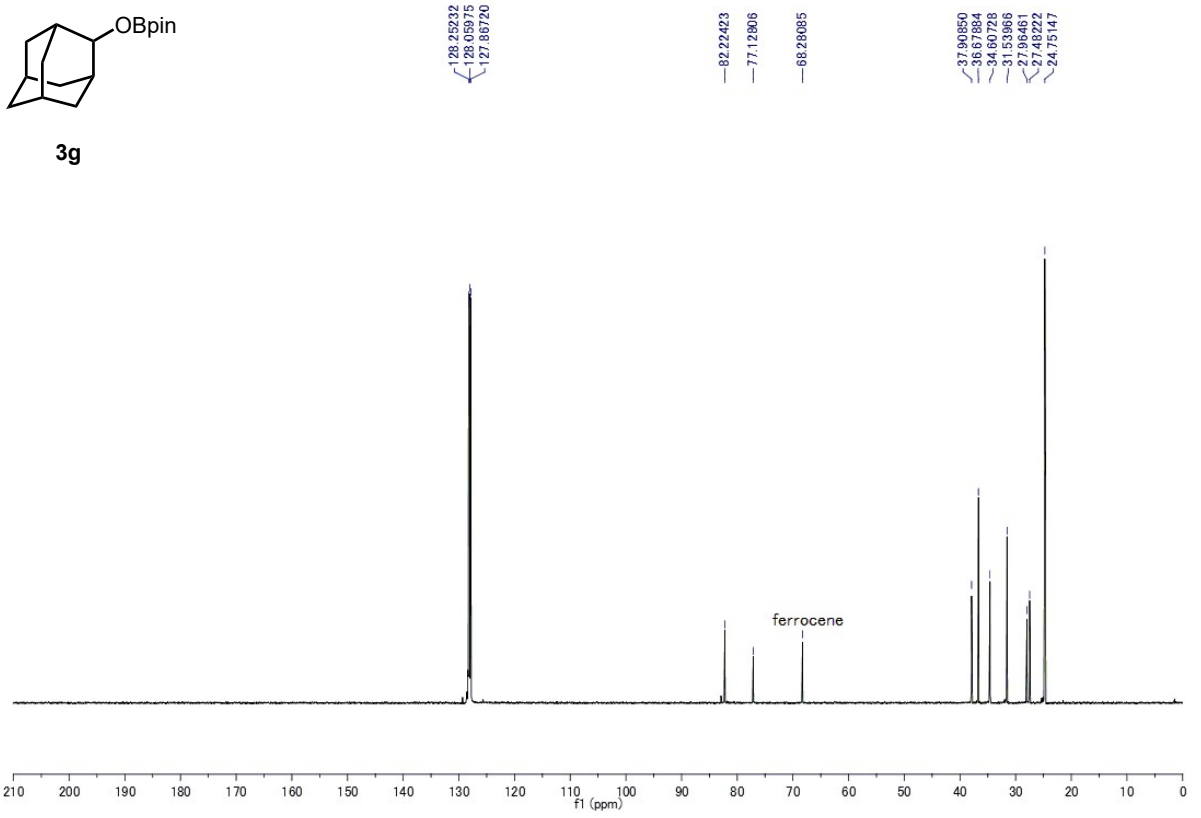


Figure S13. $^{13}C\{^{1}H\}$ NMR spectra of **3g** (126 MHz, 25 °C, C_6D_6).

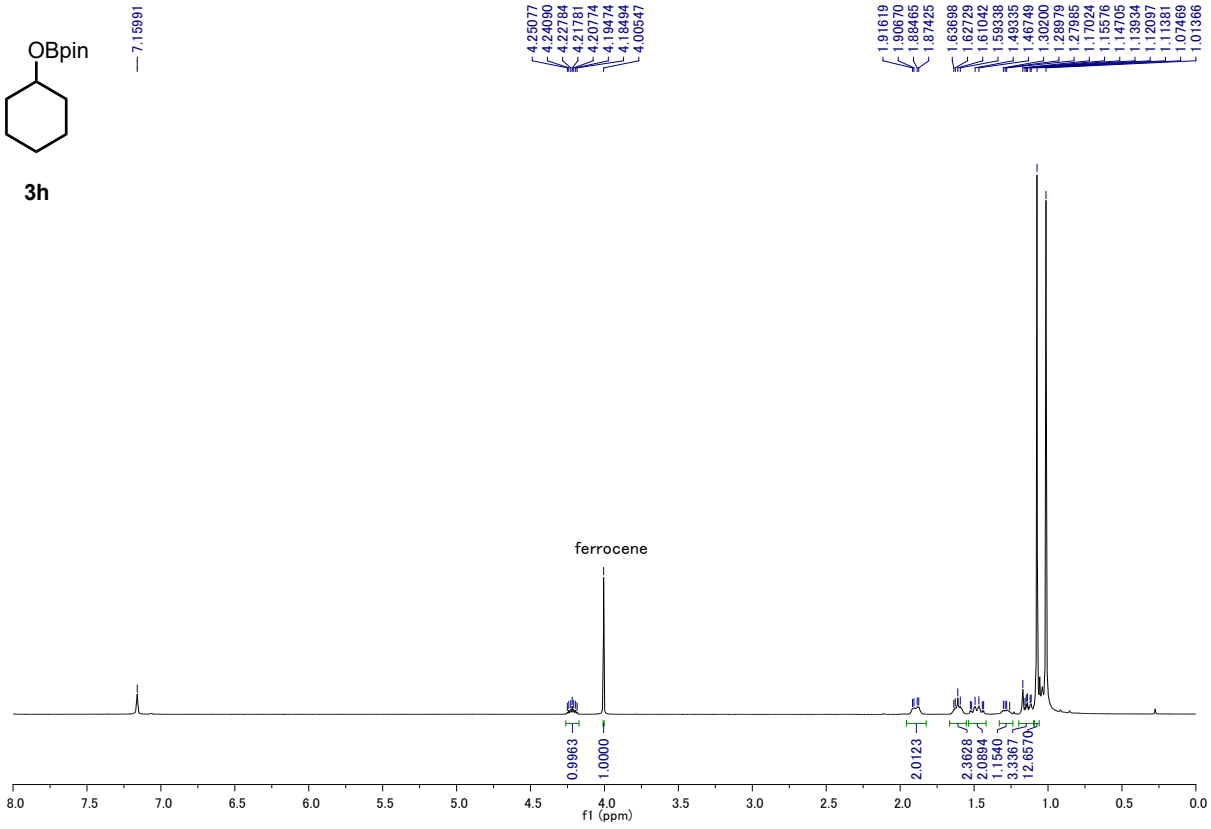


Figure S14. ^{1}H NMR spectra of **3h** (400 MHz, 25 °C, C_6D_6).

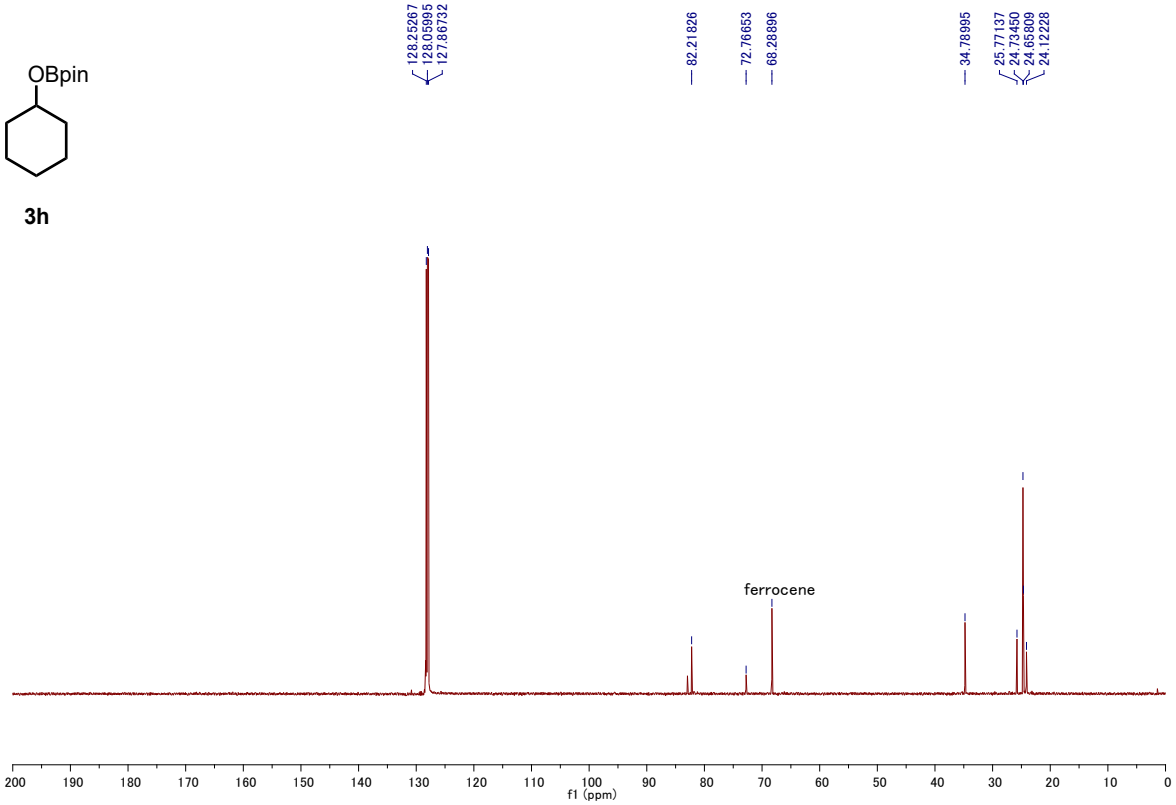


Figure S15. $^{13}C\{^{1}H\}$ NMR spectra of **3h** (126 MHz, 25 °C, C_6D_6).

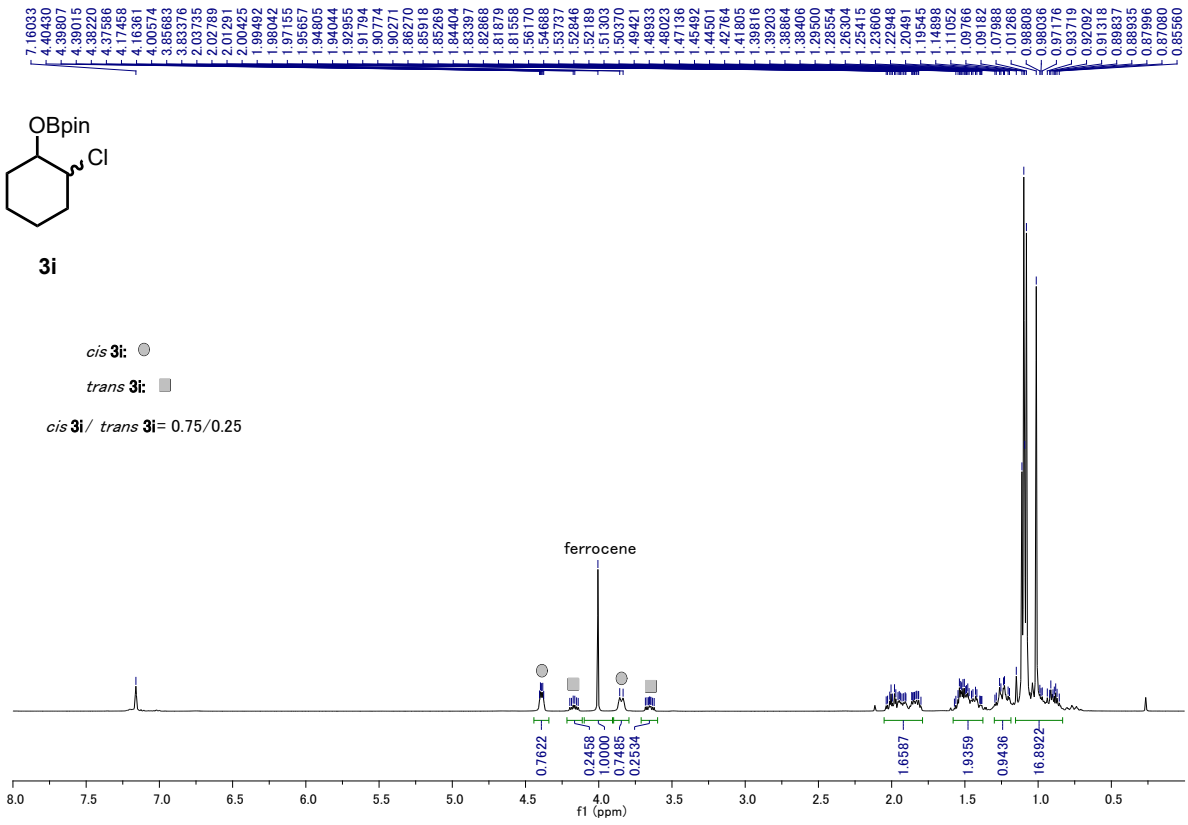


Figure S16. ^{1}H NMR spectra of **3i** (400 MHz, 25 °C, C_6D_6).

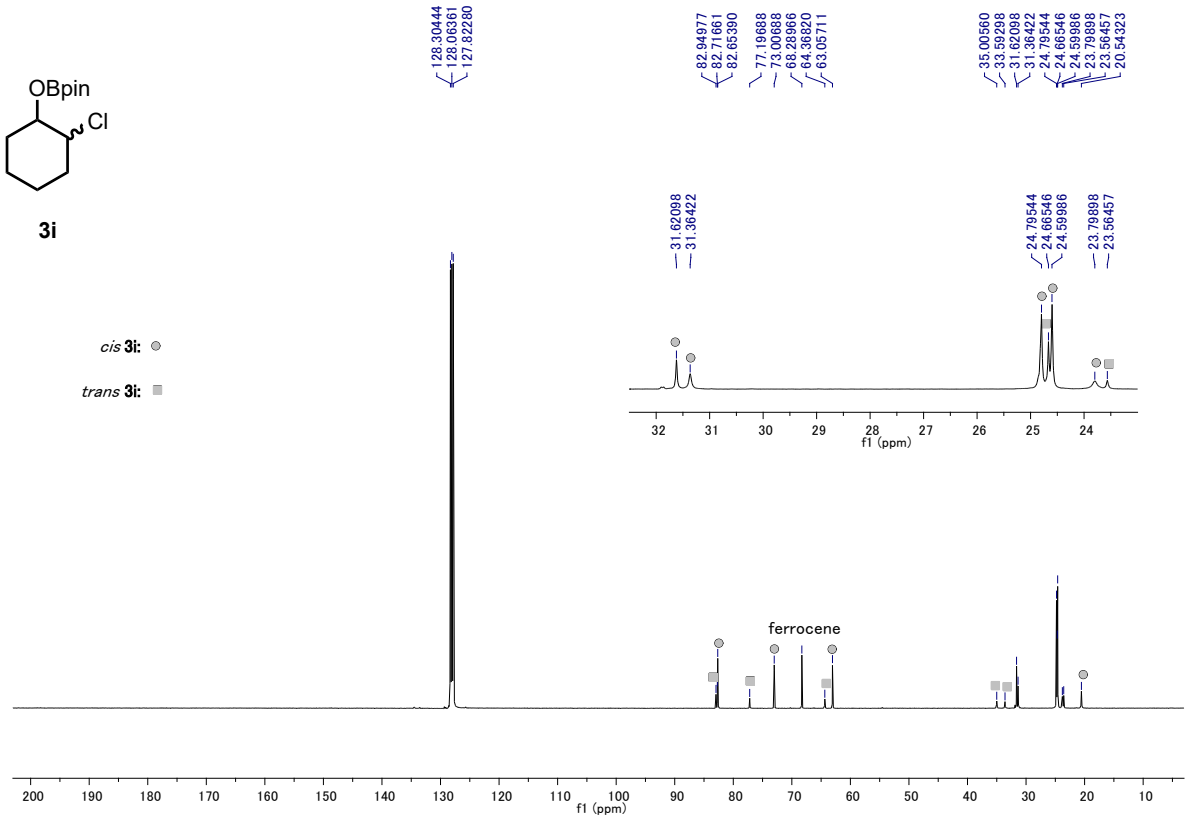


Figure S17. $^{13}C\{^{1}H\}$ NMR spectra of **3i** (100 MHz, 25 °C, C_6D_6).

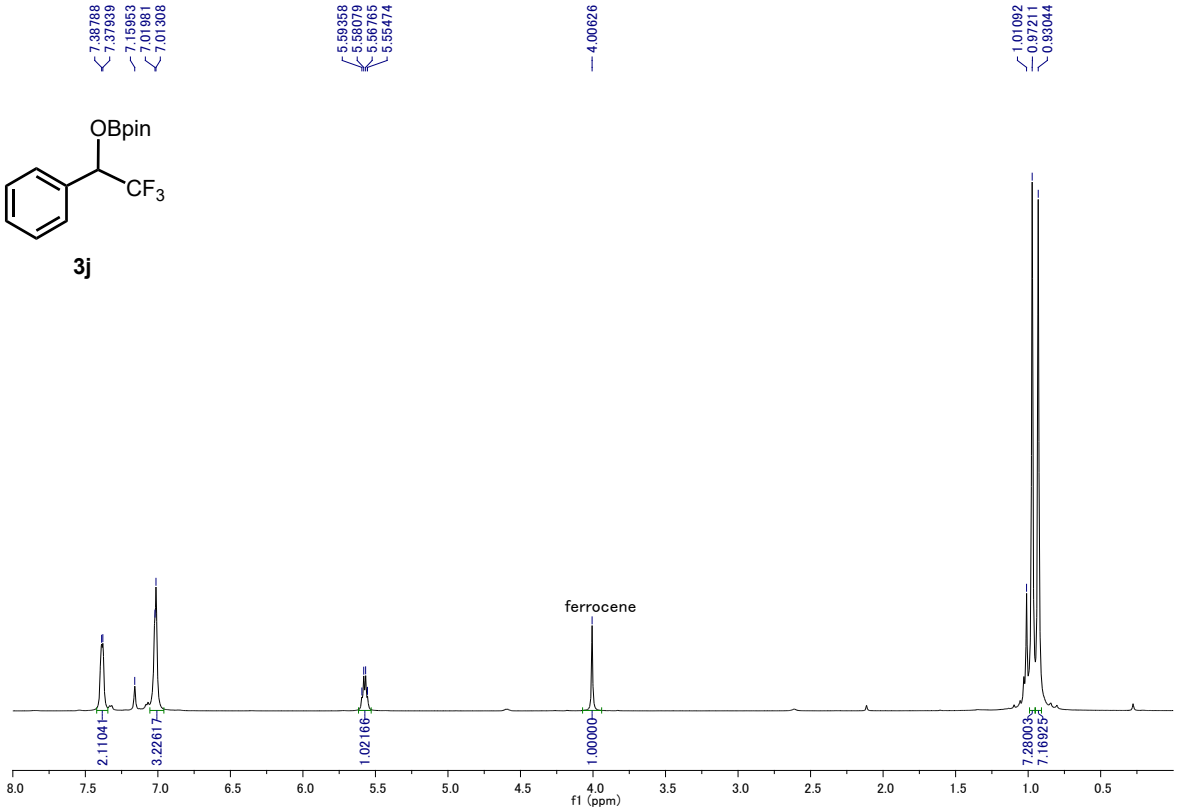


Figure S18. ^{1}H NMR spectra of **3j** (500 MHz, 25 °C, C_6D_6).

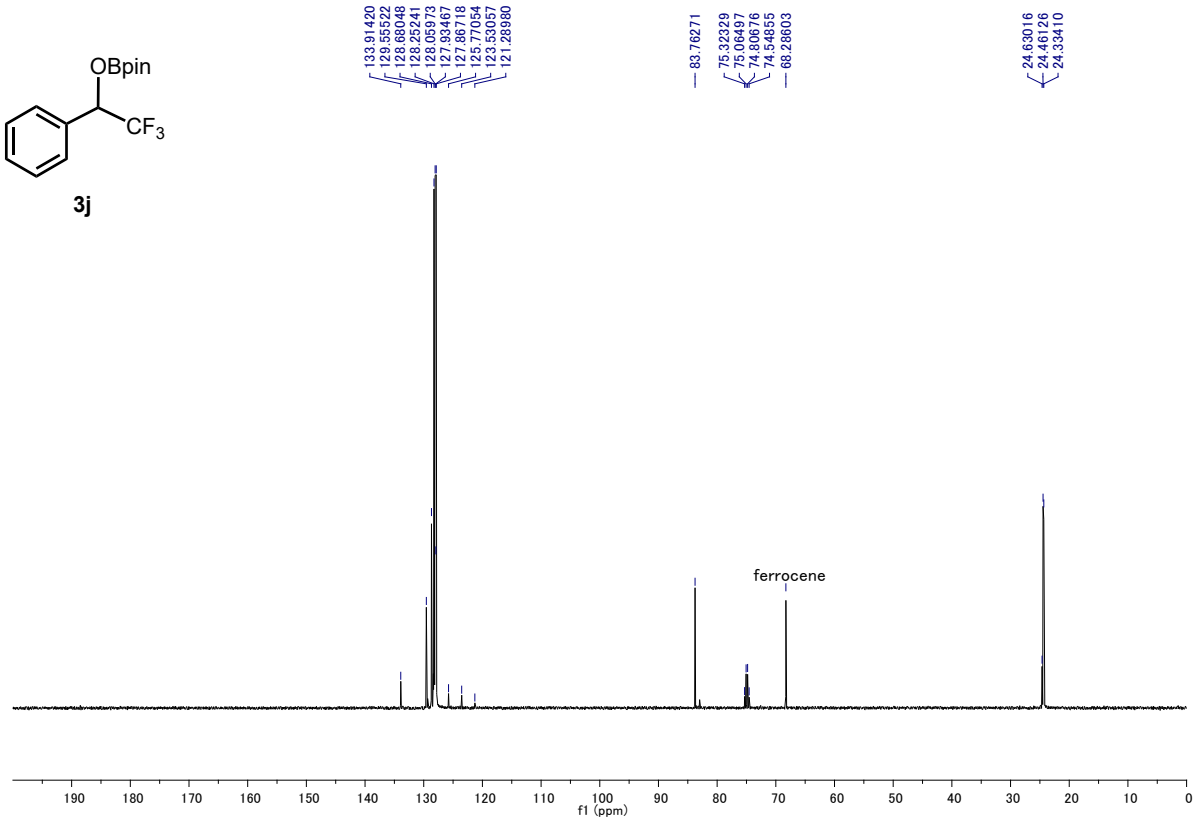


Figure S19. $^{13}C\{^{1}H\}$ NMR spectra of **3j** (126 MHz, 25 °C, C_6D_6).

(b) aldehydes

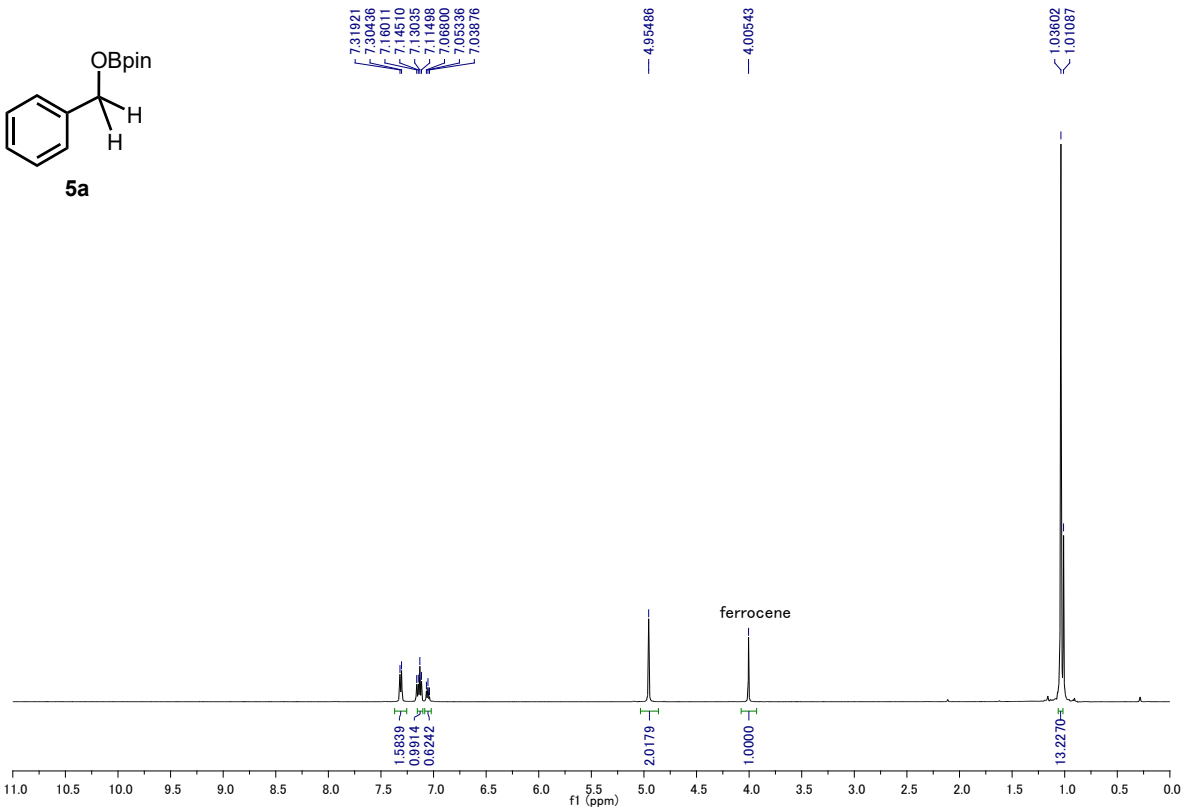


Figure S20. ^{1}H NMR spectra of **5a** (500 MHz, 25 °C, C_6D_6).

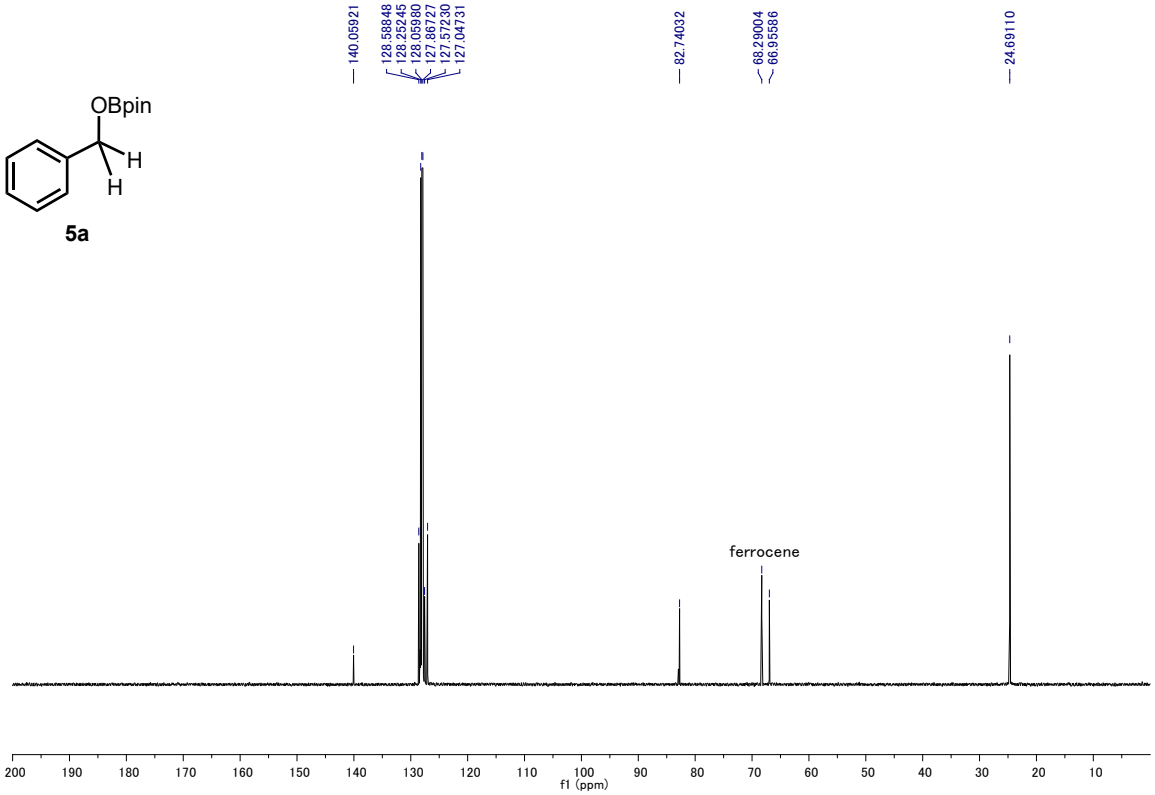


Figure S21. $^{13}C\{^{1}H\}$ NMR spectra of **5a** (126 MHz, 25 °C, C_6D_6).

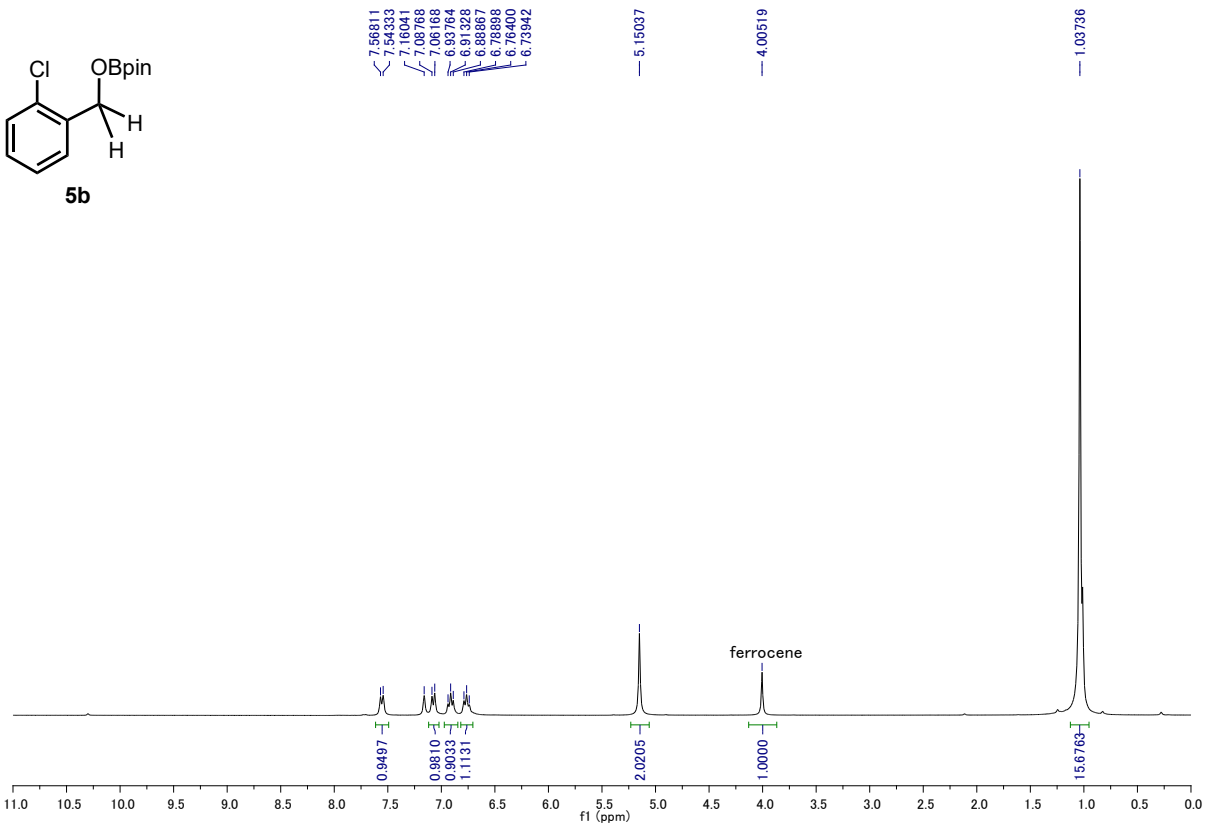


Figure S22. ^{1}H NMR spectra of **5b** (300 MHz, 25 °C, C_6D_6).

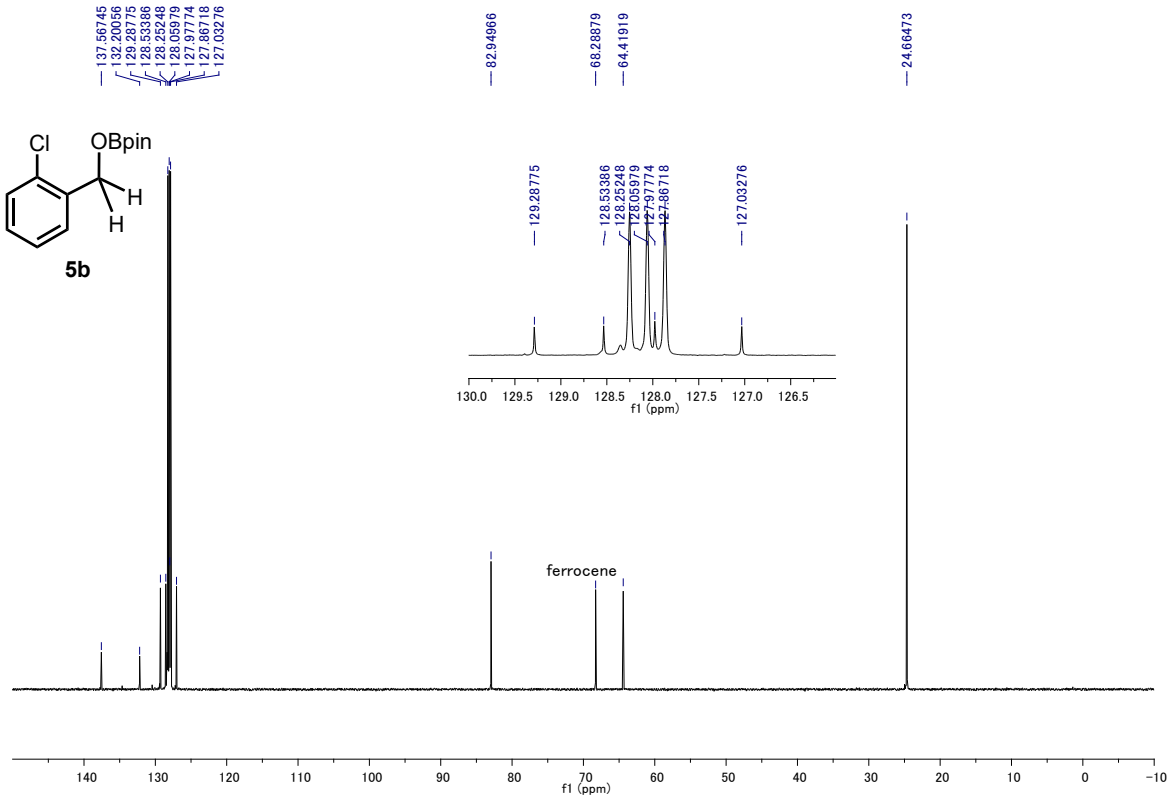


Figure S23. $^{13}C\{^{1}H\}$ NMR spectra of **5b** (126 MHz, 25 °C, C_6D_6).

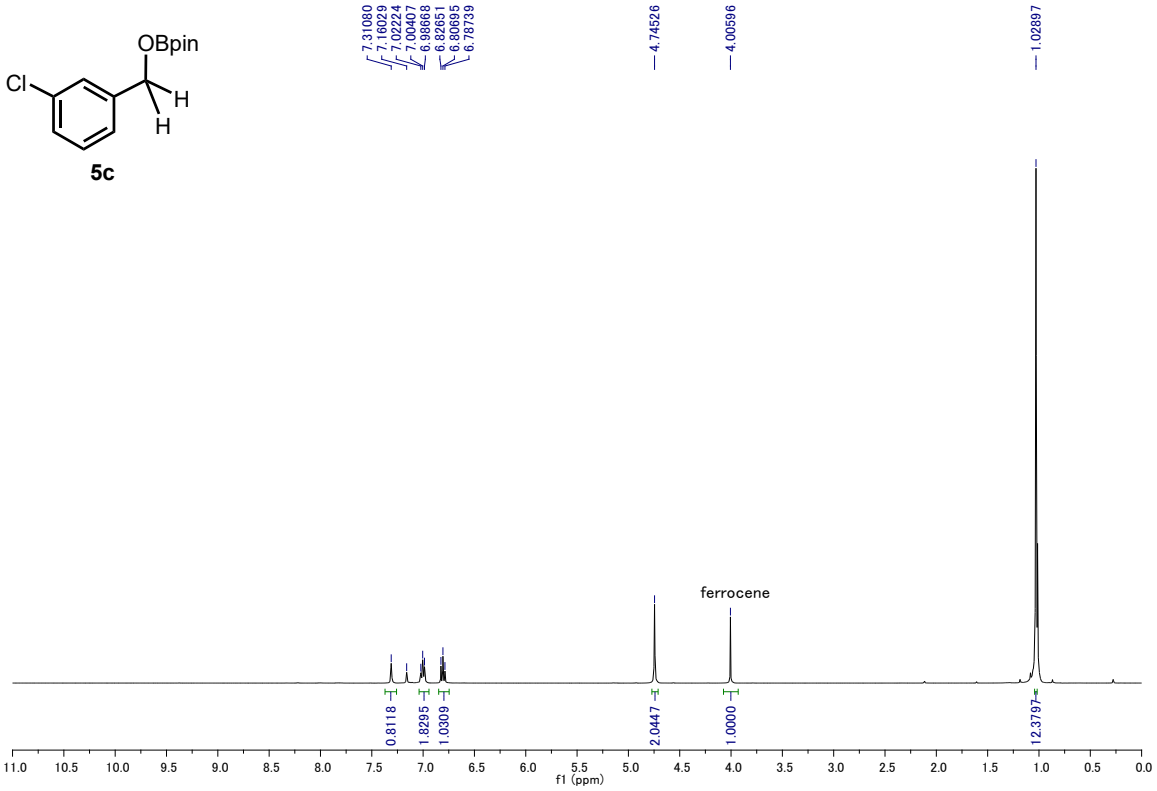


Figure S24. ^{1}H NMR spectra of **5c** (400 MHz, 25 °C, C_6D_6).

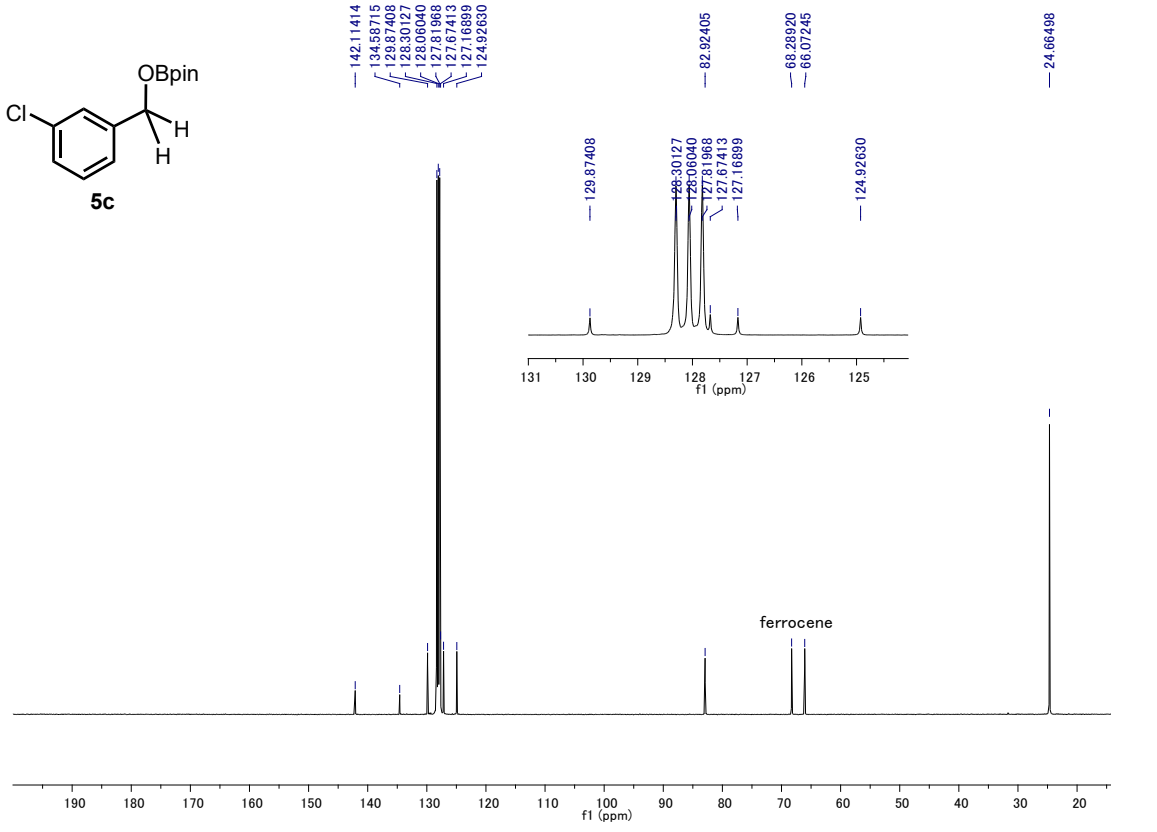


Figure S25. $^{13}C\{^{1}H\}$ NMR spectra of **5c** (101 MHz, 25 °C, C_6D_6).

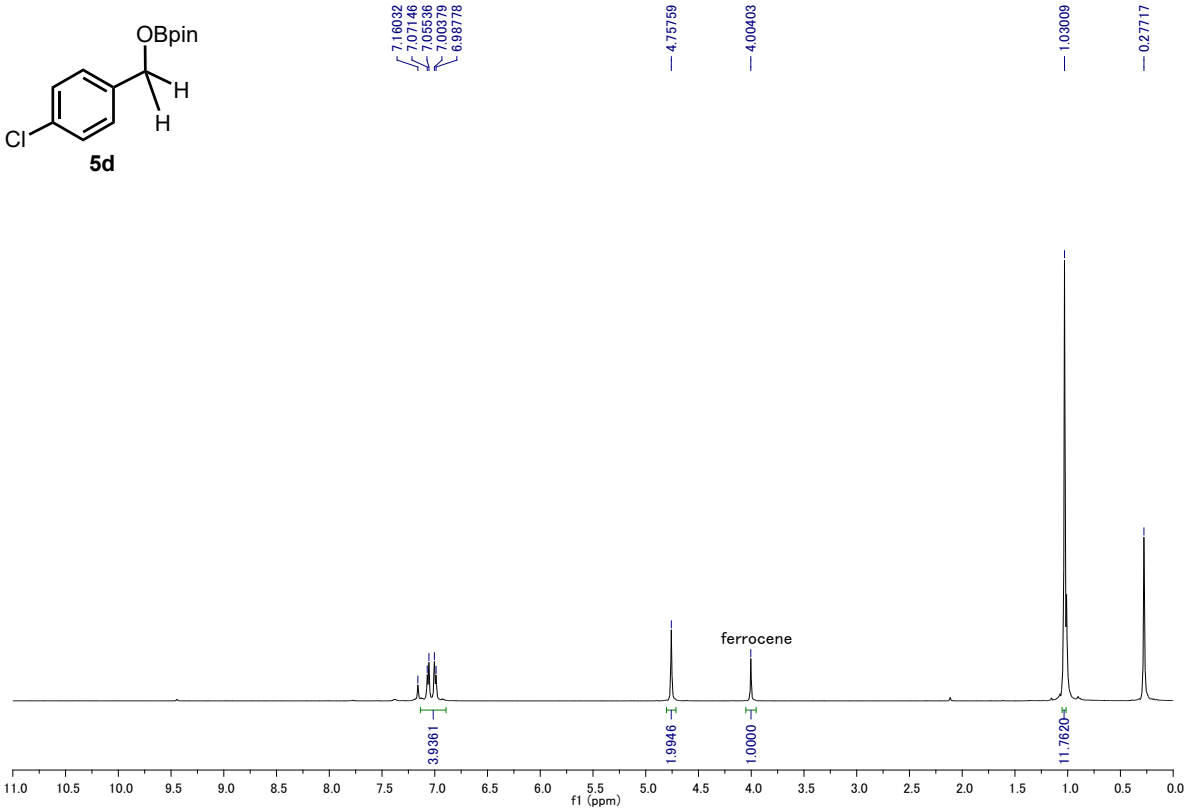


Figure S26. ^{1}H NMR spectra of **5d** (500 MHz, 25 °C, C_6D_6).

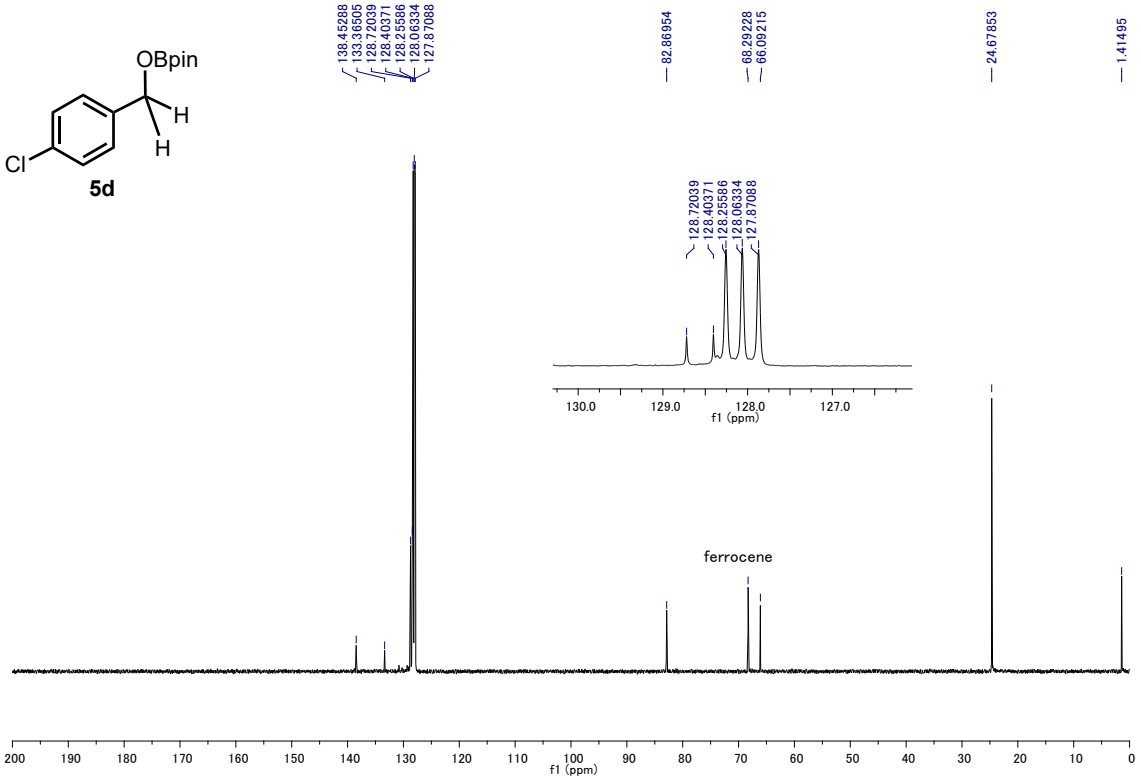


Figure S27. $^{13}C\{^{1}H\}$ NMR spectra of **5d** (126 MHz, 25 °C, C_6D_6).

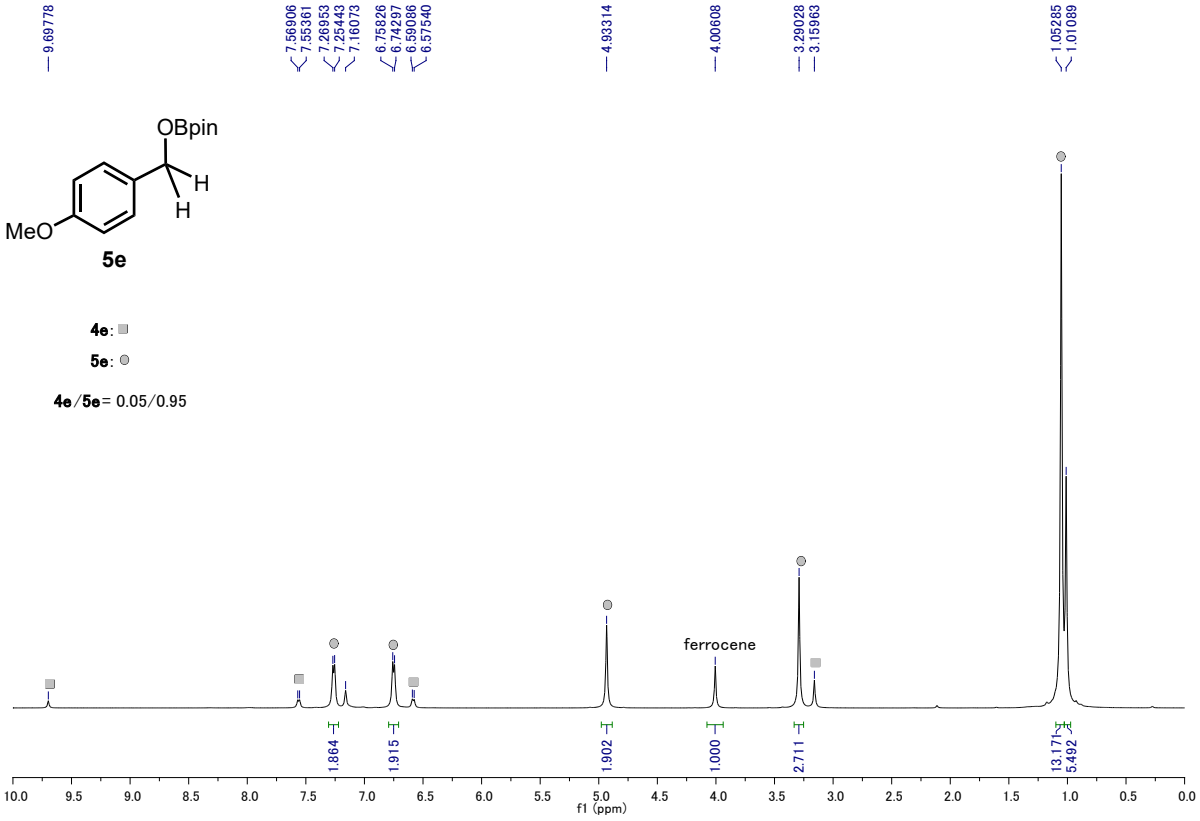


Figure S28. ^{1}H NMR spectra of **5e** (500 MHz, 25 °C, C_6D_6).

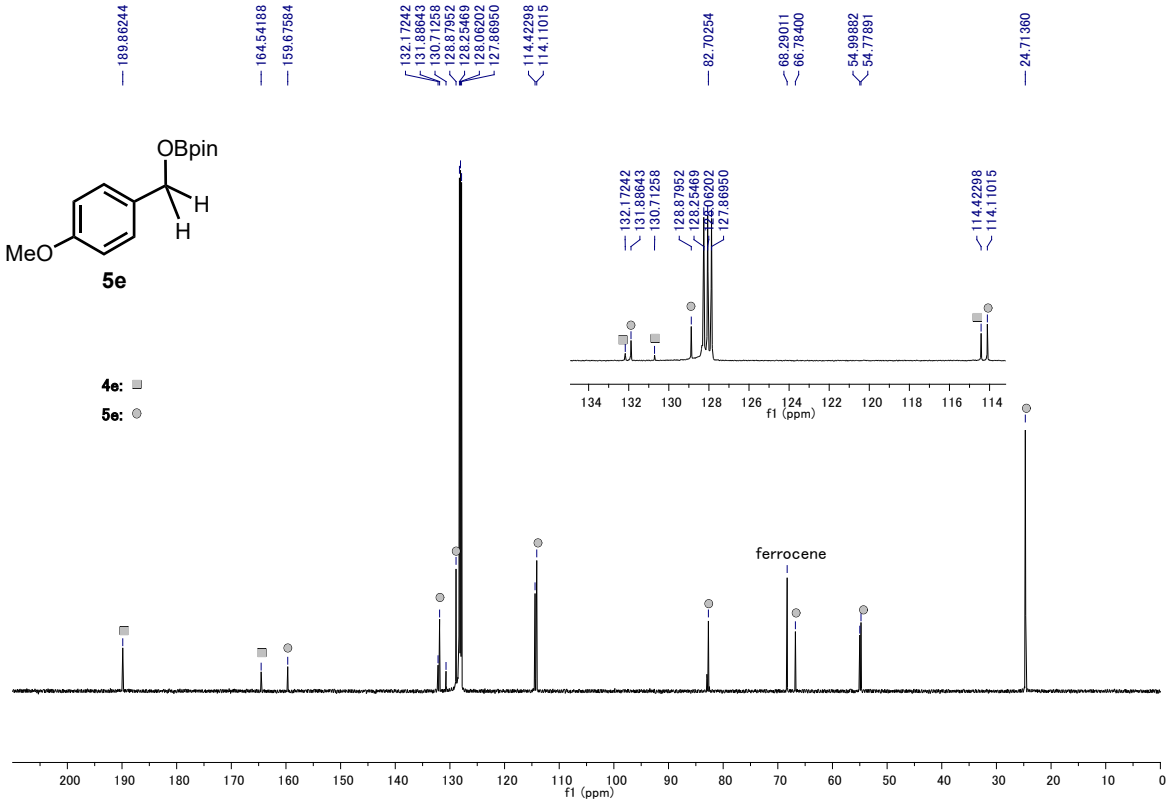


Figure S29. $^{13}C\{^{1}H\}$ NMR spectra of **5e** (126 MHz, 25 °C, C_6D_6).

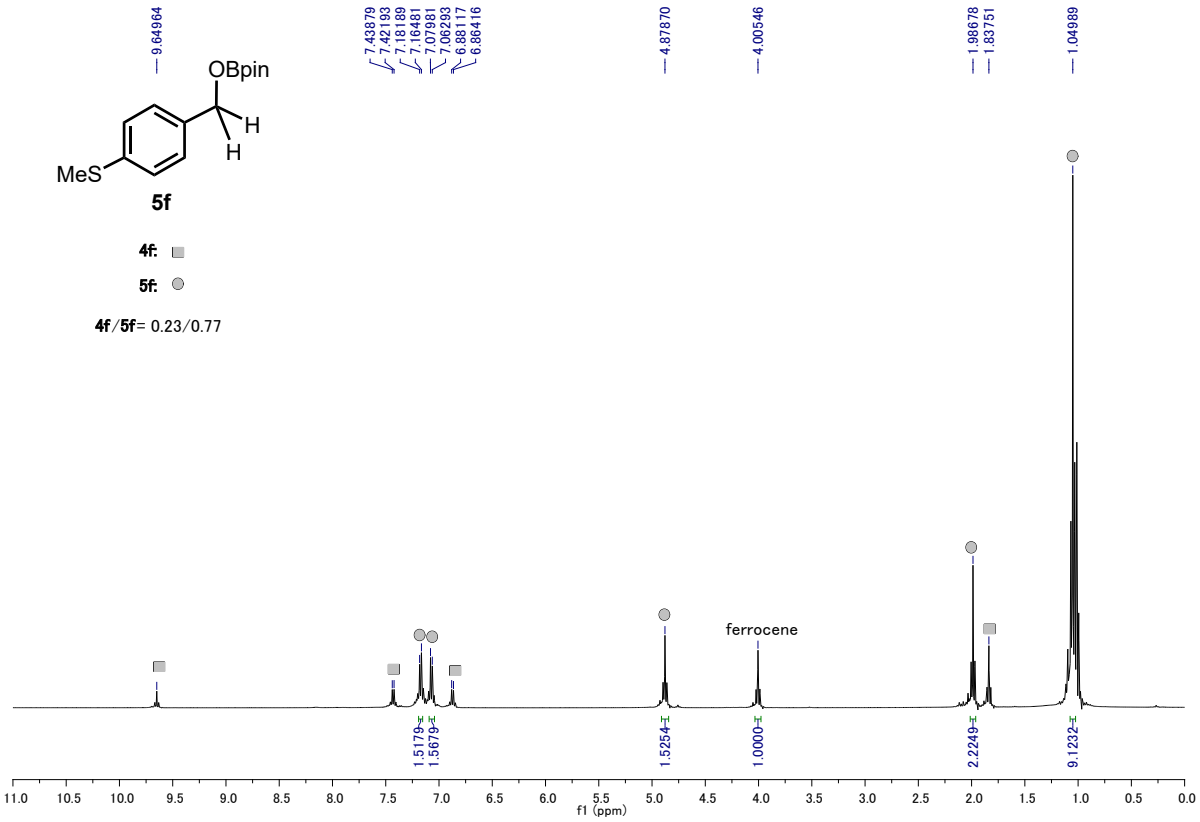


Figure S30. ^{1}H NMR spectra of **5f** (500 MHz, 25 °C, C_6D_6).

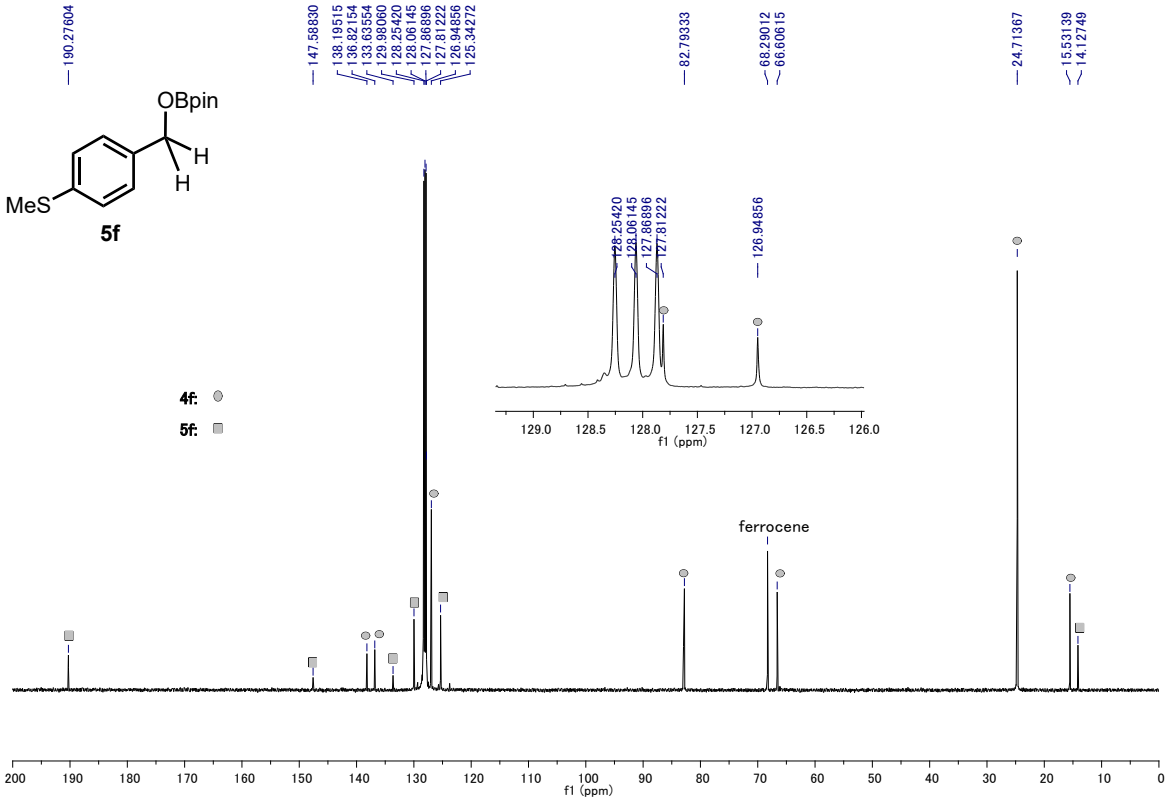


Figure S31. $^{13}C\{^{1}H\}$ NMR spectra of **5f** (126 MHz, 25 °C, C_6D_6).

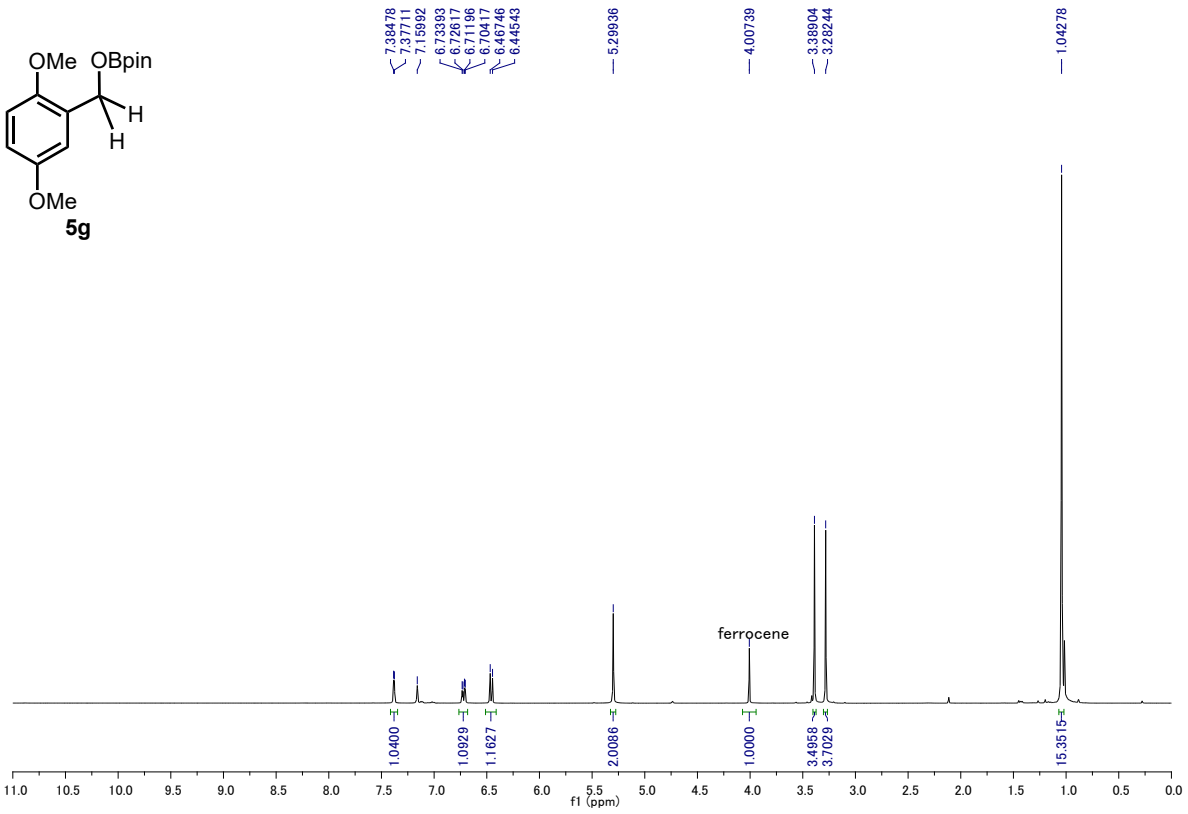


Figure S32. ^{1}H NMR spectra of **5g** (400 MHz, 25 °C, C_6D_6).

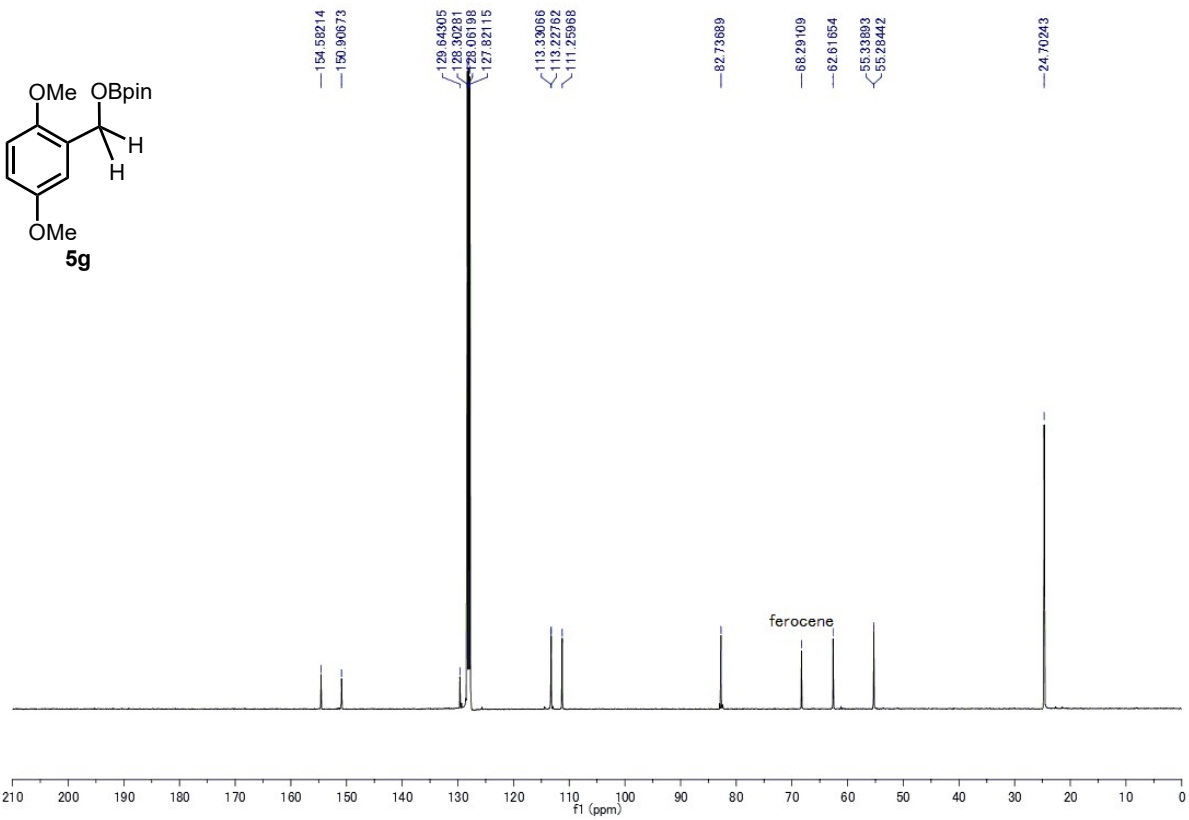


Figure S33. $^{13}C\{^{1}H\}$ NMR spectra of **5g** (101 MHz, 25 °C, C_6D_6).

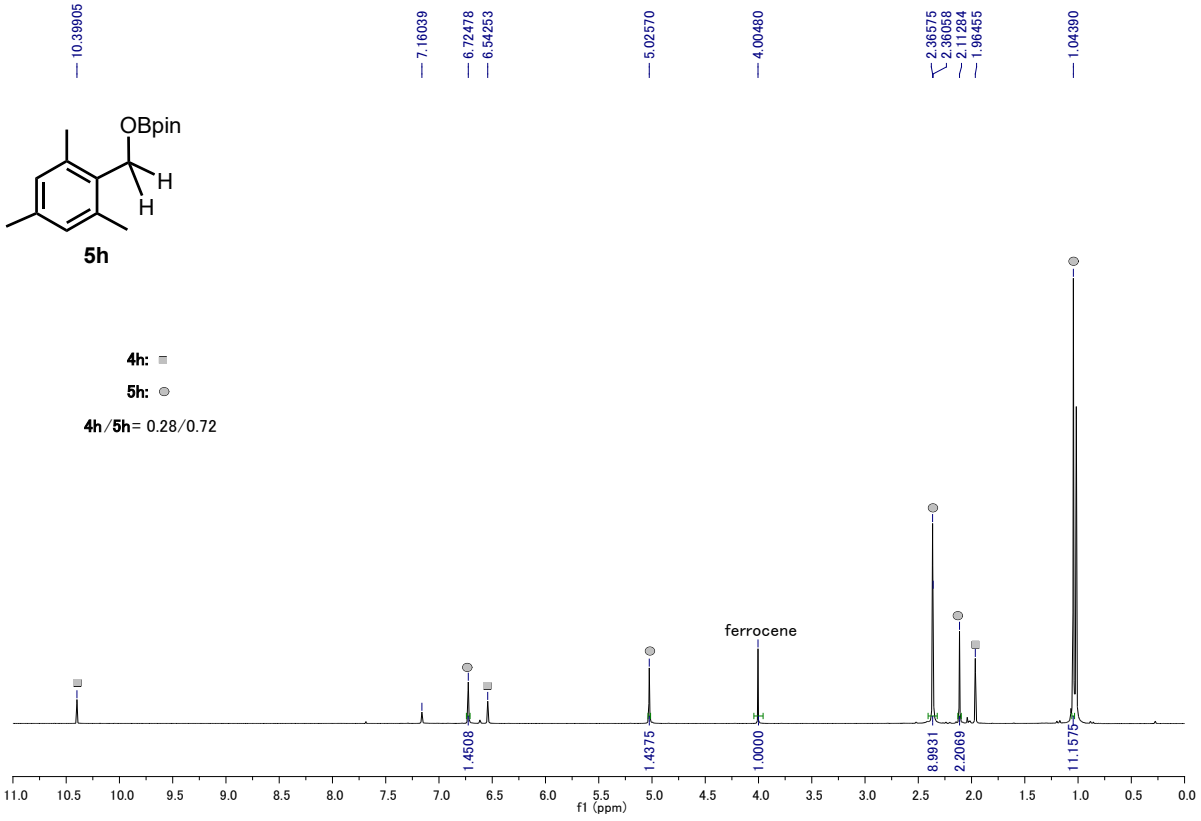


Figure S34. ^{1}H NMR spectra of **5h** (400 MHz, 25 °C, C_6D_6).

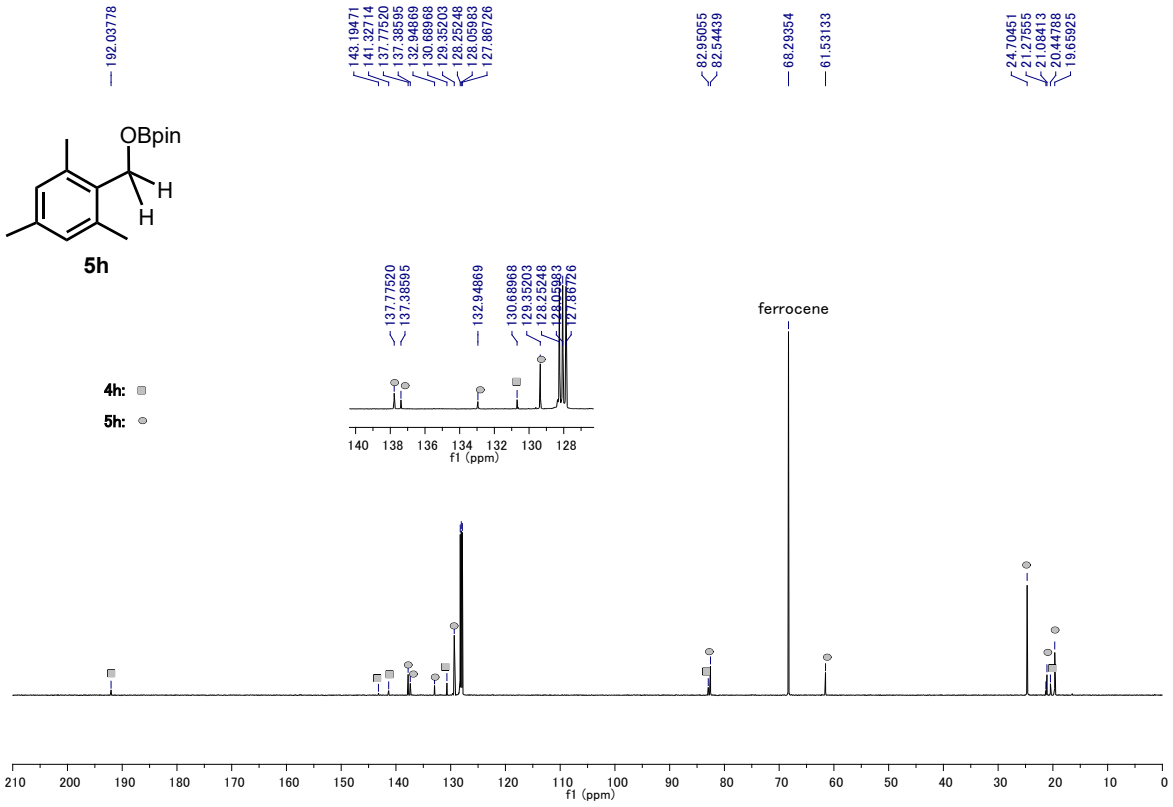


Figure S35. $^{13}C\{^{1}H\}$ NMR spectra of **5h** (126 MHz, 25 °C, C_6D_6).

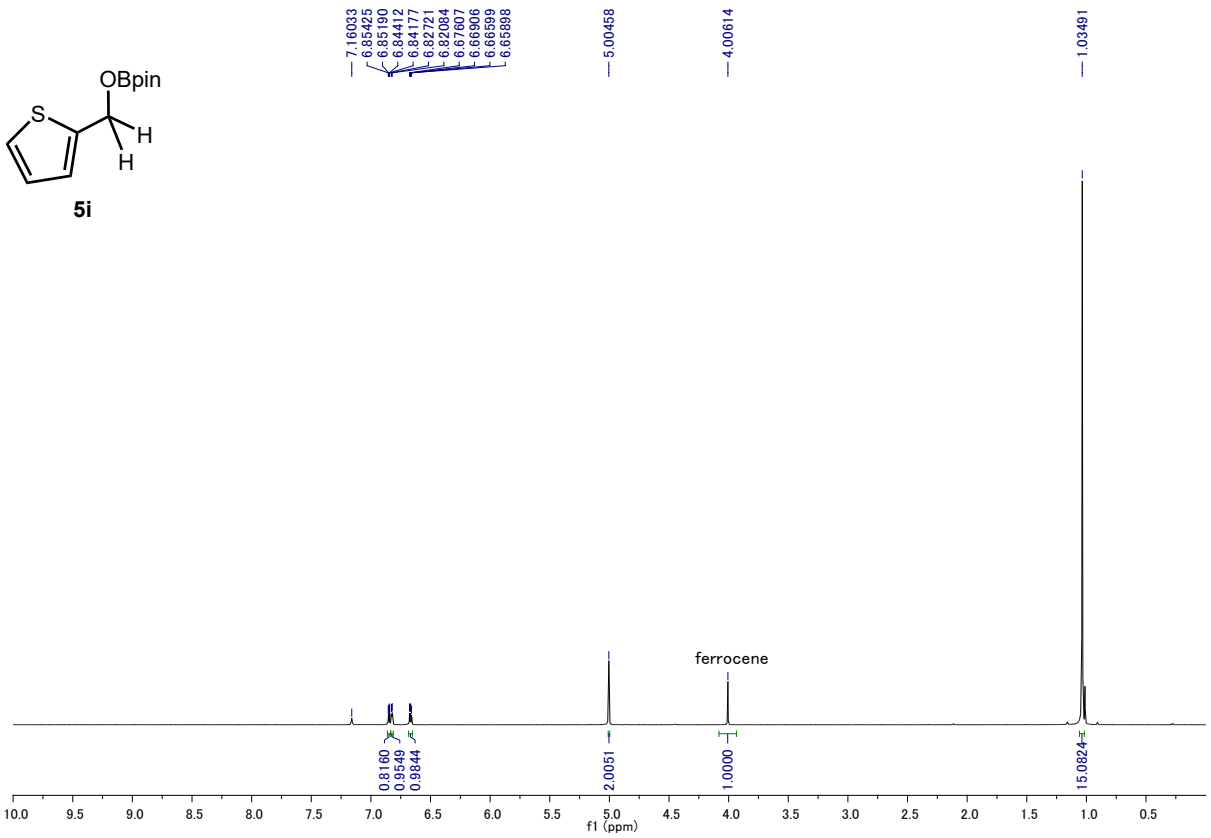


Figure S36. ^{1}H NMR spectra of **5i** (500 MHz, 25 °C, C_6D_6).

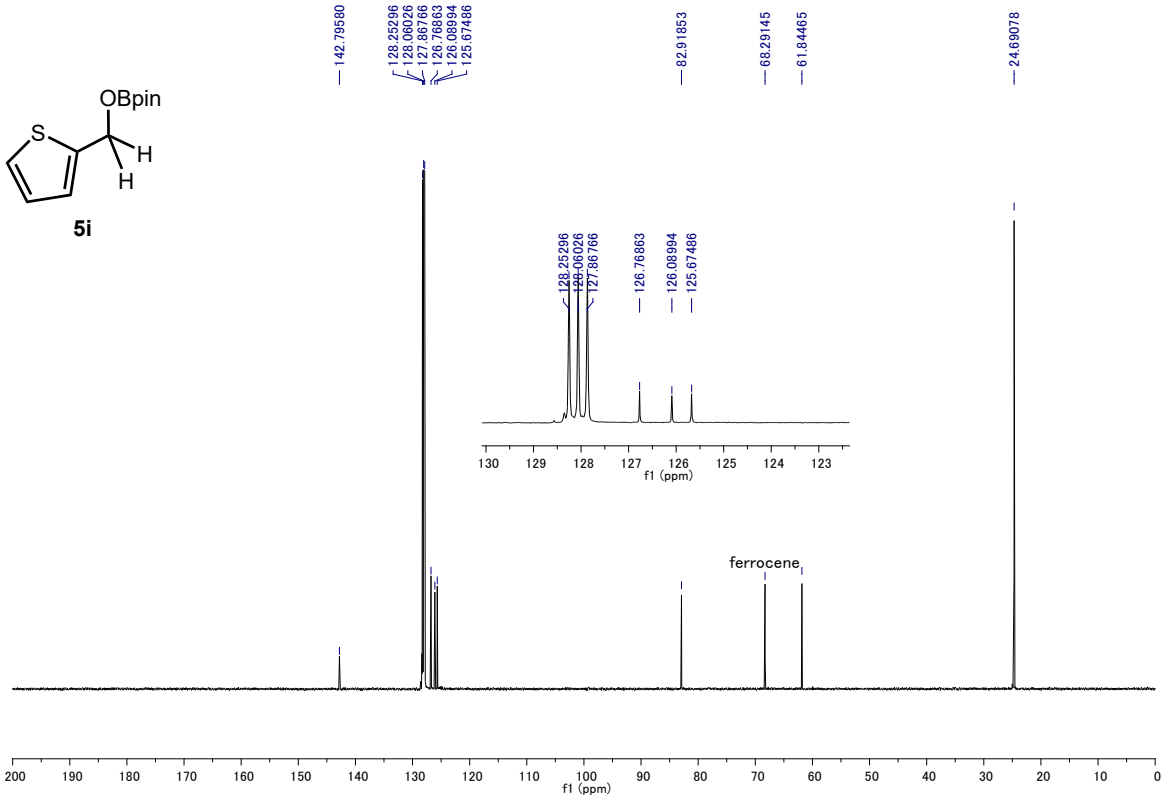


Figure S37. $^{13}C\{^{1}H\}$ NMR spectra of **5i** (126 MHz, 25 °C, C_6D_6)

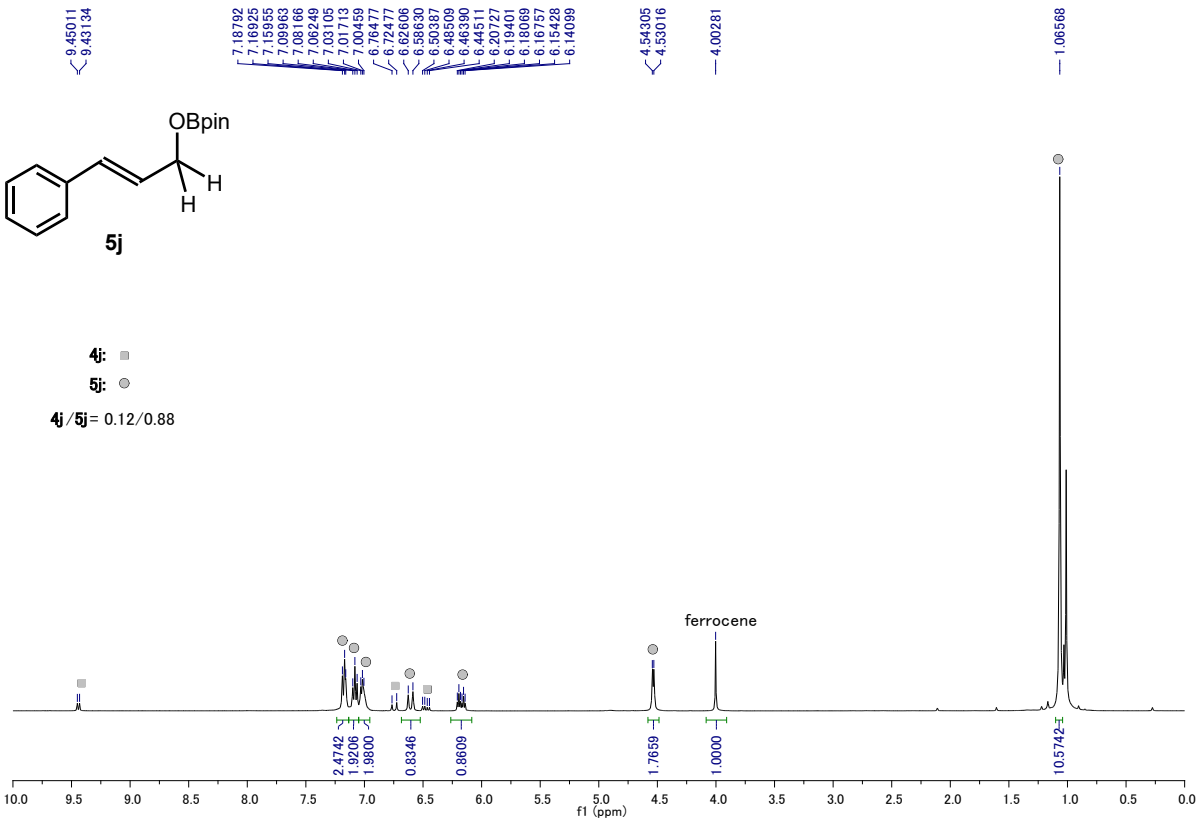


Figure S38. ^{1}H NMR spectra of **5j** (400 MHz, 25 °C, C_6D_6).

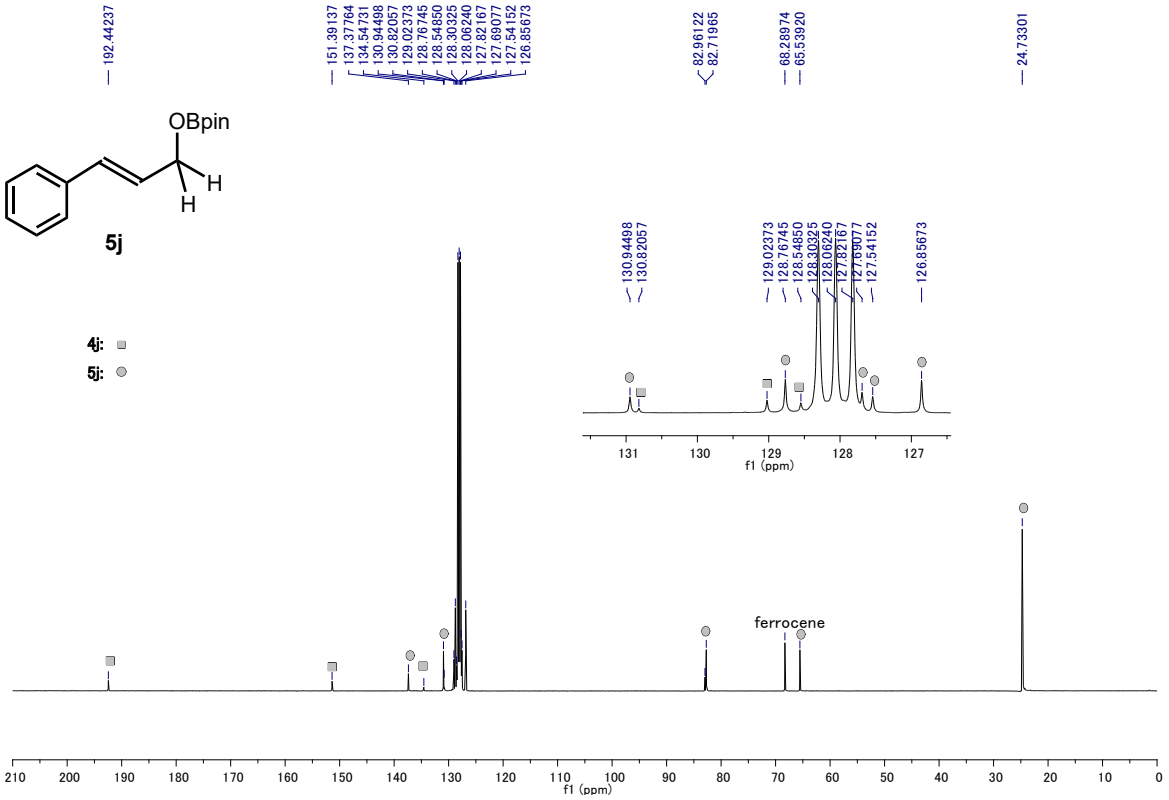


Figure S39. $^{13}C\{^{1}H\}$ NMR spectra of **5j** (101 MHz, 25 °C, C_6D_6).

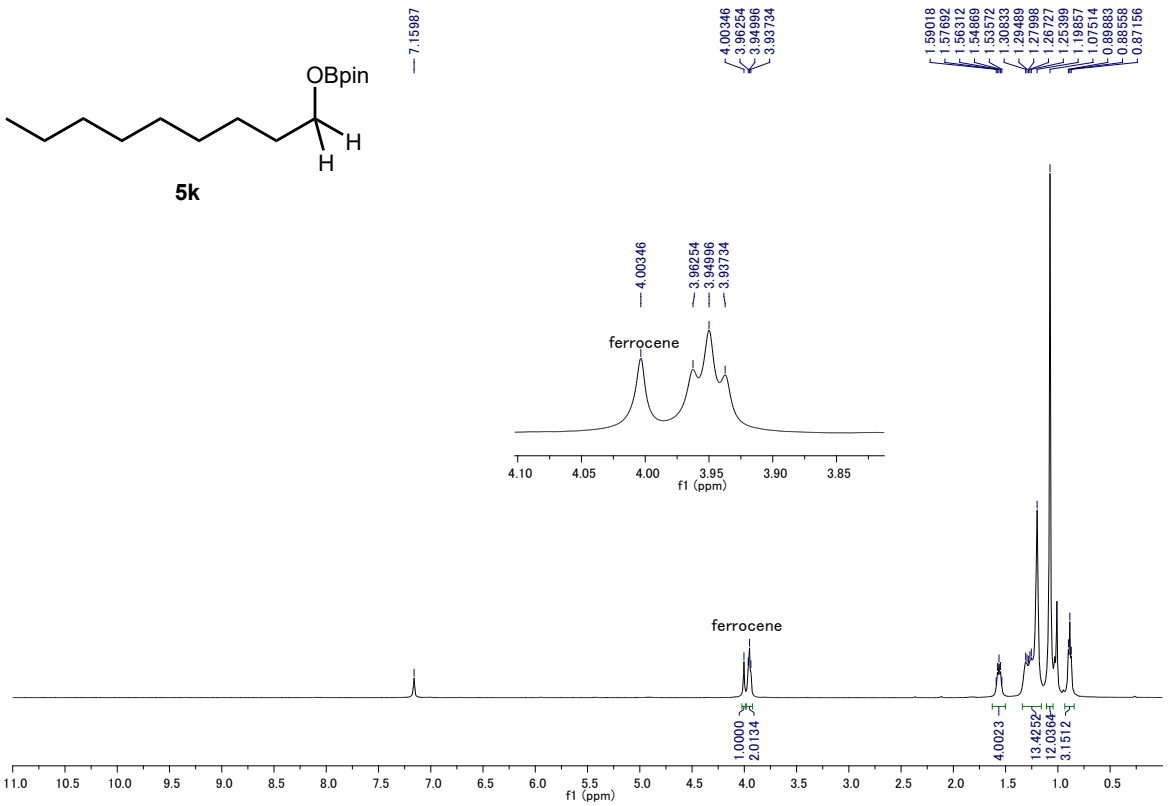


Figure S40. ^{1}H NMR spectra of **5k** (500 MHz, 25 °C, C_6D_6).

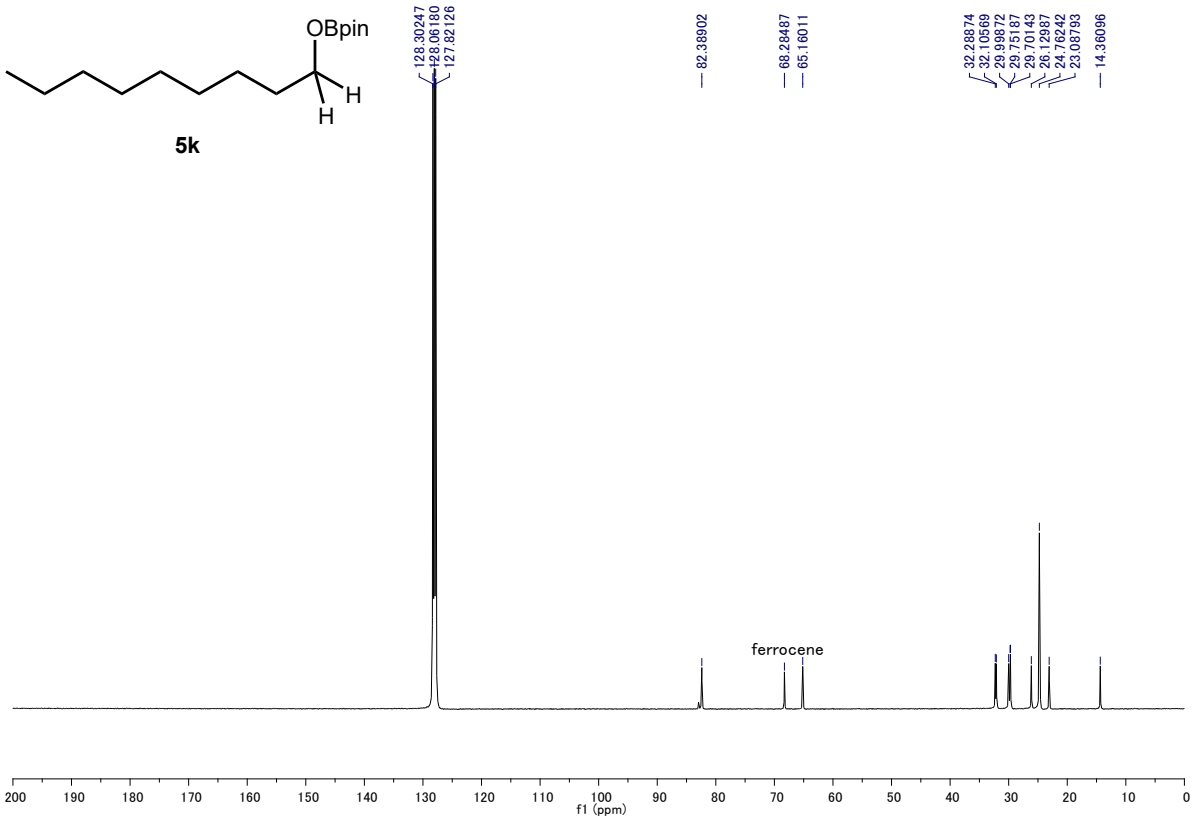


Figure S41. $^{13}C\{^{1}H\}$ NMR spectra of **5k** (101 MHz, 25 °C, C_6D_6).

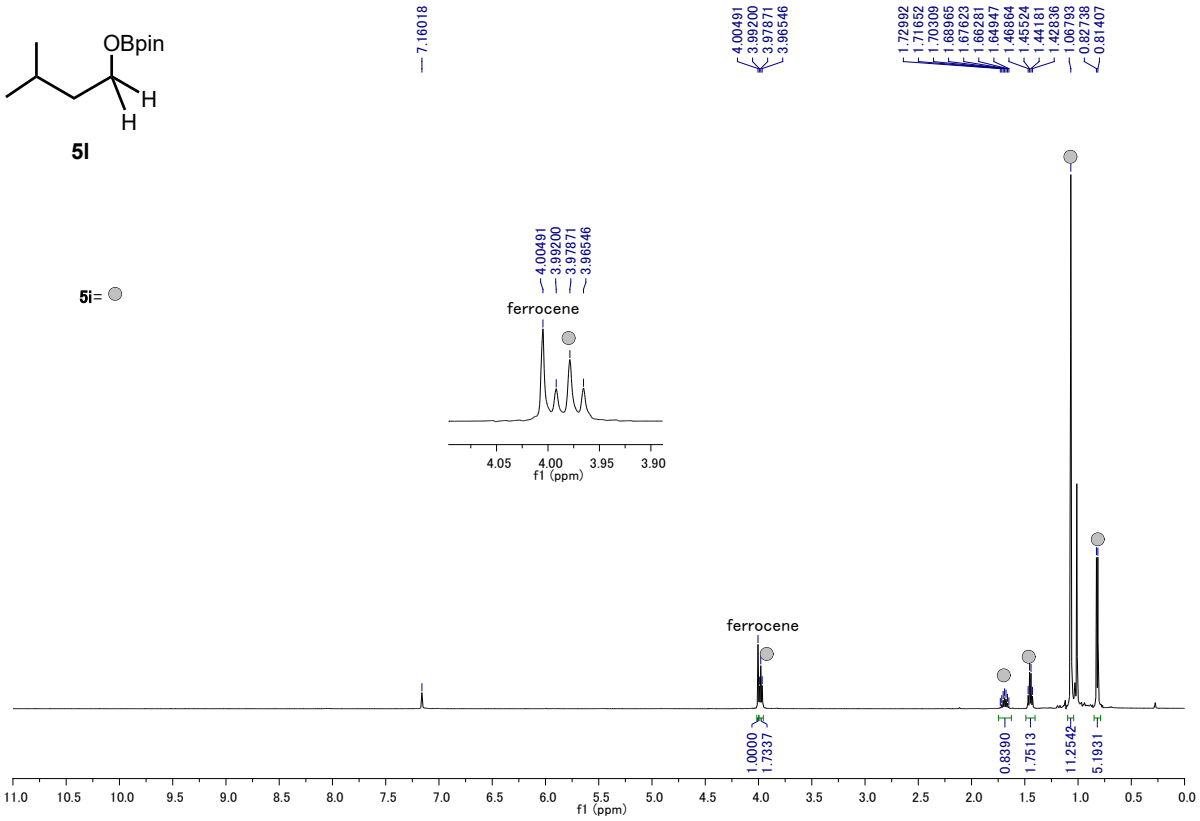


Figure S42. ^{1}H NMR spectra of **5l** (500 MHz, 25 °C, C_6D_6).

Figure S43. $^{13}C\{^{1}H\}$ NMR spectra of **5l** (126 MHz, 25 °C, C_6D_6).

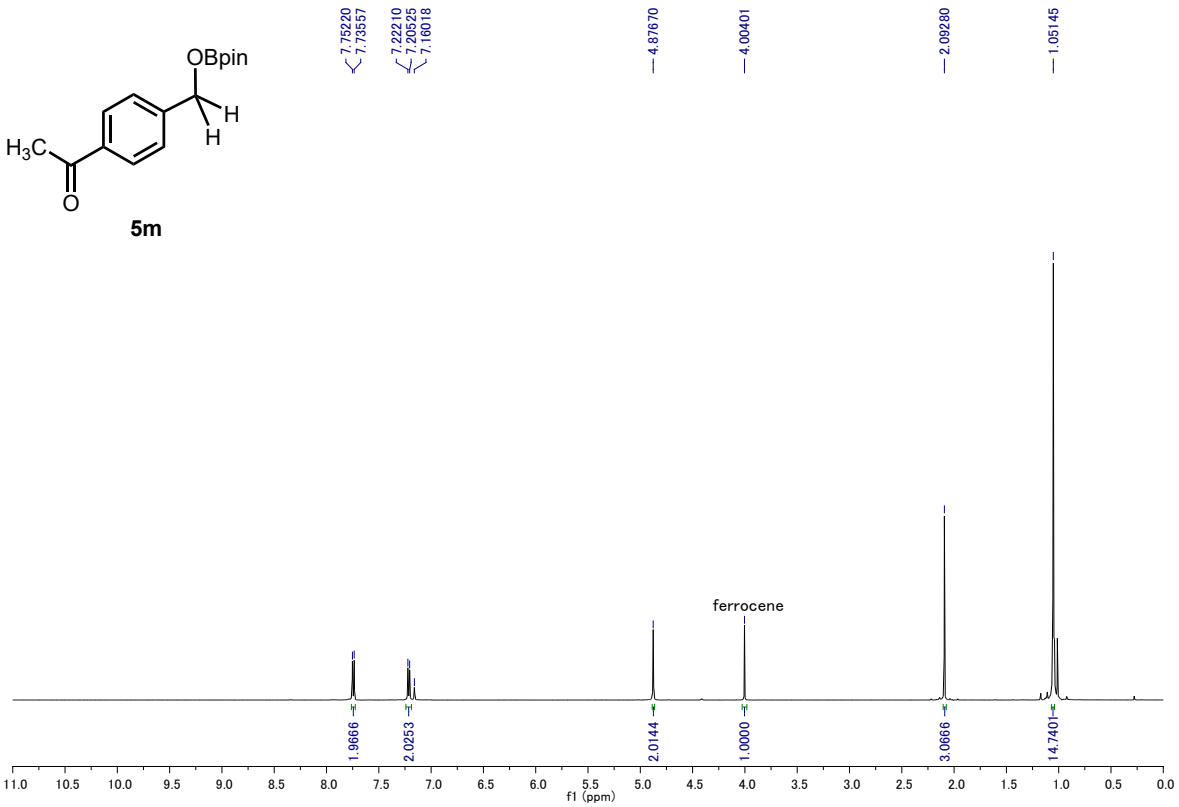


Figure S44. ^{1}H NMR spectra of **5m** (500 MHz, 25 °C, C_6D_6).

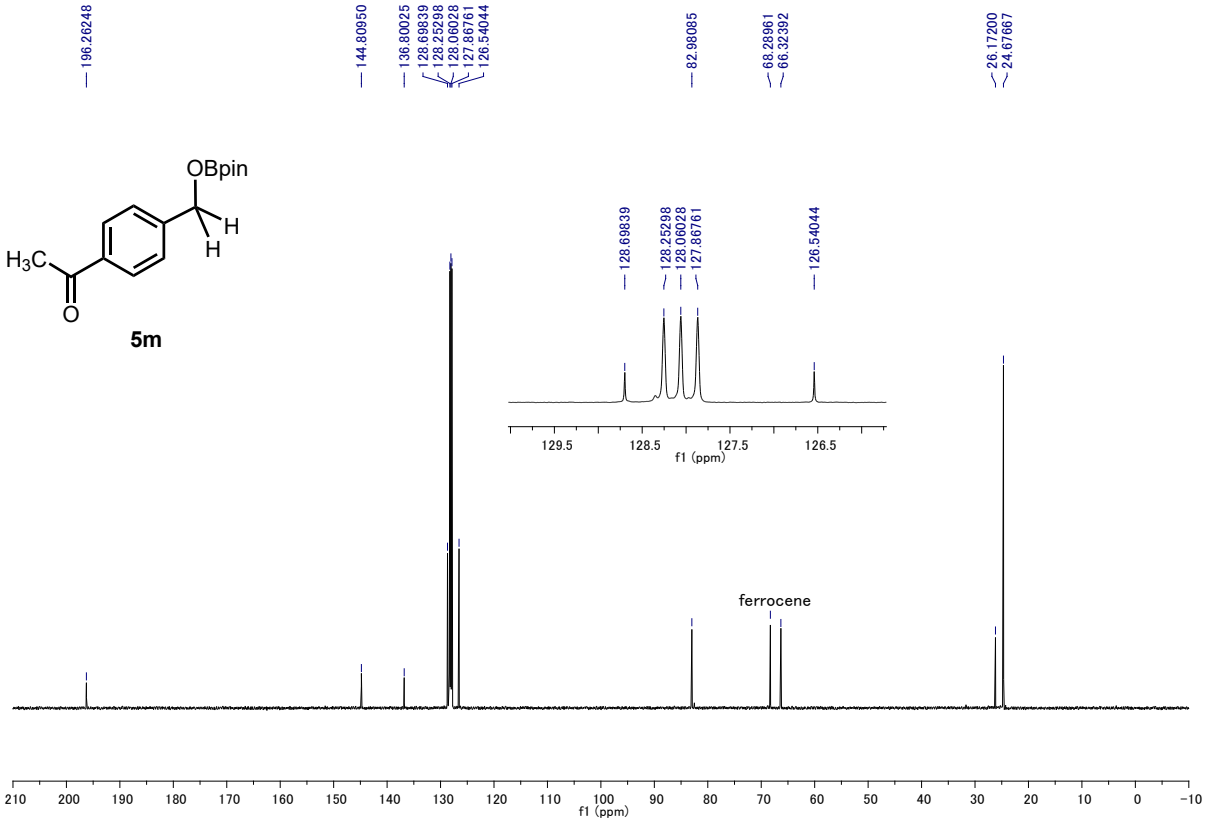


Figure S45. $^{13}C\{^{1}H\}$ NMR spectra of **5m** (126 MHz, 25 °C, C_6D_6).

(c) imines

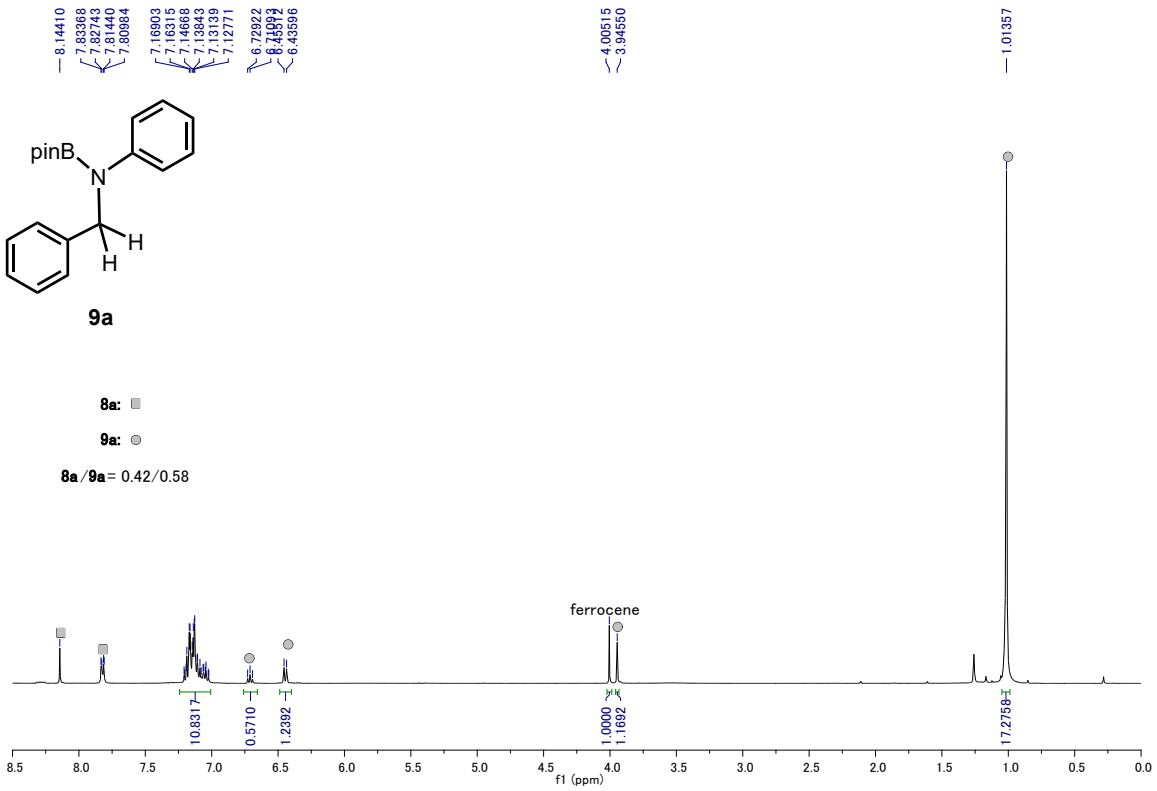


Figure S46. ^{1}H NMR spectra of **9a** (400 MHz, 25 °C, C_6D_6).

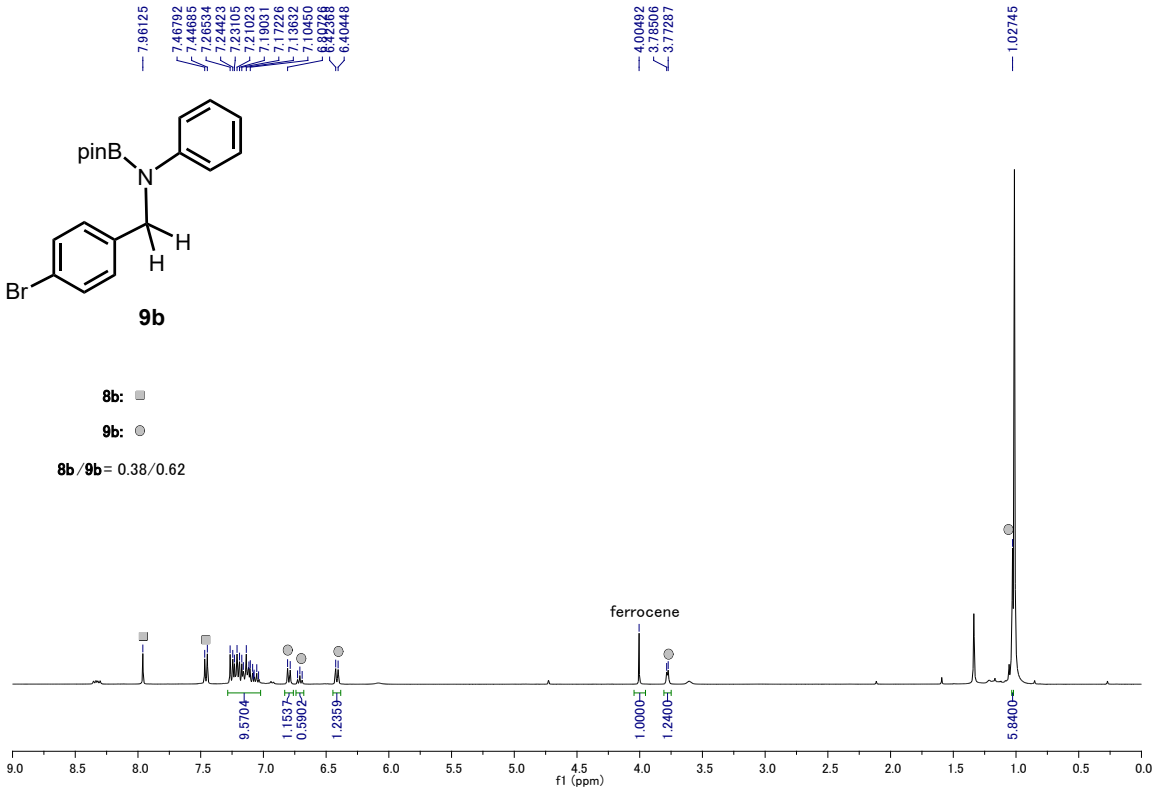


Figure S47. ^{1}H NMR spectra of **9b** (400 MHz, 25 °C, C_6D_6).

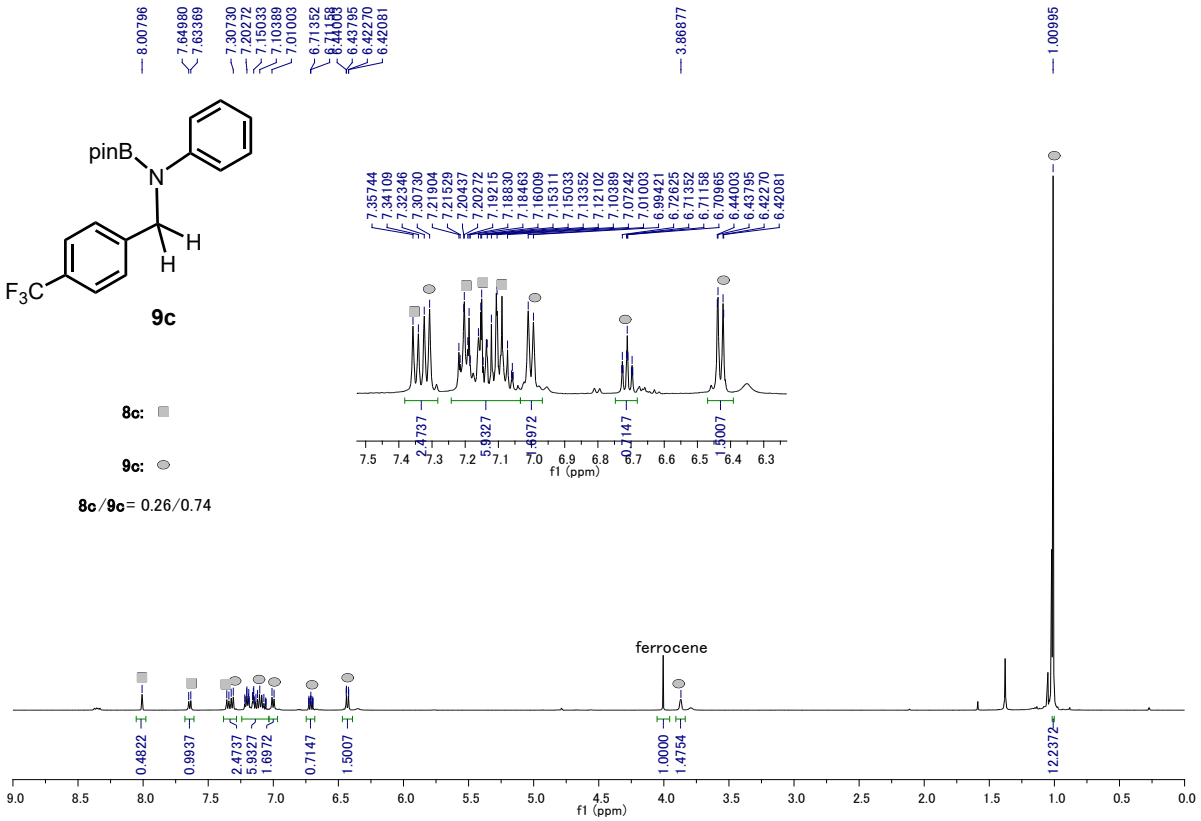


Figure S48. ^{1}H NMR spectra of **9c** (500 MHz, 25 °C, C_6D_6).

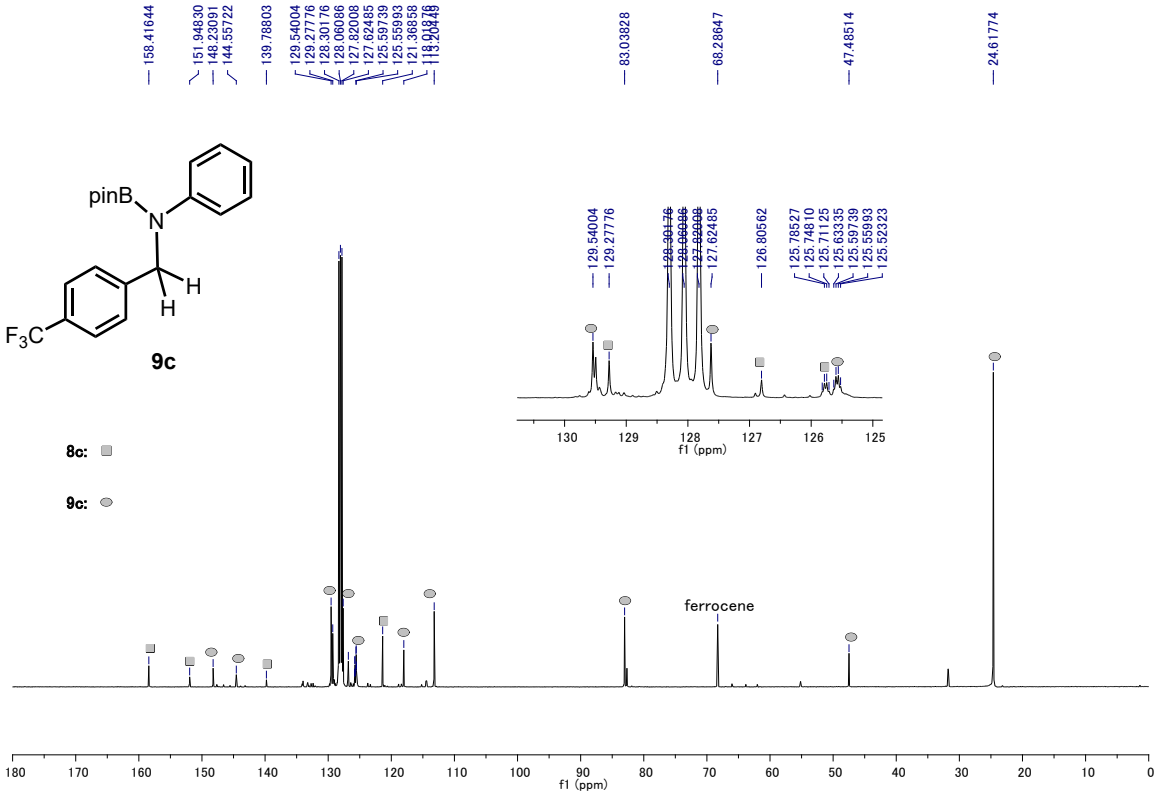
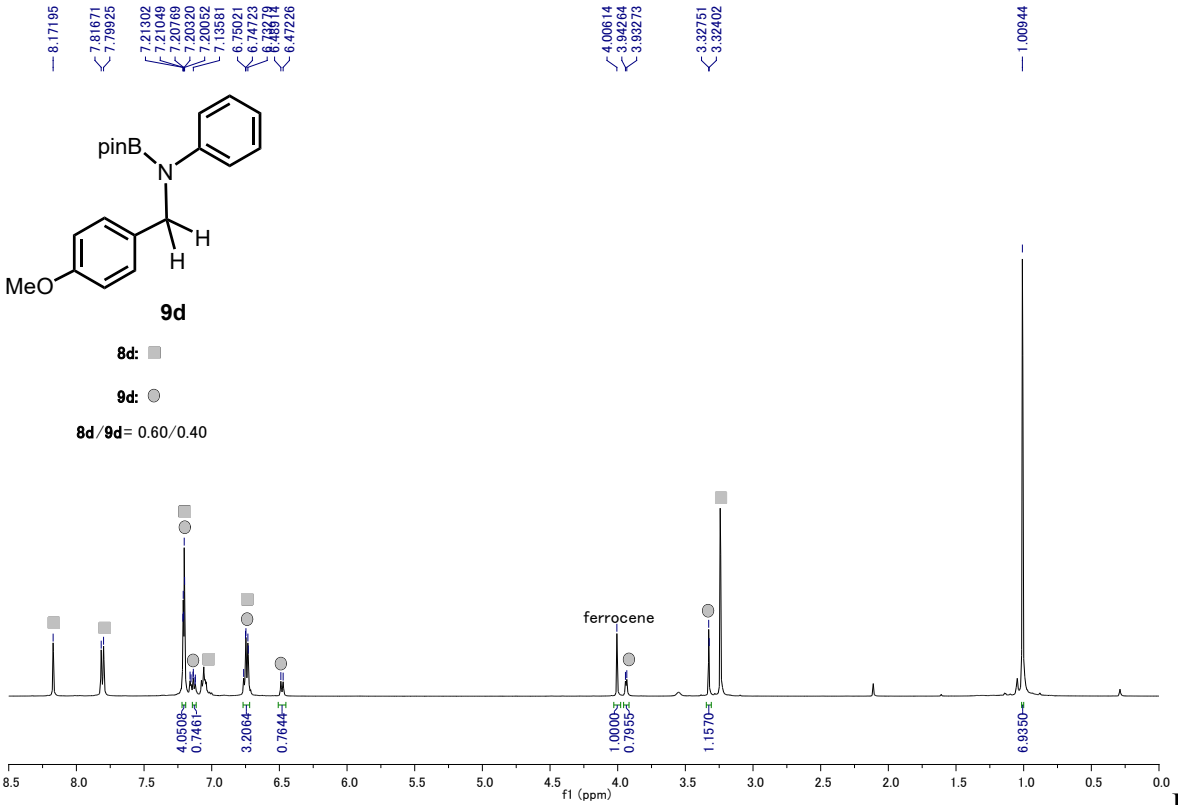
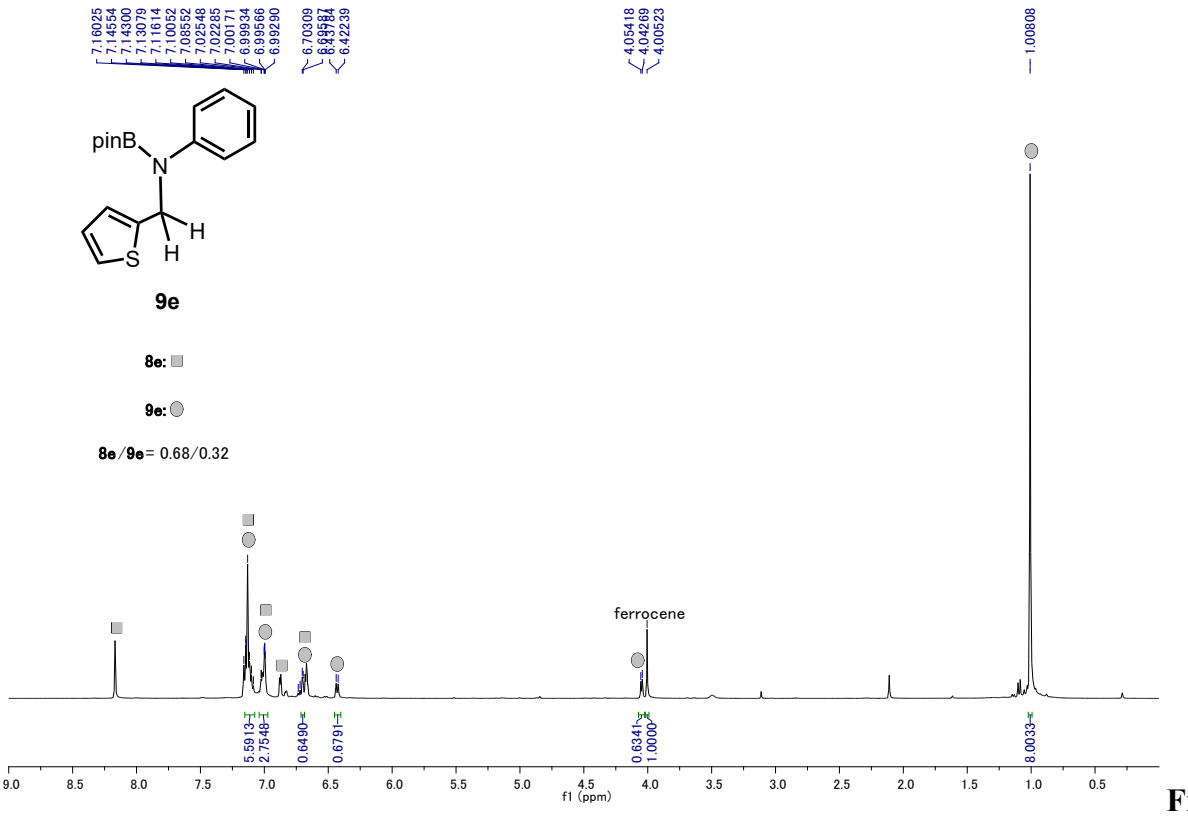


Figure S49. $^{13}C\{^{1}H\}$ NMR spectra of **9c** (126 MHz, 25 °C, C_6D_6).



Fi

gure S50. ^{1}H NMR spectra of **9d** (500 MHz, 25 °C, C_6D_6).



Fi

gure S51. ^{1}H NMR spectra of **9e** (500 MHz, 25 °C, C_6D_6).

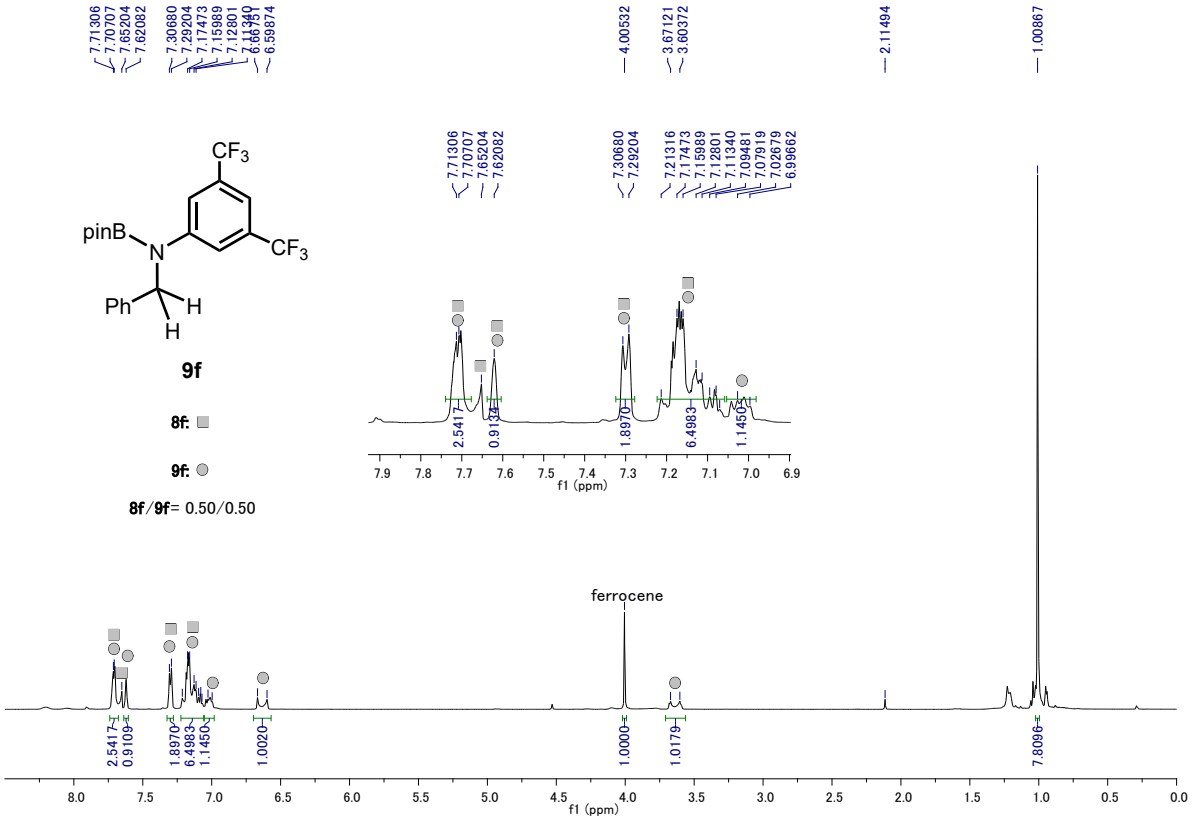


Figure S52. ^{1}H NMR spectra of **9f** (500 MHz, 25 °C, C_6D_6).

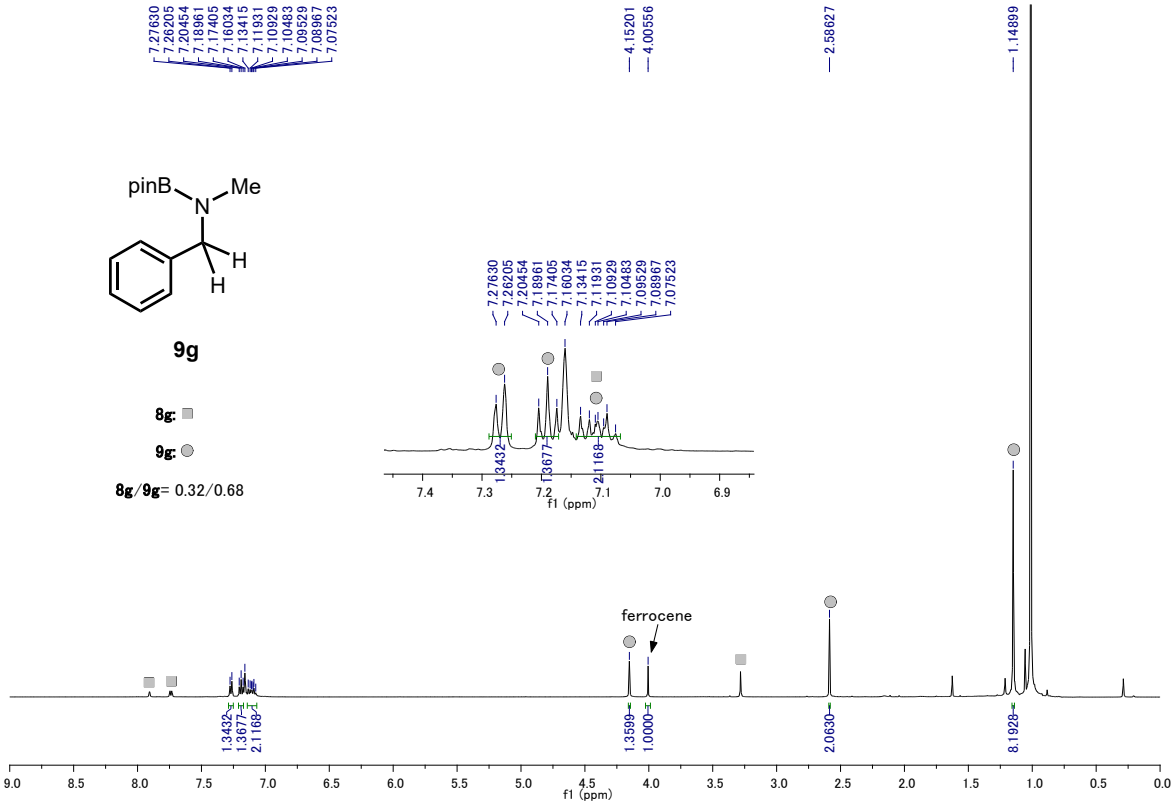
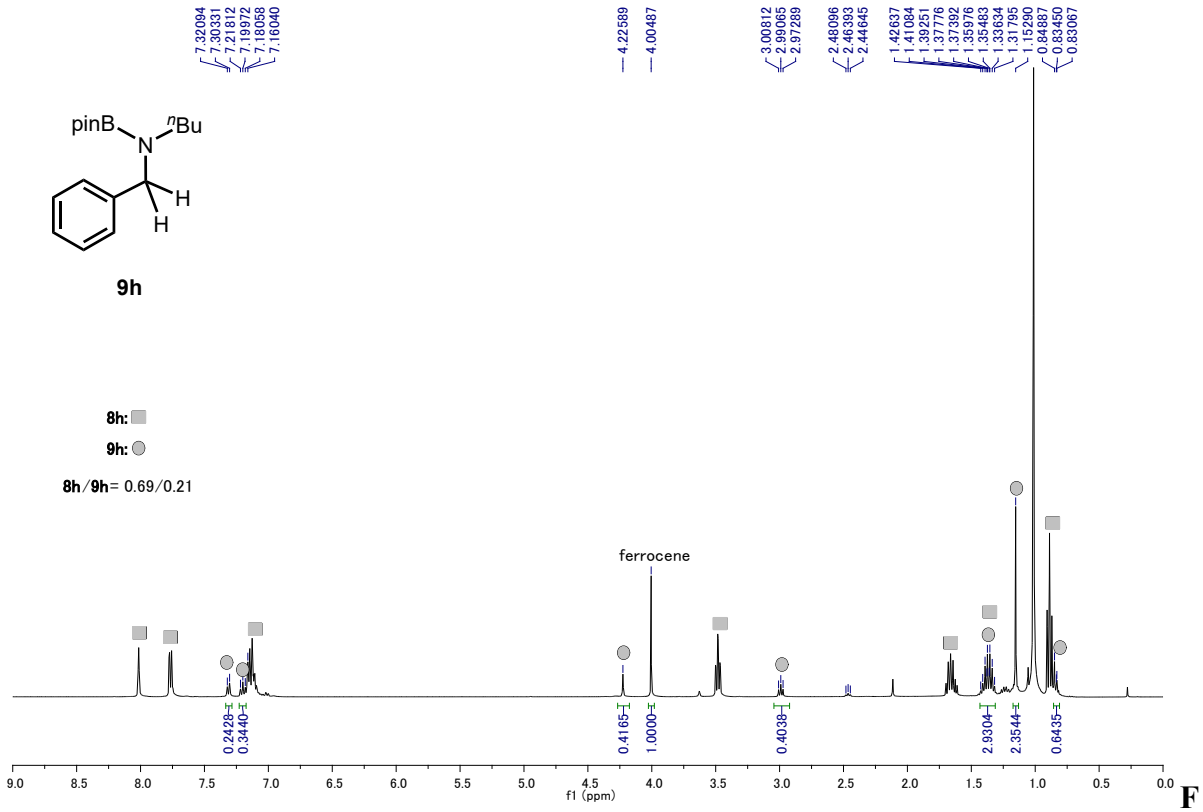


Figure S53. ^{1}H NMR spectra of **9g** (500 MHz, 25 °C, C_6D_6).



igure S54. ^{1}H NMR spectra of **9h** (400 MHz, 25 °C, C_6D_6).

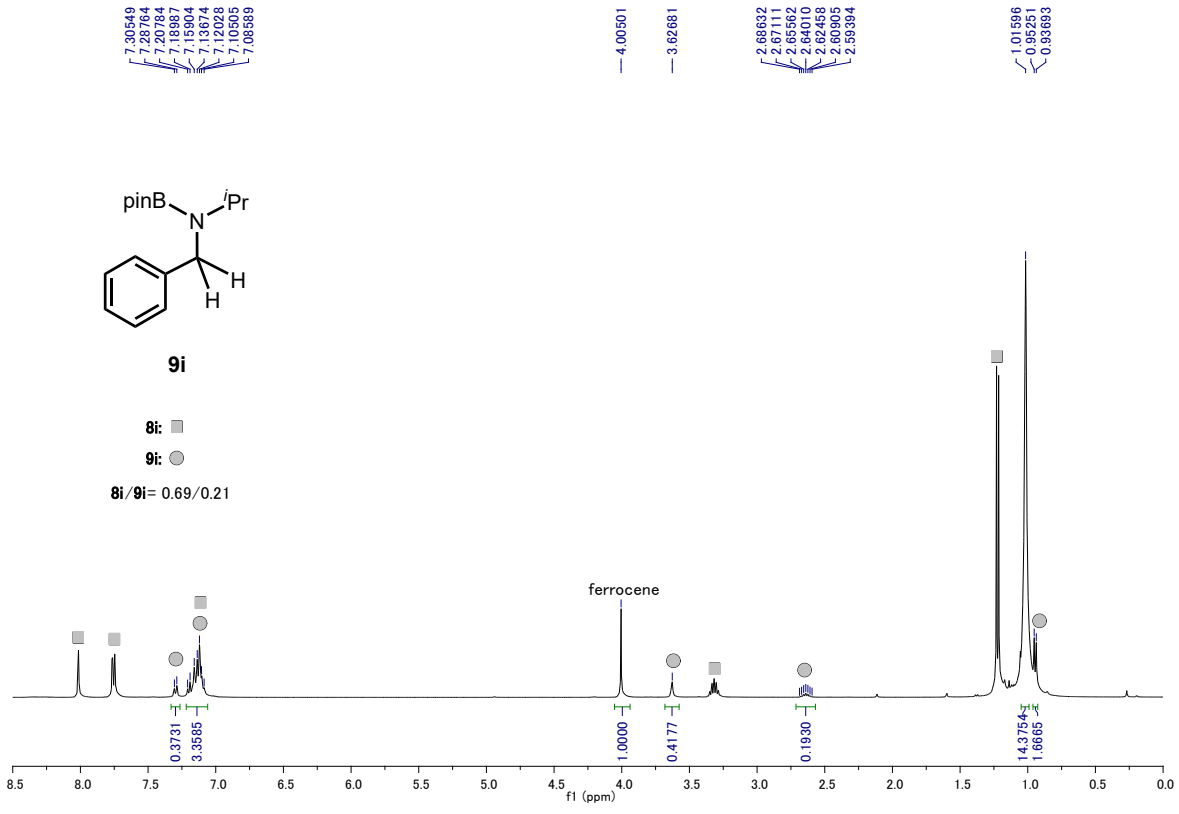


Figure S55. ^{1}H NMR spectra of **9i** (500 MHz, 25 °C, C_6D_6).

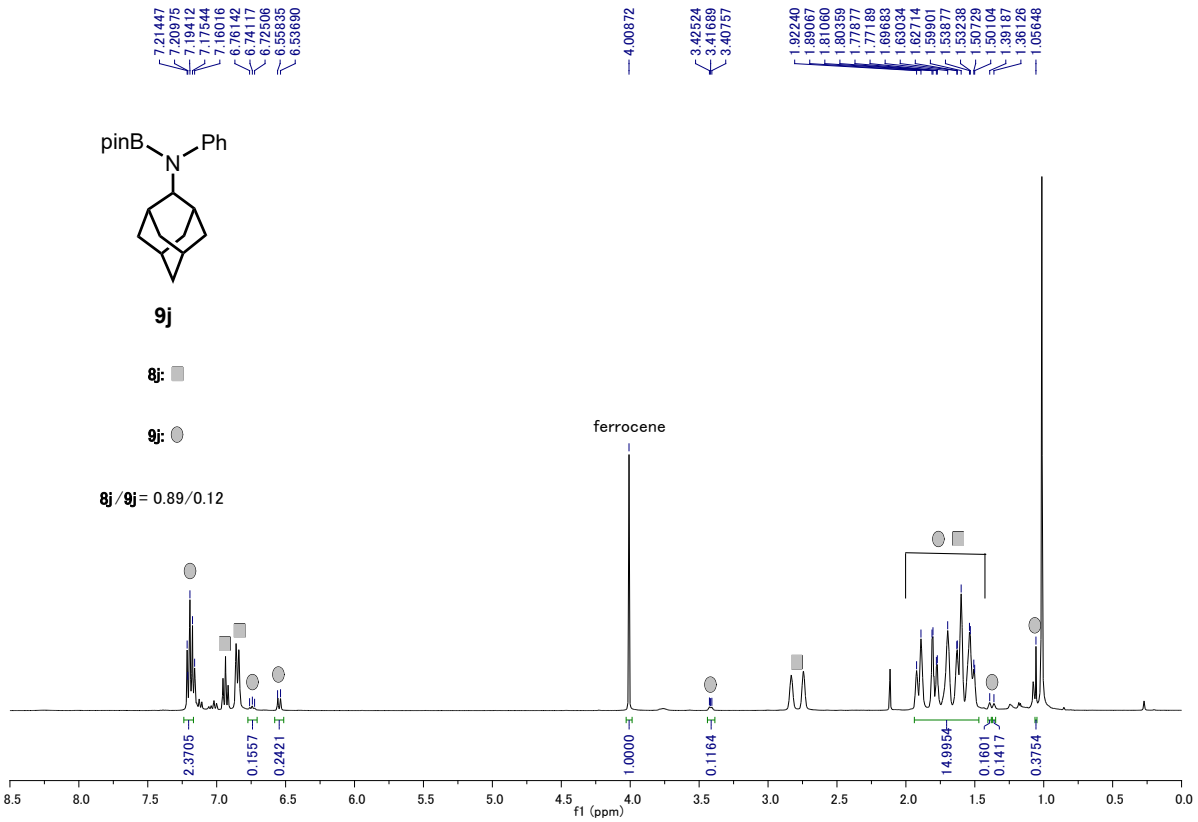


Figure S56. ^{1}H NMR spectra of **9j** (400 MHz, 25 °C, C_6D_6).

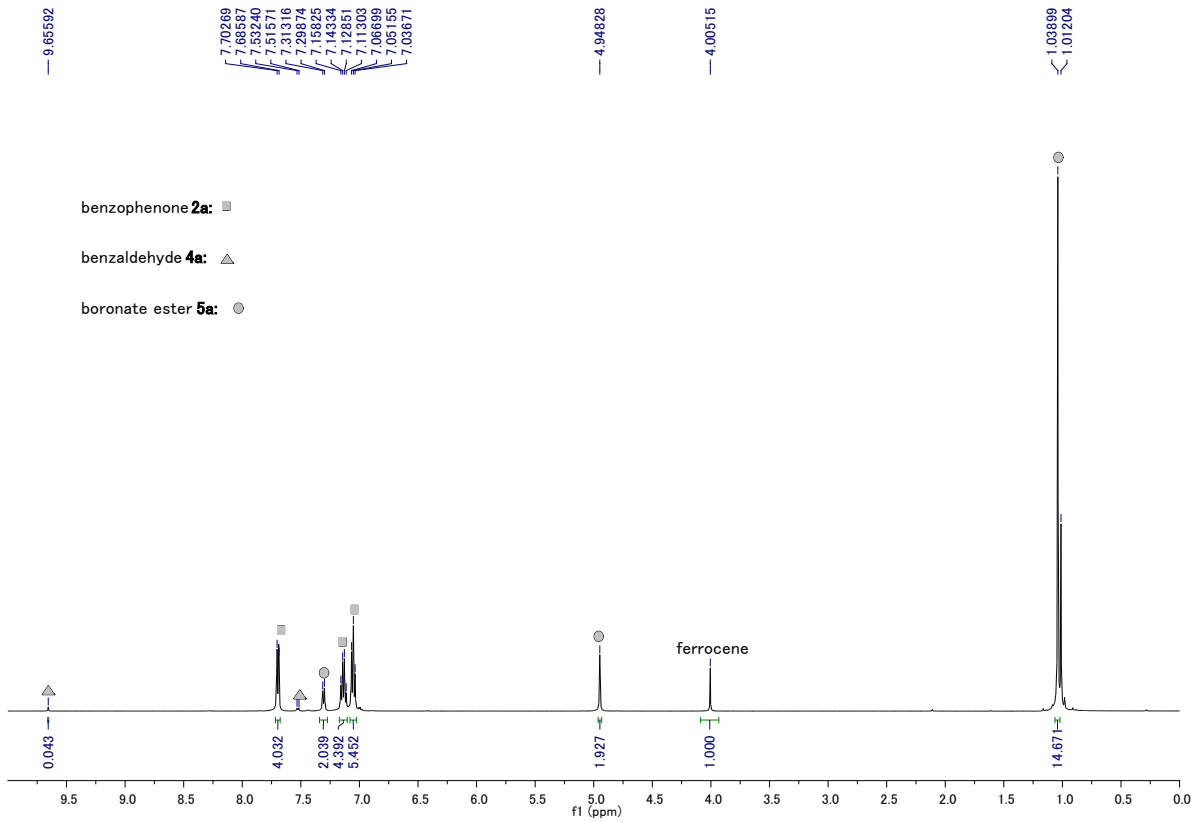


Figure S57. ^{1}H NMR spectra (500 MHz, 25 °C, C_6D_6) in the hydroboration of a mixture of benzophenone **2a** and benzaldehyde **4a** with HBpin in the presence of 0.5 mol % of **1**.

S4. Spectroscopic data and NMR charts of tin(II) hydride **10**

Generation of **10**: In a J. Young NMR tube, K[B(*sec*-Bu)$_3$H] (102 μL, 0.10 mmol, 1.0 M solution in THF) was added to a THF-d_8 solution of **1** (49.5 mg, 0.10 mmol) at –80 ˚C. The reaction mixture immediately turned to dark yellow from colorless solution and gradually turned to dark brown at –50 ˚C. The formation of **10** was confirmed by ^{1}H, ^{31}P, and ^{119}Sn NMR spectroscopies at –20 ˚C. Unfortunately, our attempts to isolate **10** proved unsuccessful due to its thermal instability at ambient temperature. ^{1}H NMR (500 MHz, –20 ˚C, THF-d_8): δ 0.83 (s, 18H, ^{t}Bu), 7.54–7.59 (m, 6H, Ar), 8.09 (m, 4H, Ar). 14.8 (br s, 1H, SnH) ^{31}P{^{1}H} NMR (202 MHz, –20 ˚C, THF-d_8) δ 27.2 ^{119}Sn{^{1}H} NMR (186 MHz, –20 ˚C, THF-d_8) δ 307.1.

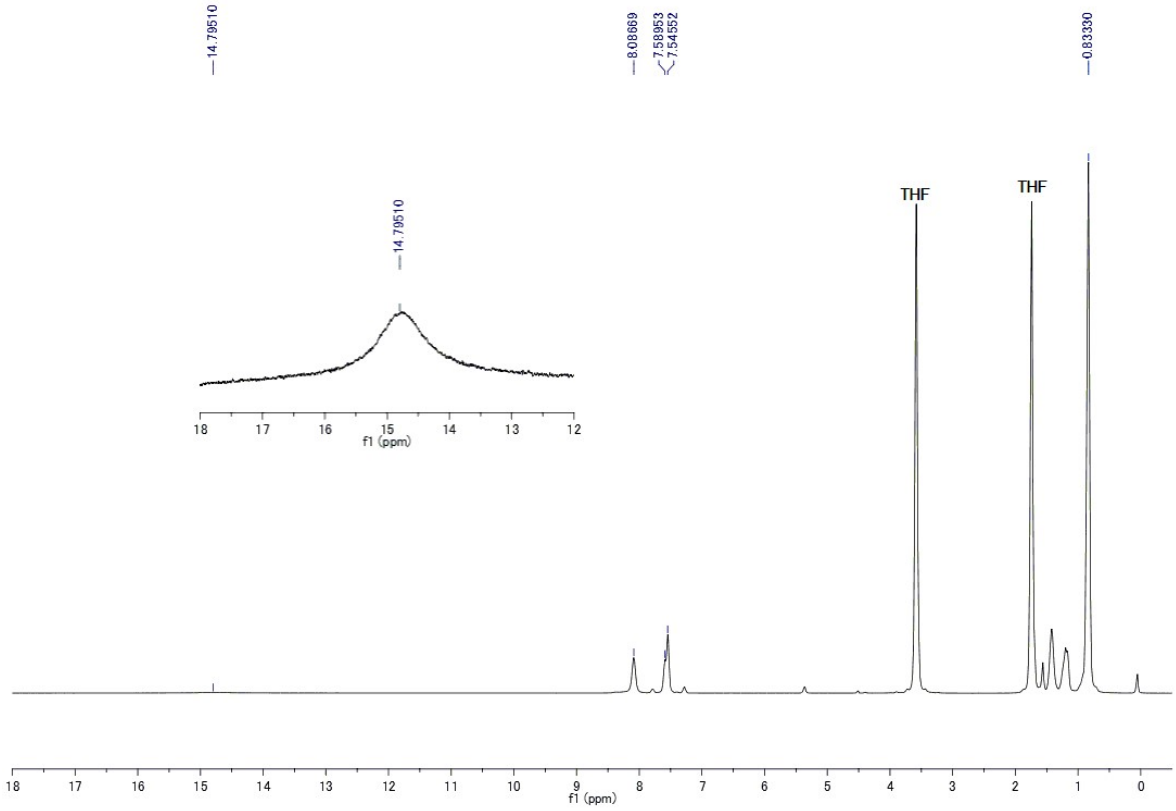


Figure S58. ^{1}H NMR spectra (500 MHz, –20 °C, THF-d_8).

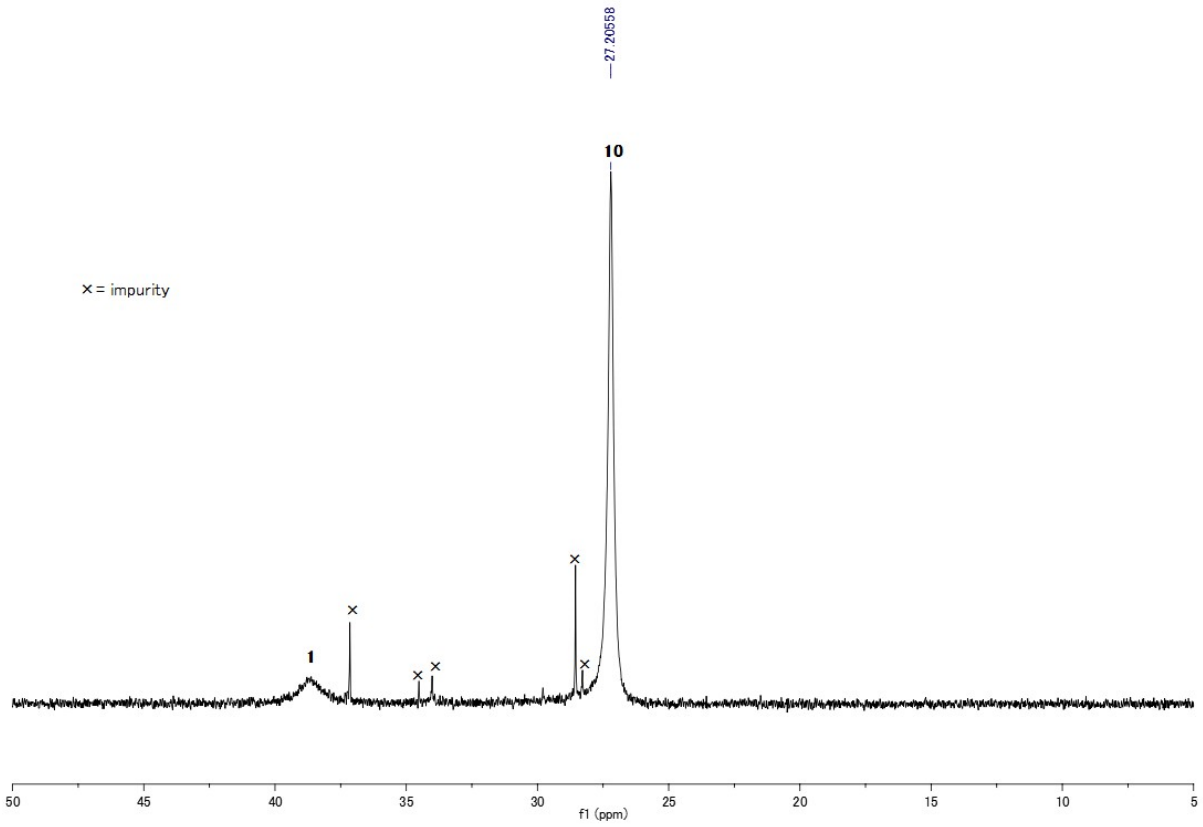


Figure S59. $^{31}P\{^{1}H\}$ NMR spectra (202 MHz, –20 °C, THF-d_8).

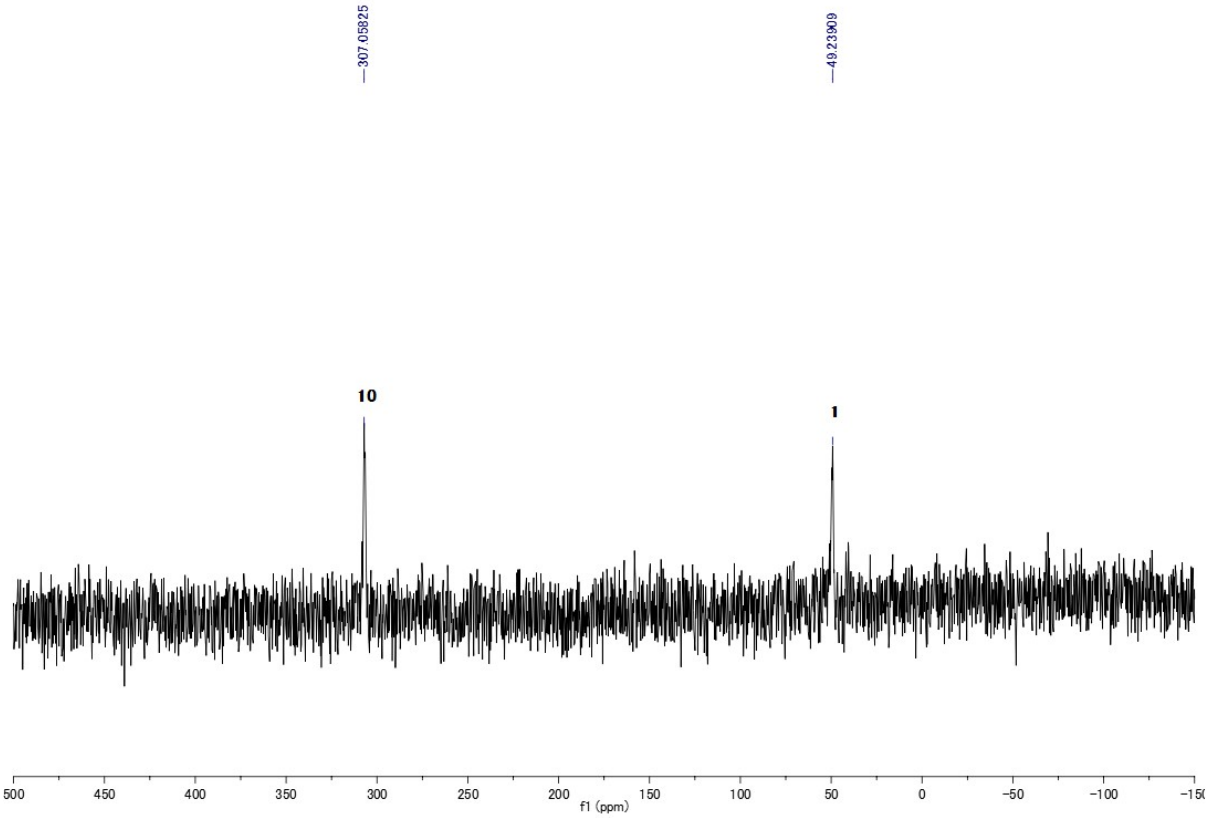


Figure S60. $^{119}Sn\{^{1}H\}$ NMR spectra (186 MHz, –20 °C, THF-d_8).

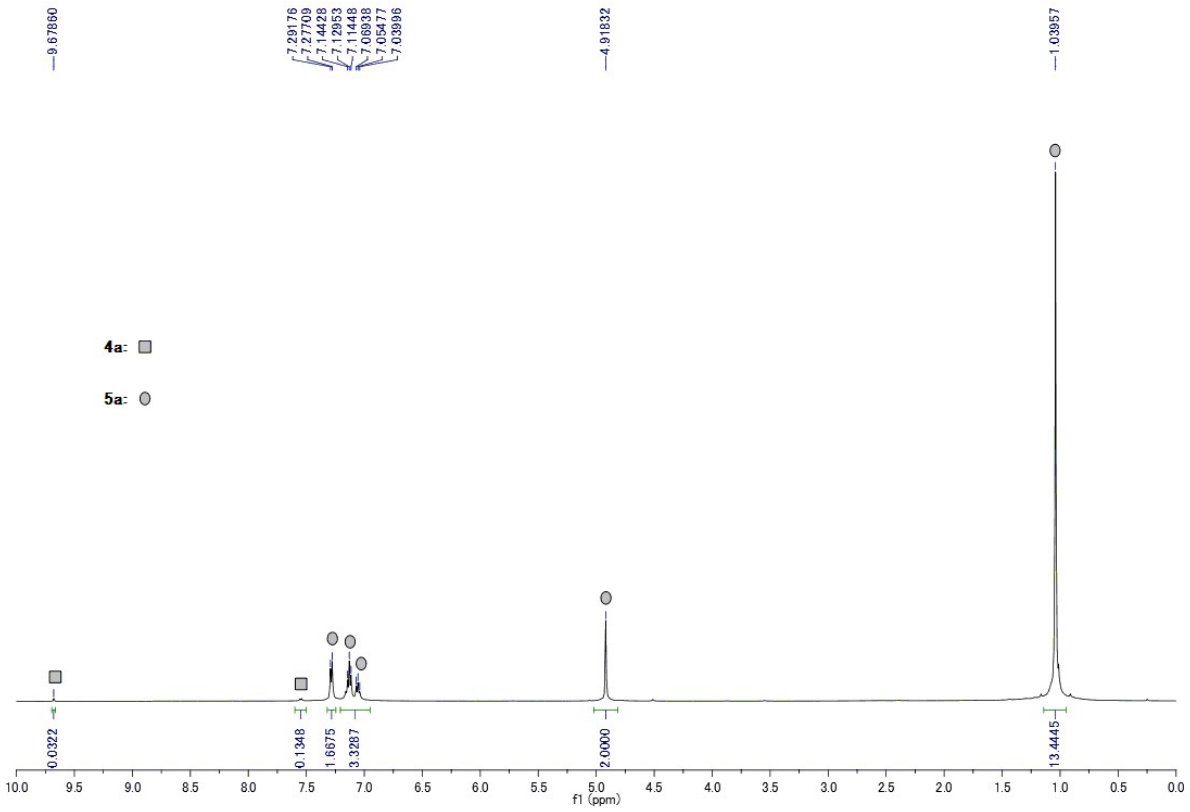


Figure S61. ^{1}H NMR spectra (500 MHz, 25 °C, C_6D_6) in the hydroboration of benzaldehyde **4a** with HBpin in the presence of 0.5 mol % of **10**.

S5. NMR charts of reaction of tin(II) hydride **10** with benzophenone **2a**

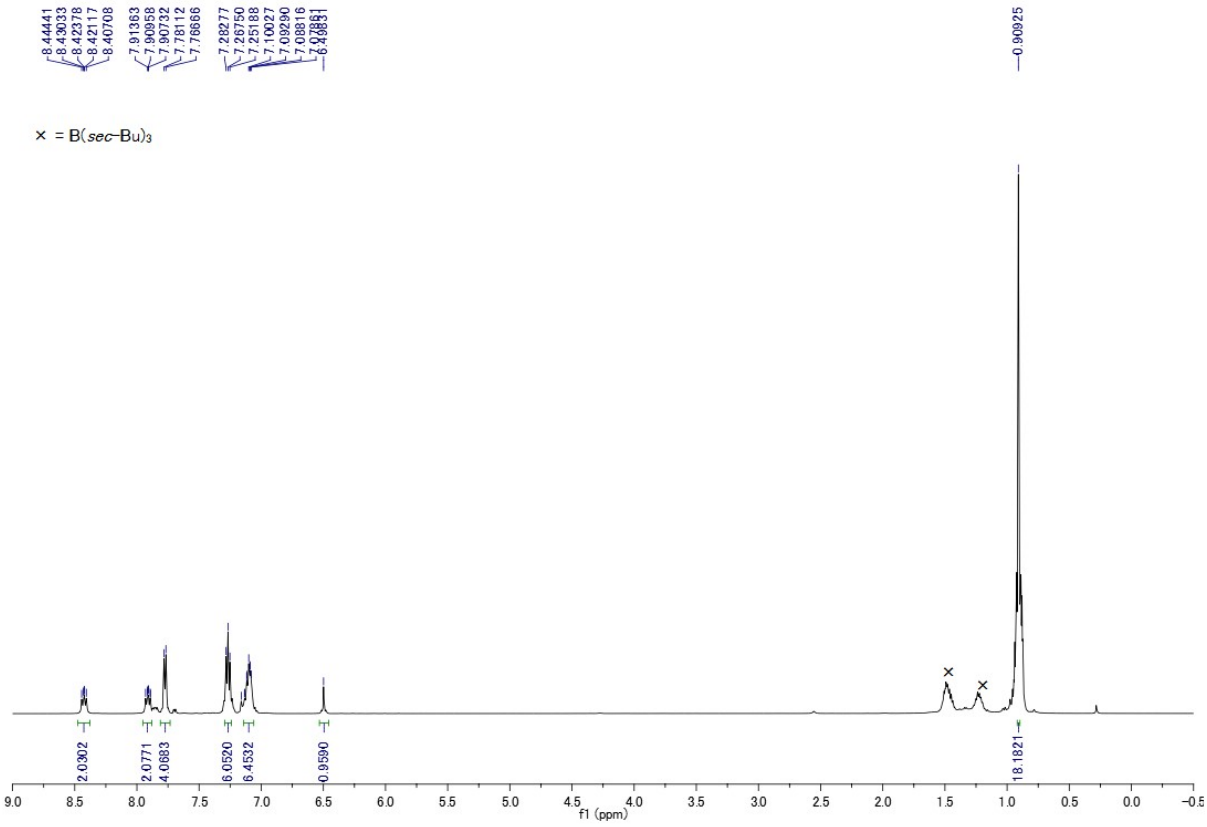


Figure S62. ^{1}H NMR spectra of **13** (500 MHz, 25 °C, C_6D_6).

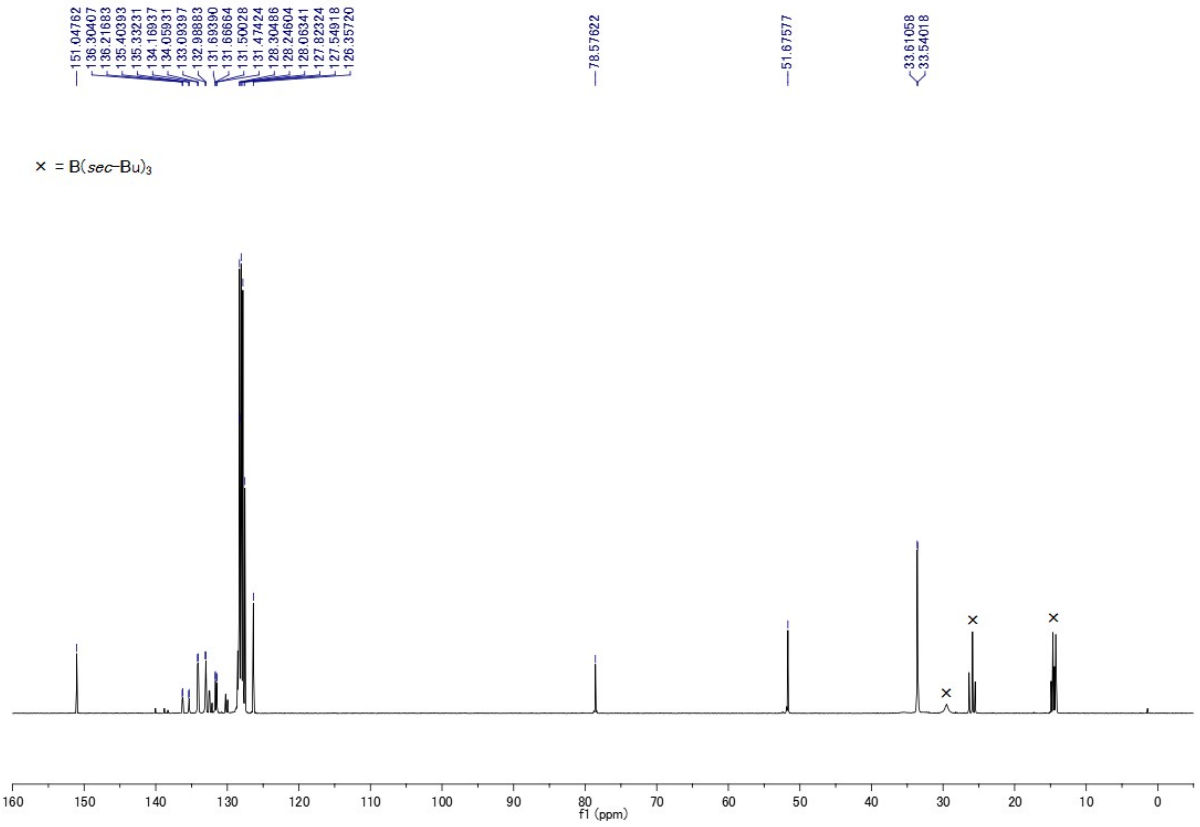


Figure S63. $^{13}C\{^{1}H\}$ NMR spectra of **13** (101 MHz, 25 °C, C_6D_6).

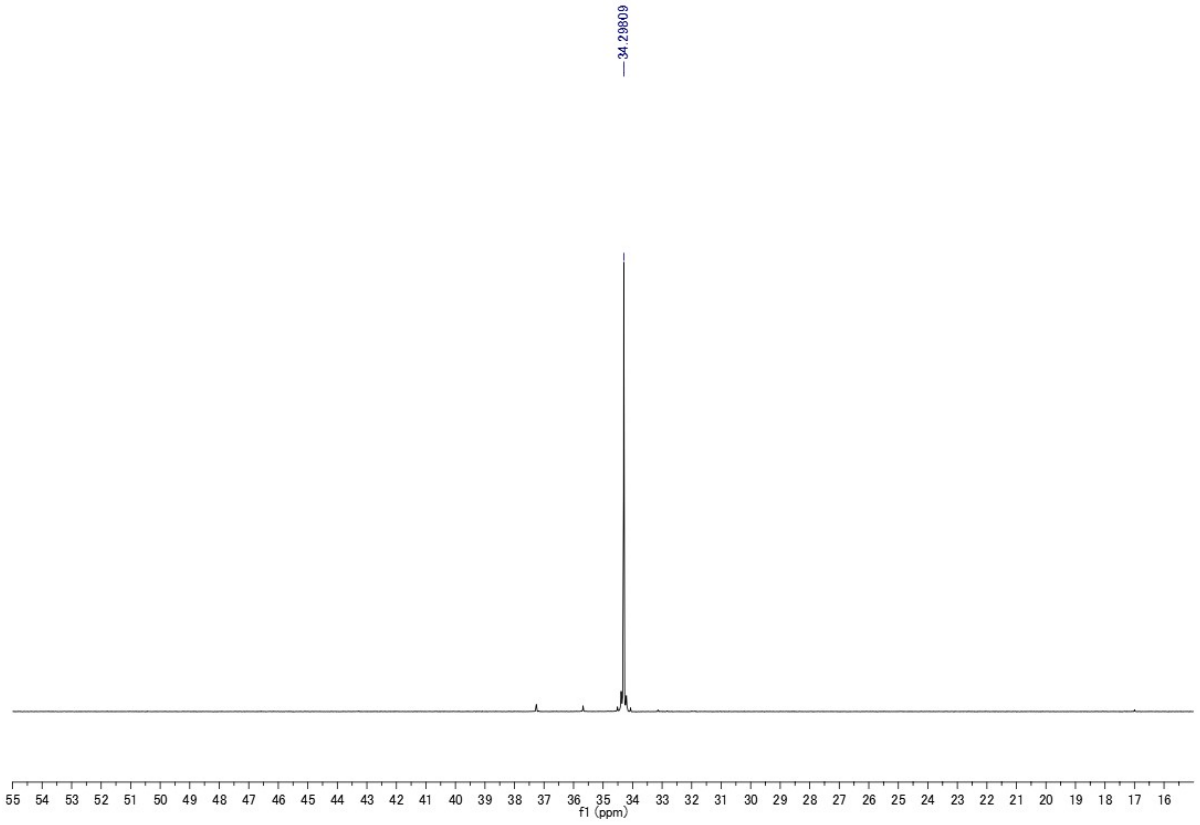


Figure S64. $^{31}P\{^{1}H\}$ NMR spectra of **13** (202 MHz, 25 °C, C_6D_6).

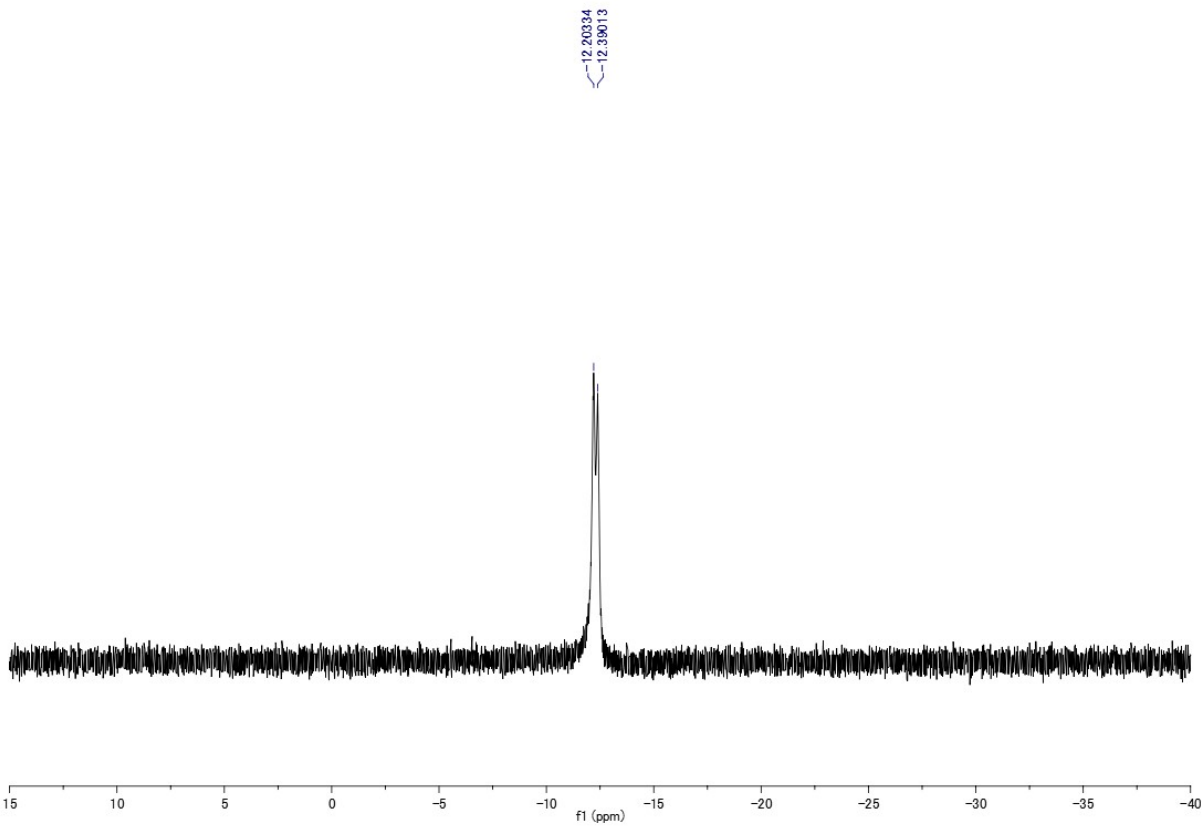


Figure S65. $^{119}Sn\{^{1}H\}$ NMR spectra of **13** (186 MHz, 25 °C, C_6D_6).

S6. Computational results

Table S1. Natural bonding orbital occupancy of tin(II) catalyst **10**, benzaldehyde **4a**, **TS-12a**, acetophenone **2d**, and **TS-12b**.

Occupancy	10	benzaldehyde 4a	TS-12a	acetophenone 2d	TS-12b
σ(Sn-H)	1.99	-	1.59	-	1.62
π*(C=O)	-	0.09	0.44	0.11	0.44

Table S2. Natural population analysis (*q*) on Sn, H(Sn), C(=O), O(=C), and Ph(CO)R (R = H or CH_3) fragment of tin(II) catalyst **10**, benzaldehyde **4a**, **TS-12a**, acetophenone **2d**, and **TS-12b**.

q	10	benzaldehyde 4a	TS-12a	acetophenone 2d	TS-12b
Sn	0.88	-	1.19	-	1.19
H(Sn)	-0.36	-	-0.26	-	-0.28
C(=O)	-	0.42	0.24	0.58	0.44
O(=C)	-	-0.55	-0.73	-0.57	-0.74
Ph(CO)R	-	0.00	-0.37	0.00	-0.35

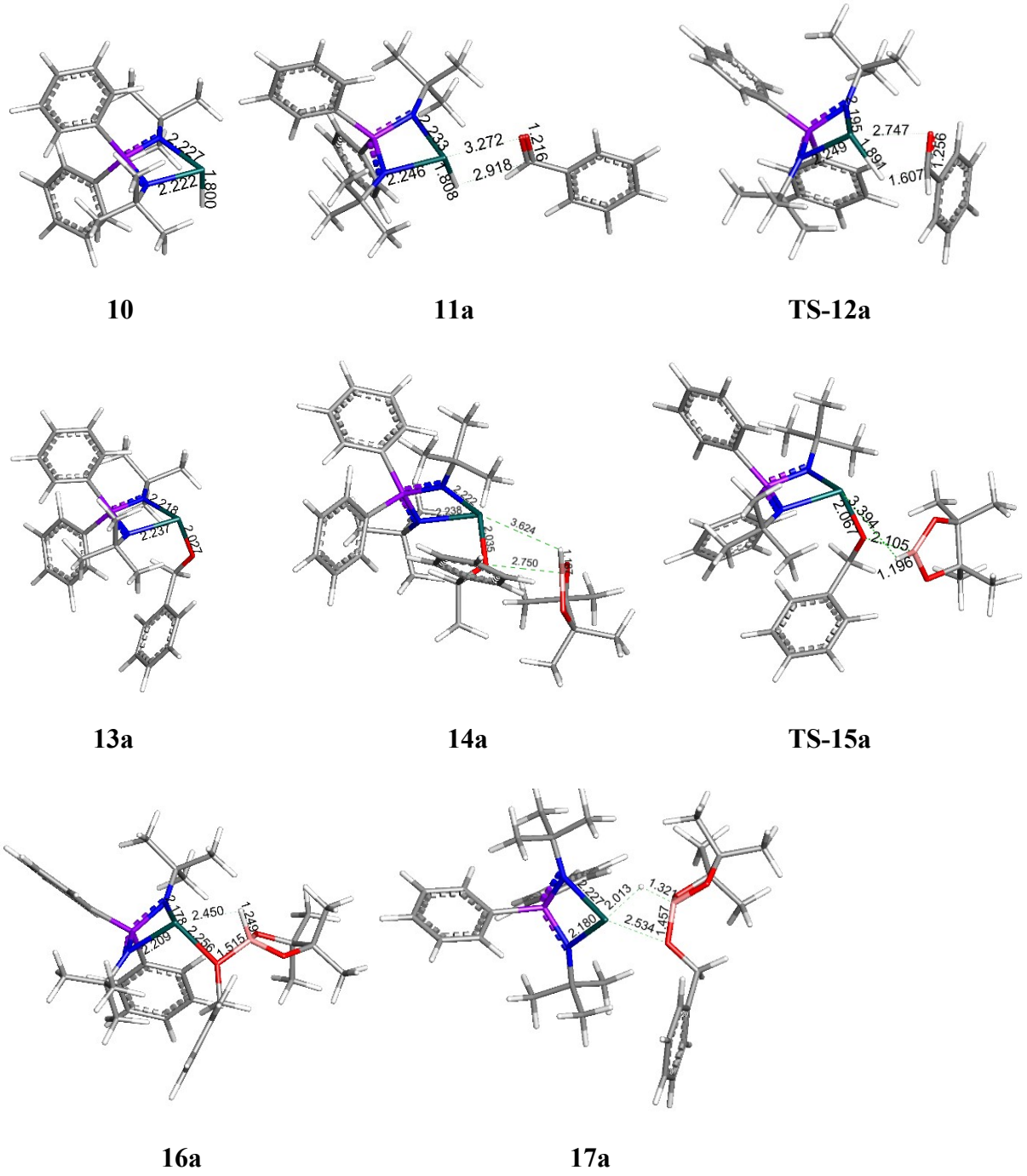
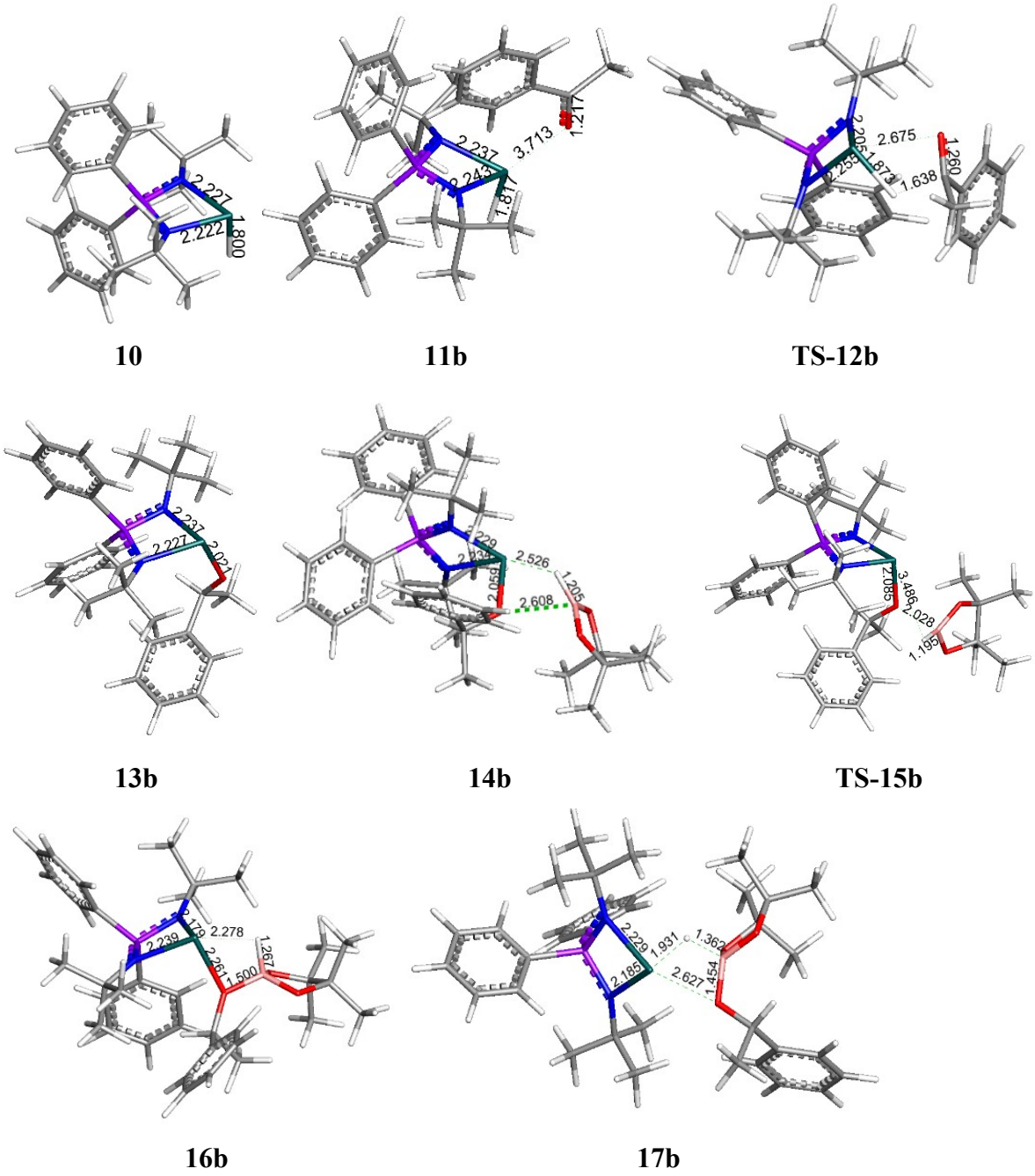


Figure S66. Optimized geometries of intermediates and transition states in the hydroboration of benzaldehyde **4a** with HBpin by tin(II) catalyst **10**.



10 **11b** **TS-12b**

13b **14b** **TS-15b**

16b **17b**

Figure S67. Optimized geometries of intermediates and transition states in the hydroboration of acetophenone **2d** with HBpin by tin(II) catalyst **10**.

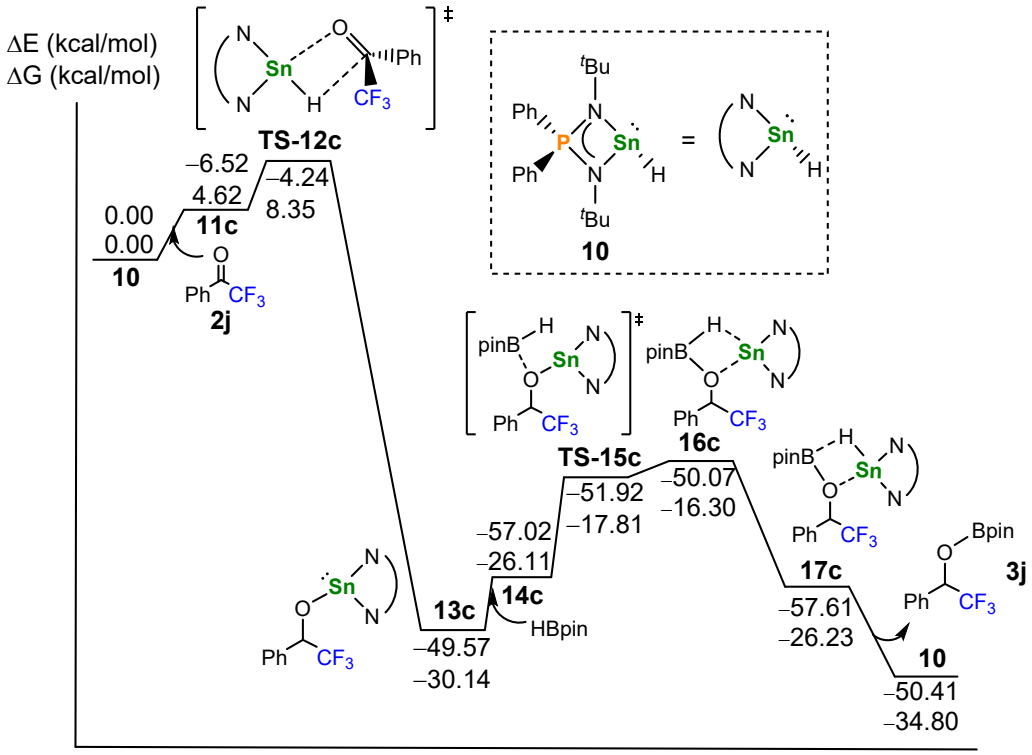


Figure S68. Solvent corrected free energy profile in toluene for the reaction of 2,2,2-trifluoroacetophenone **2j** with HBpin by tin(II) hydride **10**.

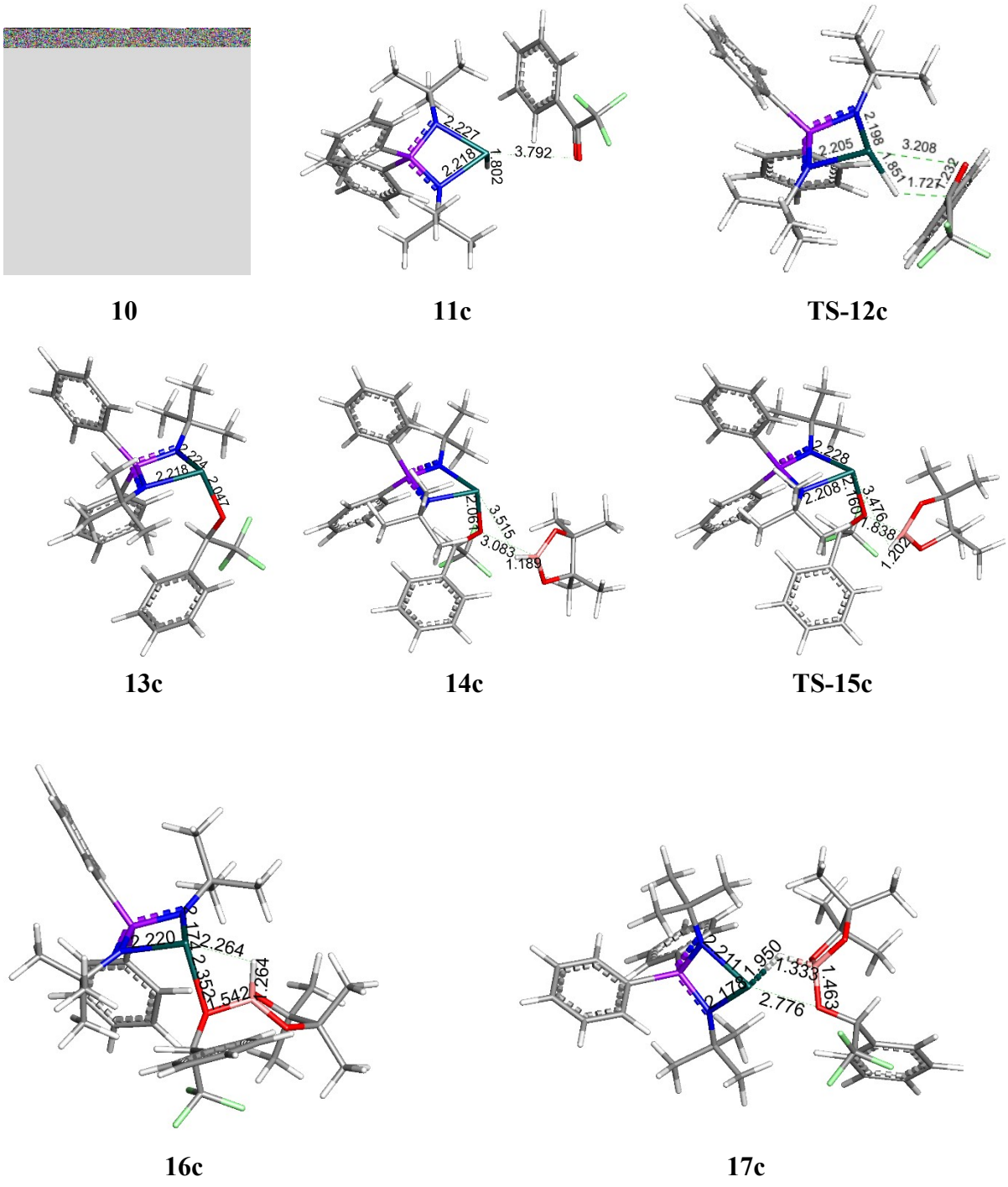


Figure S69. Optimized geometries of intermediates and transition states in the hydroboration of 2,2,2-trifluoroacetophenone **2j** with HBpin by tin(II) catalyst **10**.

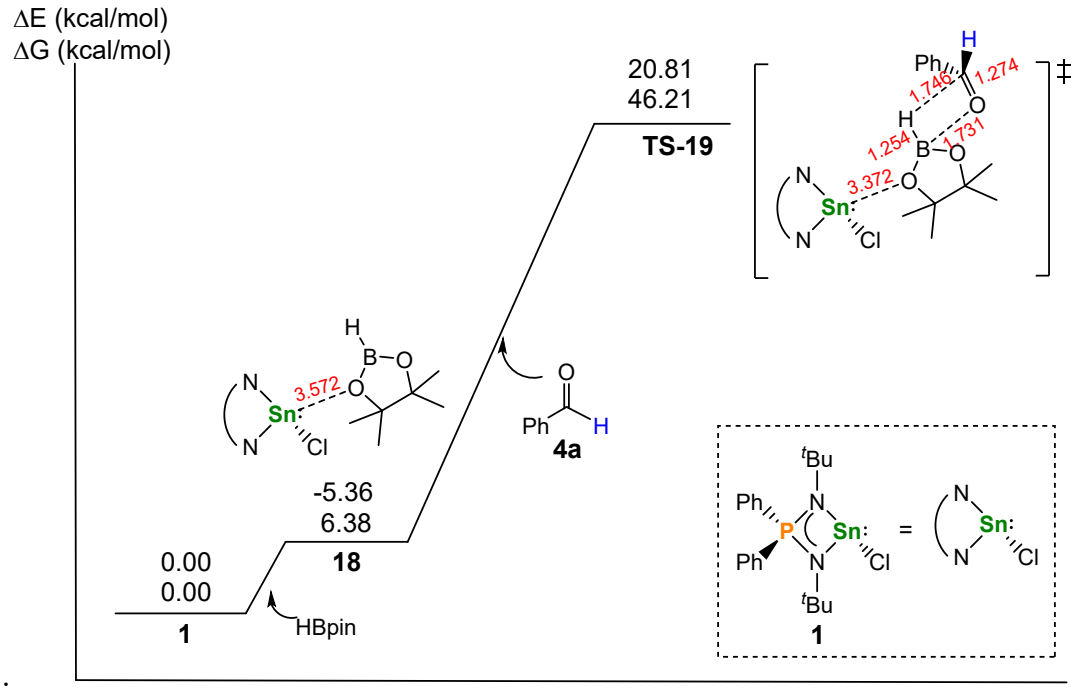


Figure S70. Solvent corrected free energy profile in toluene for the hydroboration of benzaldehyde **4a** with HBpin in the presence of tin complex **1.**

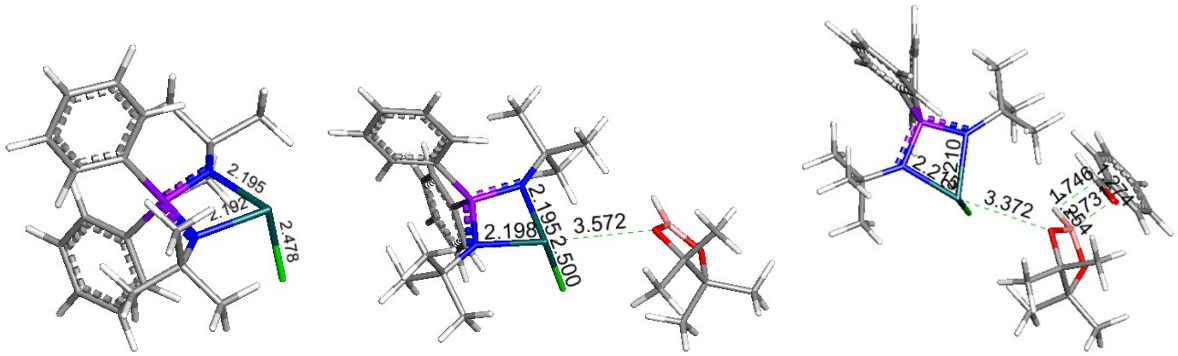


Figure S71. Optimized geometries of intermediates and transition states in the hydroboration of benzaldehyde **4a** with HBpin in the presence of tin complex **1.**

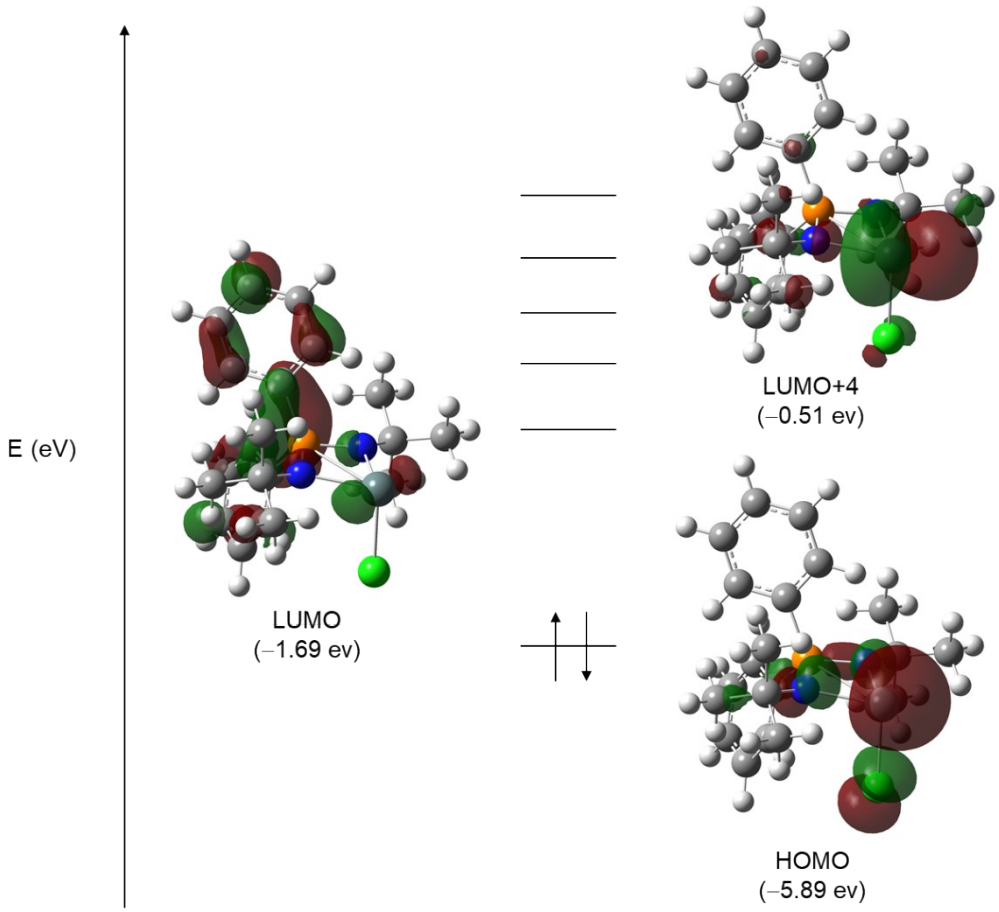


Figure S72. Molecular orbital diagrams for tin(II) chloride **1** using B3LYP functional and 6-31+G(d,p) basis set for C, H, N, P, Cl and LANL2DZ basis set for Sn.

Tin(II) hydride **10**

53

scf done: -1444.566332

C	-0.973434	3.243396	-2.377817
C	-0.462346	2.077047	-1.819461
C	-1.145675	1.435012	-0.780248
C	-2.168324	3.779818	-1.901823
C	-2.852087	3.148559	-0.865926
C	-2.341675	1.981279	-0.305180
H	-0.437016	3.737274	-3.182332
H	0.477454	1.658948	-2.170079
H	-2.566251	4.691439	-2.337740
H	-3.781460	3.566430	-0.490792
H	-2.878486	1.500632	0.507786
C	-3.774670	-2.137817	0.588046
C	-3.423948	-2.935085	1.674282
C	-2.169309	-2.795434	2.264427
C	-2.871634	-1.202244	0.090458
C	-1.611119	-1.055316	0.677368
C	-1.266924	-1.861799	1.767730
H	-4.750838	-2.244951	0.124802
H	-4.128410	-3.665919	2.060334
H	-1.893026	-3.417234	3.110659
H	-3.154671	-0.586525	-0.758652
H	-0.283512	-1.751050	2.216571
Sn	2.579200	-0.360703	0.092346
P	-0.301656	0.019840	-0.000070
N	0.696478	-0.734742	-1.027008
N	0.781167	0.447471	1.128955
C	0.430435	-1.726343	-2.075955
C	-0.778592	-1.333322	-2.938000
C	0.204529	-3.122041	-1.470252
C	1.674221	-1.760907	-2.975212
C	1.872492	1.242574	3.124461
C	-0.602640	1.443687	2.936202
C	0.889453	2.899991	1.530286
H	0.121385	-3.881410	-2.257029
H	-0.712504	-3.149997	-0.872914

H	1.043632	-3.389893	-0.818512
H	1.539658	-2.472570	-3.797183
H	2.558969	-2.077240	-2.407800
H	1.869775	-0.769512	-3.397344
H	1.862282	1.973759	3.939972
H	2.841956	1.329861	2.617033
H	1.798181	0.237091	3.552030
H	-0.610632	2.210864	3.718392
H	-0.735667	0.465477	3.409049
H	0.987977	3.659907	2.314723
H	0.033367	3.170377	0.904624
H	1.787145	2.925110	0.903289
H	-0.918073	-2.061330	-3.745142
H	-0.637077	-0.344389	-3.385160
H	-1.702050	-1.317372	-2.350373
C	0.715292	1.502238	2.149853
H	-1.464196	1.629936	2.286500
H	2.889173	1.180999	-0.784010

Benzaldehyde **4a**

14

scf done: -345.468459

C	-2.897398	0.503227	-0.019651
C	-1.748672	-0.294942	-0.064881
C	-1.863048	-1.687365	-0.066543
C	-4.150843	-0.093855	0.023555
C	-4.261641	-1.486814	0.021771
C	-3.119864	-2.284992	-0.023218
H	-2.783690	1.582785	-0.019265
H	-0.965557	-2.300791	-0.101857
H	-5.045181	0.520214	0.058729
H	-5.242934	-1.950365	0.055614
H	-3.211070	-3.366414	-0.024412
O	-0.192986	1.517823	-0.113839
C	-0.402971	0.323636	-0.111348
H	0.442334	-0.396041	-0.145302

Acetophenone **2d**

17

scf done: -384.783658

C	-2.865867	0.490637	-0.087537
C	-1.708215	-0.294358	-0.033270
C	-1.827571	-1.683335	0.084657
C	-4.120858	-0.103209	-0.024933
C	-4.232157	-1.489235	0.092626
C	-3.085243	-2.278500	0.147370
H	-2.756691	1.566283	-0.179091
H	-0.943138	-2.311072	0.128594
H	-5.013717	0.512781	-0.067601
H	-5.212208	-1.954124	0.141567
H	-3.169677	-3.356717	0.238756
C	0.882279	-0.445945	-0.046245
O	-0.309903	1.605151	-0.207079
H	0.908270	-1.162374	-0.873939
H	0.925019	-1.015498	0.887932
H	1.747796	0.213448	-0.109792
C	-0.376042	0.393385	-0.104470

2,2,2-Trifluoroacetophenone **2j**

17

scf done: -682.429748635

C	1.679991922	1.273394874	-0.000023686
C	0.666948507	0.304469044	-0.000011171
C	1.006922192	-1.054667864	0.000010190
C	3.014082504	0.889883162	-0.000018308
C	3.347861103	-0.465186074	0.000003274
C	2.345953800	-1.433247493	0.000018213
C	-1.898889068	-0.233860656	-0.000011075
O	-1.031224423	1.971415835	0.000039774
C	-0.733495875	0.800112862	-0.000014837
F	-3.079570285	0.370731773	-0.000044764
F	-1.835703593	-1.026966581	-1.087962639
F	-1.835719961	-1.026888442	1.088004010

H	1.400298298	2.321587475	-0.000038975
H	0.241978649	-1.821724071	0.000020489
H	3.793856279	1.644221907	-0.000030473
H	4.391060358	-0.765890932	0.000009307
H	2.605295849	-2.486798926	0.000036418

HBpin

22

scf done: -411.772795

B	-0.082545	0.089470	-0.754392
O	0.674762	1.178781	-0.426527
O	0.567395	-1.098963	-0.573240
C	2.024685	0.709316	-0.195033
C	1.800265	-0.811405	0.129339
H	-1.197549	0.167997	-1.157557
C	2.641283	1.520017	0.935711
C	2.801703	0.942284	-1.492095
C	2.889031	-1.742232	-0.384633
C	1.536603	-1.080501	1.612062
H	2.736889	2.564183	0.626077
H	3.639889	1.141745	1.178421
H	2.025316	1.489090	1.836093
H	2.754895	2.004829	-1.744373
H	2.369444	0.376678	-2.322554
H	3.852012	0.656707	-1.383029
H	2.635097	-2.775238	-0.132220
H	3.850406	-1.501983	0.081468
H	2.997545	-1.675606	-1.468534
H	0.748959	-0.428955	2.001326
H	2.440713	-0.932579	2.209810
H	1.208523	-2.116636	1.728784

Intermediate **11a**

67

scf done: -1790.043133

C	-4.703146	1.657952	-2.145377

C	-3.471983	1.242753	-1.651587
C	-3.395512	0.196943	-0.725256
C	-5.872857	1.035342	-1.713607
C	-5.807085	-0.002136	-0.787687
C	-4.573681	-0.419477	-0.293935
H	-4.751076	2.468311	-2.866456
H	-2.554457	1.727602	-1.974406
H	-6.835053	1.360335	-2.098380
H	-6.716600	-0.487026	-0.445963
H	-4.536067	-1.225685	0.432940
C	-2.280295	-4.254005	0.123875
C	-1.365599	-4.608419	1.111490
C	-0.636544	-3.620535	1.771466
C	-2.464690	-2.913908	-0.207318
C	-1.740083	-1.916997	0.451983
C	-0.822209	-2.282043	1.444925
H	-2.849504	-5.020631	-0.393415
H	-1.218410	-5.654225	1.364684
H	0.080570	-3.894427	2.539488
H	-3.174091	-2.651321	-0.986912
H	-0.245355	-1.505528	1.940491
Sn	0.556745	1.596533	0.354456
P	-1.750293	-0.152394	-0.017881
N	-0.547988	0.239443	-1.033361
N	-1.361303	0.809668	1.217889
C	-0.044711	-0.474361	-2.216416
C	-1.188470	-1.008167	-3.092110
C	0.873559	-1.639791	-1.808951
C	0.760254	0.540772	-3.039363
C	-1.161435	1.832785	3.388691
C	-2.954291	0.145621	3.007673
C	-3.109805	2.412520	1.928400
H	1.349867	-2.085044	-2.690719
H	0.314889	-2.424929	-1.289191
H	1.656809	-1.278288	-1.135000
H	1.138246	0.077200	-3.957742
H	1.621811	0.912055	-2.474135
H	0.129502	1.393921	-3.312831

H	-1.685093	2.184025	4.284642
H	-0.602167	2.682324	2.977050
H	-0.446329	1.056452	3.681917
H	-3.493285	0.515659	3.887235
H	-2.290982	-0.665906	3.323183
H	-3.620930	2.842443	2.798289
H	-3.871072	2.046050	1.232157
H	-2.547166	3.208659	1.428233
H	-0.778778	-1.494887	-3.984117
H	-1.850310	-0.198822	-3.415679
H	-1.790408	-1.752549	-2.560688
C	-2.154946	1.283985	2.354799
H	-3.697212	-0.267773	2.317282
H	1.452432	0.253246	1.168099
O	3.498922	0.947747	-0.922686
C	7.747632	0.564945	-0.744264
C	8.255942	-0.370939	0.160510
C	7.393636	-1.131574	0.948201
C	6.374924	0.742063	-0.862532
C	5.506182	-0.019480	-0.072757
C	6.017452	-0.954640	0.830512
H	8.425550	1.154403	-1.353427
H	9.329411	-0.505973	0.252127
H	7.791980	-1.856489	1.650850
H	5.955234	1.463927	-1.556217
H	5.334744	-1.539949	1.441726
C	4.040834	0.156633	-0.175109
H	3.425663	-0.478720	0.492572

Intermediate **11b**

70

scf done: -1829.357217

C	1.268022	2.929087	-1.917805
C	0.559201	1.802054	-1.513206
C	-0.310668	1.858343	-0.419128
C	1.124448	4.128502	-1.225831
C	0.285850	4.189522	-0.114207

C	-0.423806	3.060768	0.288306
H	1.939696	2.866943	-2.768547
H	0.673505	0.861399	-2.044135
H	1.670457	5.011579	-1.544624
H	0.176266	5.119244	0.436383
H	-1.073705	3.128240	1.155499
C	-4.812646	2.273344	0.550916
C	-5.572877	1.271614	1.146710
C	-4.998966	0.029563	1.412278
C	-3.476381	2.040626	0.232504
C	-2.884077	0.806996	0.520030
C	-3.666077	-0.203418	1.097832
H	-5.259657	3.237193	0.326674
H	-6.615160	1.453403	1.391737
H	-5.592579	-0.762825	1.857789
H	-2.907027	2.822921	-0.259300
H	-3.227872	-1.182407	1.271061
Sn	-0.365792	-2.479467	-0.162696
P	-1.197433	0.312920	0.015932
N	-1.210889	-0.710491	-1.239516
N	-0.407681	-0.615517	1.084307
C	-2.027891	-0.717452	-2.463351
C	-2.267878	0.692019	-3.027396
C	-3.389286	-1.388385	-2.211604
C	-1.250830	-1.530896	-3.508846
C	-1.363327	-0.905461	3.364856
C	0.244357	0.949572	2.905521
C	1.020522	-1.424755	2.864159
H	-3.934327	-1.520980	-3.153765
H	-4.007760	-0.783354	-1.541426
H	-3.254788	-2.370754	-1.745911
H	-1.794231	-1.563071	-4.459756
H	-1.101840	-2.564920	-3.174351
H	-0.264154	-1.087933	-3.681492
H	-1.096495	-0.956344	4.427014
H	-1.718726	-1.892932	3.050348
H	-2.187115	-0.192940	3.259465
H	0.504238	1.001957	3.968742

H	-0.590071	1.640744	2.739946
H	1.273590	-1.345828	3.927302
H	1.909997	-1.196981	2.271152
H	0.751010	-2.470509	2.667535
H	-2.872887	0.626011	-3.938538
H	-1.328574	1.191716	-3.280247
H	-2.813915	1.321238	-2.316543
C	-0.144845	-0.483885	2.525242
H	1.104919	1.293379	2.324458
H	-1.979902	-2.987748	0.498972
O	3.311503	-2.242742	0.292334
C	5.438107	-2.370493	-0.763913
H	6.328506	-2.330048	-0.126753
H	5.152719	-3.412673	-0.907115
H	5.697533	-1.918446	-1.726136
C	3.276220	1.937970	0.580020
C	4.484422	2.616943	0.431444
C	5.638307	1.918816	0.079933
C	3.218818	0.562584	0.388328
C	4.375416	-0.147691	0.047022
C	5.582254	0.541687	-0.117557
H	2.373056	2.485578	0.829399
H	4.524395	3.691582	0.582733
H	6.580846	2.444010	-0.039619
H	2.276304	0.030420	0.488572
H	6.487965	0.007484	-0.387436
C	4.287759	-1.636042	-0.108177

Intermediate **11c**

70

scf done: -2127.0088108

C	3.668679290	1.838835019	3.279813783
C	2.794152532	1.228931941	2.388111734
C	3.277368446	0.638618958	1.214968410
C	5.034968863	1.866842638	3.006593369
C	5.524193534	1.284034332	1.840587892
C	4.648801440	0.673309447	0.946321689

C	4.232062423	-3.269332888	-1.162379758
C	3.695868589	-3.502436372	-2.426319239
C	2.726998902	-2.643804350	-2.942037490
C	3.797677990	-2.180398283	-0.411010201
C	2.827777333	-1.313418362	-0.923289381
C	2.294227240	-1.554381839	-2.195028937
Sn	-0.721911487	0.840645714	-0.377223756
P	2.032962025	0.015857469	0.038145525
N	0.669833935	-0.458562588	0.778645013
N	1.406014129	1.163126014	-0.915322622
C	0.362301987	-1.711464317	1.480477032
C	1.442850293	-2.054521363	2.515794582
C	0.191694478	-2.882599234	0.496338083
C	-0.965592828	-1.481779400	2.214444245
C	1.043087773	2.786115434	-2.661058404
C	3.333793420	1.868294128	-2.316397905
C	2.340272074	3.438207080	-0.621488652
C	2.040951312	2.293143803	-1.603825217
O	-4.190598738	0.764126206	-1.907464773
C	-5.022058040	1.642409131	0.132174465
C	-3.342299046	-3.070220098	-0.438868208
C	-3.811170881	-3.417971182	0.827003573
C	-4.486623384	-2.479970172	1.605740319
C	-3.552395671	-1.788003208	-0.930108785
C	-4.226305771	-0.838730040	-0.149169000
C	-4.690504826	-1.190916167	1.125655117
C	-4.430901480	0.503986538	-0.751989701
F	-4.994179154	2.807670776	-0.502398785
F	-6.310075567	1.363173054	0.434535863
F	-4.357217742	1.780884746	1.292011633
H	3.284363906	2.295578478	4.186748970
H	1.725912246	1.209910854	2.586609387
H	5.718476213	2.344656464	3.702178909
H	6.588116911	1.306720897	1.624715082
H	5.040481343	0.226263081	0.037078079
H	4.986892958	-3.937537878	-0.758766098
H	4.032930023	-4.354556061	-3.009222998
H	2.304188654	-2.825511265	-3.925409321

H	4.215198362	-2.014199684	0.578202974
H	1.525182678	-0.889949394	-2.579678591
H	-0.218932007	-3.761355682	1.009001492
H	1.144963982	-3.168995478	0.042084858
H	-0.494262086	-2.594921027	-0.306932100
H	-1.250175275	-2.369245870	2.790851166
H	-1.776575414	-1.279972354	1.504091291
H	-0.887411805	-0.627784530	2.895969309
H	1.466136108	3.617141498	-3.235729116
H	0.119781645	3.147359817	-2.190482725
H	0.784848915	1.977634045	-3.353626645
H	3.759578203	2.715926317	-2.864854834
H	3.141490466	1.057227440	-3.025701162
H	2.715483439	4.321009108	-1.152750895
H	3.091882350	3.140231951	0.116298171
H	1.427710571	3.719907259	-0.084432948
H	1.176324037	-2.971975568	3.052727120
H	1.557561177	-1.246740959	3.245630796
H	2.414405523	-2.223824119	2.039033976
H	4.090461638	1.528025618	-1.601664497
H	-0.938793278	-0.384328110	-1.681143660
H	-2.803240184	-3.795066009	-1.039702358
H	-3.644171986	-4.419694337	1.211035969
H	-4.850245476	-2.749094952	2.591954879
H	-3.185175065	-1.496740166	-1.907858555
H	-5.214395432	-0.473445008	1.745551544

Transition state **TS-12a**

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scf done: -1790.036183

C	-0.664135	-4.297038	0.432167
C	-1.234478	-3.031205	0.346524
C	-0.456012	-1.924540	-0.013696
C	0.689775	-4.468190	0.155648
C	1.470424	-3.372124	-0.203534
C	0.904110	-2.103423	-0.283698
H	-1.277850	-5.147477	0.713694

H	-2.291517	-2.909500	0.563370
H	1.137909	-5.455235	0.221588
H	2.526177	-3.496934	-0.416279
H	1.521063	-1.248907	-0.547913
C	-4.683884	-1.299641	-1.734436
C	-5.551557	-0.340924	-1.216451
C	-5.083402	0.600341	-0.302416
C	-3.349253	-1.315919	-1.341123
C	-2.872275	-0.374872	-0.423003
C	-3.749853	0.583737	0.091481
H	-5.044499	-2.032712	-2.449588
H	-6.592615	-0.327265	-1.525193
H	-5.758198	1.349099	0.101293
H	-2.677281	-2.058068	-1.762203
H	-3.374361	1.318682	0.798350
Sn	0.368174	2.201880	0.648092
P	-1.111856	-0.225167	0.027387
N	-0.904746	0.527844	1.444548
N	-0.291627	0.818578	-0.923946
C	-0.972704	0.008441	2.817689
C	-2.288973	-0.739902	3.072969
C	-0.918654	1.229168	3.747712
C	0.220969	-0.909990	3.138296
C	-1.778373	1.529259	-2.817522
C	-0.052832	-0.279752	-3.128707
C	0.633703	2.093408	-2.775021
H	-1.023284	0.924082	4.794419
H	-1.722980	1.932984	3.506963
H	0.040265	1.754201	3.651656
H	0.243267	-1.151324	4.207791
H	1.159900	-0.411896	2.871950
H	0.168215	-1.849867	2.581078
H	-1.744349	1.857456	-3.862741
H	-2.074578	2.384520	-2.199781
H	-2.553201	0.763739	-2.735402
H	-0.118595	-0.128062	-4.212083
H	-0.746556	-1.086332	-2.863754
H	0.672379	2.196102	-3.865121

H	1.630024	1.853978	-2.398917
H	0.359075	3.070481	-2.359326
H	-2.343622	-1.071055	4.116232
H	-2.370287	-1.630330	2.441085
H	-3.150185	-0.095730	2.868494
C	-0.389465	1.020974	-2.385930
H	0.961805	-0.610849	-2.883324
H	1.925138	1.268378	1.177146
O	2.836704	2.628722	-0.478611
C	4.329172	-1.119122	-1.819959
C	4.750739	-2.044464	-0.867107
C	4.643716	-1.740872	0.491894
C	3.813849	0.112367	-1.418168
C	3.707471	0.419831	-0.062100
C	4.123696	-0.514356	0.889781
H	4.417079	-1.349060	-2.877625
H	5.164683	-2.998595	-1.180558
H	4.964591	-2.462235	1.237314
H	3.510735	0.857599	-2.145400
H	4.029236	-0.276797	1.947147
C	3.213932	1.776702	0.363432
H	3.648297	2.108359	1.326565

Transition state **TS-12b**

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scf done: -1829.350366

C	1.292775	4.252055	0.773580
C	1.686783	2.924967	0.635851
C	0.799659	1.971285	0.123703
C	0.008324	4.636808	0.397594
C	-0.880645	3.692598	-0.110488
C	-0.491991	2.362824	-0.243354
C	5.066589	0.865183	-1.298239
C	5.723767	-0.265591	-0.820508
C	5.029812	-1.203482	-0.059043
C	3.716302	1.057402	-1.019665
C	3.011549	0.120122	-0.257935

C	3.682005	-1.010489	0.220805
Sn	-0.514971	-2.135198	0.313646
P	1.212082	0.198564	0.052643
N	0.808542	-0.646238	1.369169
N	0.324302	-0.617523	-1.048802
C	0.815626	-0.268554	2.787911
C	2.178764	0.292802	3.218150
C	0.543987	-1.552541	3.584924
C	-0.294644	0.750824	3.101412
C	1.762077	-1.574063	-2.852460
C	0.702076	0.693491	-3.125968
C	-0.704045	-1.352403	-3.126615
C	0.538911	-0.703820	-2.509980
O	-2.885551	-2.191357	-0.923847
C	-4.096777	1.721807	-1.814269
C	-4.249366	2.640868	-0.779014
C	-4.066604	2.230347	0.542620
C	-3.774074	0.395765	-1.529420
C	-3.595212	-0.022886	-0.210222
C	-3.742288	0.907794	0.823052
C	-3.294833	-1.487483	0.038123
C	-4.100701	-2.169239	1.136100
H	1.989765	4.983799	1.170790
H	2.691836	2.636122	0.929122
H	-0.300260	5.672941	0.501509
H	-1.884280	3.984187	-0.400605
H	-1.193072	1.625032	-0.625619
H	5.604614	1.598890	-1.890870
H	6.776884	-0.415203	-1.039073
H	5.538955	-2.085701	0.316834
H	3.216136	1.942891	-1.400649
H	3.132305	-1.738106	0.811672
H	0.581845	-1.354735	4.661619
H	1.289496	-2.319149	3.345748
H	-0.451484	-1.953713	3.356781
H	-0.376188	0.914601	4.182766
H	-1.254316	0.376163	2.728757
H	-0.101941	1.717004	2.625617

H	1.824233	-1.734158	-3.935052
H	1.673887	-2.553019	-2.367264
H	2.699048	-1.114428	-2.526548
H	0.827731	0.612104	-4.211375
H	1.581553	1.213276	-2.732650
H	-0.595829	-1.403916	-4.215943
H	-1.598891	-0.777171	-2.881356
H	-0.859436	-2.369752	-2.752647
H	2.181169	0.509783	4.292450
H	2.409037	1.225971	2.693628
H	2.978468	-0.424581	3.007245
H	-0.179714	1.309877	-2.924441
H	-1.995969	-1.215716	0.999037
H	-4.238486	2.033099	-2.844969
H	-4.506061	3.673464	-0.997994
H	-4.165037	2.946075	1.353266
H	-3.670403	-0.340524	-2.319121
H	-3.575161	0.603366	1.852174
H	-3.639539	-3.131253	1.370505
H	-5.105282	-2.356751	0.737961
H	-4.190739	-1.570459	2.045074

Transition state **TS-12c**

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scf done: -2127.00751161

C	2.307656853	3.839767971	1.641980567
C	2.481200101	2.512957431	1.261621004
C	1.492582057	1.852898226	0.522939192
C	1.145452057	4.517743400	1.283422355
C	0.155083034	3.865138341	0.552760710
C	0.321503183	2.535646540	0.177433551
C	5.609438128	0.292488128	-0.918932191
C	6.026976932	-1.011227671	-0.664325181
C	5.129218589	-1.940092467	-0.142711198
C	4.294932038	0.667013829	-0.655645974
C	3.387097398	-0.259041126	-0.132267120
C	3.816686064	-1.566105491	0.122277009

Sn	-0.427069129	-1.938943449	-0.210138564
P	1.610045185	0.087702241	0.099251222
N	0.946528036	-0.922066295	1.182984539
N	0.698321014	-0.322417993	-1.185740430
C	0.876205847	-0.841244991	2.648850212
C	2.265463221	-0.621959159	3.263917131
C	0.328971938	-2.189036108	3.138726278
C	-0.083419536	0.273998308	3.099884750
C	1.977979201	-1.153507946	-3.148173326
C	1.443053307	1.293297719	-2.922957198
C	-0.382782085	-0.341527478	-3.344362751
C	0.954500336	-0.131465667	-2.625527323
O	-3.203996107	-1.233424712	-1.653150456
C	-3.337661037	2.927648527	-1.796208156
C	-3.301552935	3.665772462	-0.615160965
C	-3.246575991	3.005501381	0.611684008
C	-3.334057421	1.536343772	-1.747160930
C	-3.280391290	0.869847420	-0.520545518
C	-3.228441539	1.615581143	0.661776749
C	-3.302520064	-0.639070881	-0.578551172
C	-4.088473457	-1.394756608	0.535792437
F	-3.800489454	-1.027716790	1.803749775
F	-5.407274787	-1.173166877	0.360675540
F	-3.879768424	-2.711549431	0.454984130
H	3.081312982	4.343459474	2.213424627
H	3.393592892	1.994215346	1.541073334
H	1.010336627	5.555770531	1.572565615
H	-0.754121935	4.387214612	0.274939729
H	-0.459829659	2.023183136	-0.378677141
H	6.306846317	1.019914837	-1.323067709
H	7.052544501	-1.302396441	-0.870490826
H	5.451805560	-2.957365853	0.056831059
H	3.982380109	1.686986092	-0.858782689
H	3.110493638	-2.286771914	0.525672892
H	0.286128394	-2.213406969	4.232681307
H	0.965156003	-3.013307138	2.797219123
H	-0.690776130	-2.357964298	2.768631421
H	-0.238725340	0.232691607	4.184432509

H	-1.052690187	0.153324164	2.604003001
H	0.306355569	1.265434946	2.850729454
H	2.092391396	-1.062908632	-4.234492399
H	1.644195289	-2.173246197	-2.924048747
H	2.960914318	-1.007720064	-2.689519893
H	1.578144903	1.425028718	-4.002039786
H	2.406763260	1.499999055	-2.446221687
H	-0.264341094	-0.193239553	-4.423514376
H	-1.130193371	0.363047494	-2.968828023
H	-0.774734850	-1.352988699	-3.186614410
H	2.201285995	-0.618637827	4.357683032
H	2.690345938	0.339602144	2.957260134
H	2.956799443	-1.414096096	2.958515405
H	0.718656583	2.035390265	-2.573594299
H	-1.840572816	-0.864445444	0.312383270
H	-3.383705278	3.433491700	-2.755632336
H	-3.318109793	4.751420306	-0.650530706
H	-3.204688699	3.573218823	1.536184008
H	-3.385863309	0.943619118	-2.654222676
H	-3.158248803	1.118153033	1.620795865

Intermediate **13a**

67

scf done: -1790.105462

C	1.335834	3.576295	0.286106
C	0.833166	2.310472	0.001448
C	-0.506870	2.006763	0.259106
C	0.504174	4.549314	0.834819
C	-0.832957	4.255658	1.095007
C	-1.336947	2.991101	0.807477
H	2.378823	3.795501	0.077091
H	1.484131	1.550482	-0.420407
H	0.896234	5.537563	1.056157
H	-1.485988	5.012295	1.519265
H	-2.382583	2.777910	1.010112
C	-4.546194	1.452337	-1.892462
C	-5.331311	0.312314	-1.748826

C	-4.838532	-0.787739	-1.048672
C	-3.268357	1.495201	-1.339444
C	-2.767856	0.398486	-0.632835
C	-3.565038	-0.743829	-0.495461
H	-4.925601	2.310691	-2.438504
H	-6.325389	0.278515	-2.184433
H	-5.445568	-1.681002	-0.937684
H	-2.663041	2.387776	-1.467091
H	-3.174052	-1.603847	0.042113
Sn	0.239158	-2.298794	0.329652
P	-1.052678	0.289313	-0.014639
N	-0.068113	-0.533694	-1.008990
N	-0.928017	-0.673507	1.286181
C	0.006118	-0.517189	-2.481778
C	-0.027861	0.910364	-3.047222
C	-1.135292	-1.337595	-3.108754
C	1.349573	-1.152289	-2.862511
C	-1.310926	-1.841781	3.365758
C	-2.768979	0.091440	2.783155
C	-0.369592	0.467867	3.420909
H	-0.995529	-1.427632	-4.192269
H	-2.108734	-0.871022	-2.929194
H	-1.157767	-2.347398	-2.682799
H	1.474088	-1.169453	-3.951130
H	1.412352	-2.188888	-2.506399
H	2.178164	-0.591902	-2.420110
H	-1.607986	-1.754201	4.416359
H	-0.300625	-2.268292	3.340480
H	-1.996449	-2.539040	2.870233
H	-3.060029	0.194759	3.834205
H	-3.486980	-0.570088	2.289044
H	-0.689464	0.610810	4.459953
H	-0.318029	1.450993	2.942413
H	0.636272	0.037859	3.429274
H	0.060072	0.878990	-4.138887
H	0.798509	1.510988	-2.656827
H	-0.968541	1.417797	-2.809000
C	-1.341900	-0.467955	2.682392

H	-2.849120	1.080937	2.321088
C	4.082538	-0.885714	-0.546609
C	3.588738	-0.069346	0.468103
C	4.087185	1.232621	0.588204
C	5.042042	-0.406349	-1.439075
C	5.523611	0.895284	-1.322815
C	5.043415	1.715807	-0.300276
H	3.696226	-1.896193	-0.630163
H	3.712585	1.874698	1.383449
H	5.413090	-1.053994	-2.228438
H	6.268885	1.268186	-2.019049
H	5.419921	2.729618	-0.194026
H	1.734608	0.193058	1.483982
O	2.038278	-1.827275	1.135446
C	2.533942	-0.564623	1.440567
H	2.986108	-0.589332	2.446403

Intermediate **13b**

70

scf done: -1829.413343

C	-0.067465	4.182871	1.106886
C	-0.578060	3.096993	0.402214
C	-0.523786	1.804841	0.937594
C	0.501419	3.996302	2.364934
C	0.546364	2.719635	2.917406
C	0.036795	1.635771	2.208037
H	-0.116732	5.176115	0.671017
H	-1.019763	3.268268	-0.572840
H	0.903653	4.843561	2.912008
H	0.986642	2.561490	3.897224
H	0.090875	0.642387	2.638742
C	-4.812703	1.937339	-0.644395
C	-5.381293	0.980467	-1.479354
C	-4.644419	-0.142819	-1.851798
C	-3.505030	1.781218	-0.188683
C	-2.751018	0.669898	-0.574405
C	-3.340101	-0.296560	-1.399602

H	-5.387693	2.806780	-0.340154
H	-6.399717	1.105135	-1.834987
H	-5.086037	-0.897793	-2.494981
H	-3.084429	2.521178	0.484429
H	-2.768517	-1.175530	-1.686957
Sn	0.275897	-2.250724	-0.435635
P	-1.058688	0.309792	0.014208
N	-0.043359	-0.168278	-1.156977
N	-0.985721	-1.017637	0.939775
C	0.285674	0.346602	-2.498419
C	0.303260	1.876957	-2.547676
C	-0.713925	-0.176154	-3.544436
C	1.688060	-0.163007	-2.858141
C	-2.795810	-2.599572	1.468771
C	-2.713463	-0.426493	2.676950
C	-0.932822	-2.140035	3.084325
H	-0.394095	0.102744	-4.555161
H	-1.713285	0.238406	-3.380712
H	-0.781293	-1.269510	-3.498627
H	1.962818	0.164104	-3.867108
H	1.729584	-1.259937	-2.847224
H	2.431264	0.211746	-2.152127
H	-3.424405	-3.013868	2.265528
H	-2.229701	-3.425913	1.023423
H	-3.450200	-2.178350	0.697994
H	-3.281924	-0.862185	3.505689
H	-3.433804	-0.005758	1.968180
H	-1.518035	-2.590239	3.894386
H	-0.268725	-1.383167	3.515968
H	-0.300432	-2.919930	2.644464
H	0.647309	2.216171	-3.531057
H	0.980161	2.281721	-1.788952
H	-0.703122	2.285826	-2.397106
C	-1.851350	-1.517764	2.021545
H	-2.109094	0.389778	3.082043
O	2.033006	-2.001805	0.532184
C	2.434481	-0.834496	1.199273
C	3.109689	-1.214440	2.518420

H	2.413786	-1.792624	3.134649
H	3.422835	-0.321198	3.070948
H	3.993260	-1.831257	2.324802
C	4.389789	-0.590841	-0.386326
C	3.354380	0.010809	0.333593
C	3.176538	1.391483	0.231208
C	5.226249	0.171664	-1.196625
C	5.037742	1.550957	-1.299802
C	4.010633	2.159164	-0.581465
H	4.511186	-1.668470	-0.326644
H	2.364281	1.869717	0.772194
H	6.023095	-0.309956	-1.756285
H	5.684473	2.145315	-1.938443
H	3.849005	3.230516	-0.661925
H	1.562746	-0.214852	1.438992

Intermediate **13c**

70

scf done: -2127.08150685

C	-0.295528804	2.917065484	3.161653972
C	-0.892150839	2.360894568	2.034369990
C	-0.721691413	1.005132208	1.730030169
C	0.481148009	2.125270221	4.005437589
C	0.645289128	0.772188578	3.724374894
C	0.044108062	0.218224036	2.597657941
C	-5.208440519	1.487669363	0.996391834
C	-5.871412600	1.102996033	-0.164800883
C	-5.167148838	0.479060537	-1.193493963
C	-3.840355818	1.259705176	1.130066321
C	-3.122312552	0.652903864	0.096067850
C	-3.802852325	0.254472213	-1.061043648
Sn	0.048963462	-1.455143181	-1.732540225
P	-1.348785123	0.231735848	0.188803808
N	-0.508627061	0.611273208	-1.149808290
N	-1.062872177	-1.366395245	0.191849304
C	-0.435578739	1.816792988	-1.997646567
C	-0.500001668	3.107961176	-1.177135927

C	-1.570465428	1.826469021	-3.036008059
C	0.906683516	1.781446271	-2.740334532
C	-2.800769663	-3.087638012	-0.139994766
C	-2.525163518	-2.070756312	2.118649905
C	-0.731824560	-3.546548080	1.197166859
C	-1.779155813	-2.484274995	0.840076489
O	1.951333171	-1.434994343	-0.976561736
C	2.349279053	-0.727638187	0.143654747
C	3.204927168	-1.643732656	1.027622485
C	4.014719386	0.575737220	-1.238837468
C	3.094193324	0.553274006	-0.190478621
C	2.823113553	1.728554522	0.510567146
C	4.655820348	1.761965842	-1.583516991
C	4.376952023	2.937678373	-0.885710496
C	3.460285551	2.918342373	0.163421023
F	2.516243255	-2.739919049	1.408666914
F	4.327012102	-2.071802924	0.428482266
F	3.575813960	-1.010844076	2.167132281
H	-0.437696590	3.971350346	3.378921338
H	-1.491553882	2.996958987	1.392763791
H	0.952847309	2.562065332	4.880379270
H	1.251832049	0.145407398	4.370361991
H	0.186444988	-0.834690552	2.378513341
H	-5.755447905	1.961158257	1.805979711
H	-6.937546560	1.281148688	-0.267521342
H	-5.681158598	0.166787532	-2.097236758
H	-3.341122891	1.538962003	2.052116084
H	-3.256813936	-0.239164937	-1.860723802
H	-1.433177742	2.649106243	-3.747153641
H	-2.546782525	1.953721304	-2.559261657
H	-1.580703802	0.887213427	-3.601727234
H	0.982199699	2.631959882	-3.426591671
H	1.007428429	0.867259290	-3.339679487
H	1.741276874	1.822045249	-2.038904958
H	-3.298290802	-3.957356530	0.304253682
H	-2.309568796	-3.417384690	-1.062947711
H	-3.567416704	-2.351654899	-0.402700564
H	-3.000818619	-2.952433595	2.561335597

H	-3.314222909	-1.341864271	1.908877056
H	-1.210658904	-4.435409788	1.623061875
H	-0.010795194	-3.157915332	1.922215529
H	-0.168059478	-3.858735533	0.310130231
H	-0.349417248	3.974026796	-1.830970809
H	0.277721969	3.119372264	-0.407571966
H	-1.483531262	3.223750713	-0.705820490
H	-1.850117629	-1.646848466	2.867250127
H	4.200970745	-0.338291282	-1.793129785
H	2.097313917	1.719188465	1.319558709
H	5.369783708	1.772476414	-2.401581659
H	4.871131267	3.864819237	-1.160318671
H	3.233256399	3.831153965	0.706476500
H	1.504507844	-0.457451919	0.787031336

Intermediate **14a**

89

scf done: -2201.888084

C	-3.705089	2.909792	2.320615
C	-3.526122	1.950338	1.328884
C	-2.516132	0.987840	1.439445
C	-2.880941	2.917007	3.444380
C	-1.882180	1.956249	3.573538
C	-1.702767	1.001388	2.576786
C	-6.062521	-1.538627	0.027760
C	-6.043303	-2.379626	-1.080546
C	-4.864419	-2.546354	-1.805591
C	-4.909075	-0.855751	0.408936
C	-3.727655	-1.000664	-0.323381
C	-3.716156	-1.862738	-1.427082
Sn	0.391105	-1.065612	-1.076445
P	-2.131045	-0.230597	0.124052
N	-1.312820	0.358181	-1.144971
N	-1.029112	-1.307213	0.635166
C	-1.656954	1.260476	-2.258929
C	-2.582012	2.397983	-1.816818
C	-2.330674	0.488135	-3.406106

C	-0.347330	1.866295	-2.782208
C	-1.464241	-3.741933	0.640950
C	-2.260838	-2.364500	2.560266
C	0.191805	-2.685045	2.195837
C	-1.160911	-2.497657	1.494825
O	1.770444	0.108648	-0.152095
C	1.607074	1.077454	0.848336
C	2.427229	3.012624	-0.549623
C	1.448399	2.479997	0.296425
C	0.329658	3.256290	0.601221
C	2.273209	4.282241	-1.098410
C	1.142526	5.045842	-0.800940
C	0.174592	4.531832	0.057397
B	4.074626	-0.225466	-1.239449
O	4.264509	-1.573609	-1.067373
O	4.734741	0.530160	-0.299704
C	4.890485	-1.766718	0.217171
C	5.539853	-0.359725	0.496709
C	5.887965	-2.913236	0.106385
C	3.785700	-2.137157	1.208097
C	5.479202	0.087218	1.951648
C	6.974563	-0.237484	-0.023250
H	-4.490497	3.652159	2.215611
H	-4.181602	1.961468	0.464781
H	-3.019320	3.668069	4.216294
H	-1.233352	1.953798	4.444215
H	-0.911721	0.265346	2.668251
H	-6.975855	-1.414757	0.601744
H	-6.943339	-2.910462	-1.375945
H	-4.840045	-3.210826	-2.663866
H	-4.932041	-0.222215	1.289956
H	-2.795281	-2.000759	-1.987535
H	-2.479049	1.143540	-4.272080
H	-3.308301	0.098316	-3.106440
H	-1.703787	-0.354415	-3.721538
H	-0.549207	2.528830	-3.631028
H	0.340686	1.085946	-3.133347
H	0.157881	2.438733	-2.002905

H	-1.481056	-4.646371	1.260477
H	-0.700025	-3.877128	-0.133421
H	-2.436936	-3.646306	0.147800
H	-2.306566	-3.284988	3.152504
H	-3.245750	-2.218526	2.105155
H	0.173281	-3.557036	2.859693
H	0.447574	-1.798214	2.786533
H	0.991067	-2.836740	1.461653
H	-2.719263	3.111237	-2.636985
H	-2.160219	2.933992	-0.961826
H	-3.573342	2.011384	-1.552015
H	-2.069778	-1.535592	3.246667
H	2.502681	1.054385	1.489639
H	3.306892	2.419289	-0.777000
H	-0.440794	2.856833	1.252926
H	3.036576	4.678074	-1.762129
H	1.020368	6.033711	-1.235472
H	-0.710139	5.115204	0.297483
H	0.745205	0.845710	1.487426
H	3.559842	0.235011	-2.205926
H	5.352591	-3.841622	-0.111192
H	6.427772	-3.043753	1.050639
H	6.612358	-2.745124	-0.692644
H	3.294075	-3.046322	0.848598
H	3.031848	-1.348564	1.263167
H	4.190121	-2.334909	2.205630
H	5.921094	1.082995	2.047100
H	6.044255	-0.601117	2.589491
H	4.450700	0.136087	2.314116
H	7.041681	-0.531743	-1.074577
H	7.667465	-0.852262	0.559415
H	7.286868	0.807426	0.055258

Intermediate **14b**

92

scf done: -2241.202035

C	-4.218629	2.980709	1.603981

C	-3.849966	1.920634	0.781682
C	-2.811096	1.057538	1.148381
C	-3.558881	3.190160	2.813240
C	-2.535152	2.329281	3.198350
C	-2.166310	1.272604	2.370691
C	-5.987768	-1.913150	-0.252276
C	-5.779775	-2.911601	-1.198761
C	-4.516172	-3.082340	-1.762294
C	-4.938295	-1.079040	0.127623
C	-3.672372	-1.231218	-0.444026
C	-3.470787	-2.249261	-1.384459
Sn	0.479063	-1.089362	-0.791668
P	-2.191892	-0.280923	0.055651
N	-1.274018	0.218714	-1.182949
N	-1.087573	-1.203023	0.801948
C	-1.538824	0.932048	-2.444874
C	-2.580205	2.042640	-2.279678
C	-2.018893	-0.042820	-3.533781
C	-0.215702	1.565259	-2.900882
C	-1.108642	-3.633737	1.185046
C	-2.514603	-2.179464	2.635281
C	-0.019225	-2.058769	2.801673
C	-1.202302	-2.243182	1.837530
O	1.665081	0.262490	0.160185
C	1.224359	1.294905	1.006688
C	2.141251	1.361684	2.229065
C	2.284887	3.088995	-0.430735
C	1.173178	2.629436	0.281524
C	0.017193	3.411454	0.301717
C	2.231028	4.293128	-1.126433
C	1.066289	5.062846	-1.112865
C	-0.039412	4.621081	-0.390581
B	4.034565	-0.032939	-1.204746
O	4.078056	-1.401949	-1.168706
O	4.854475	0.555261	-0.275917
C	4.802008	-1.784474	0.020146
C	5.640715	-0.490885	0.335034
C	5.632390	-3.021746	-0.295396

C	3.766254	-2.109870	1.097731
C	5.804563	-0.186458	1.817603
C	7.005482	-0.472478	-0.357593
H	-5.023510	3.642929	1.299625
H	-4.379887	1.773776	-0.152834
H	-3.845805	4.018358	3.454206
H	-2.016483	2.481553	4.139956
H	-1.358996	0.612860	2.668438
H	-6.966716	-1.784881	0.199642
H	-6.598096	-3.561993	-1.492906
H	-4.345840	-3.865055	-2.495151
H	-5.107280	-0.324091	0.888582
H	-2.484221	-2.389227	-1.819227
H	-2.115680	0.472803	-4.496243
H	-2.993042	-0.473234	-3.281927
H	-1.300821	-0.861948	-3.658835
H	-0.352737	2.076584	-3.860092
H	0.561741	0.803438	-3.045905
H	0.149051	2.286482	-2.166682
H	-1.168031	-4.424966	1.941487
H	-0.159559	-3.753220	0.648968
H	-1.925710	-3.776304	0.469353
H	-2.501358	-2.943420	3.419950
H	-3.380299	-2.377836	1.995839
H	-0.009098	-2.846179	3.564209
H	-0.075365	-1.088215	3.307037
H	0.933575	-2.094410	2.260435
H	-2.661572	2.618756	-3.208044
H	-2.298925	2.726784	-1.473598
H	-3.570489	1.620156	-2.072634
H	-2.655851	-1.208214	3.117923
H	2.119324	0.404054	2.761020
H	1.825986	2.154824	2.916048
H	3.169136	1.562040	1.910561
H	3.189338	2.489131	-0.448928
H	-0.857597	3.061782	0.842567
H	3.099564	4.632252	-1.683727
H	1.023671	5.999995	-1.660166

H	-0.952779	5.209457	-0.373853
H	0.207912	1.080198	1.357174
H	3.447054	0.572491	-2.040403
H	4.964637	-3.859843	-0.513386
H	6.256846	-3.294646	0.562298
H	6.275007	-2.866437	-1.163868
H	3.115633	-2.908245	0.725604
H	3.142311	-1.237994	1.308387
H	4.244014	-2.456079	2.019548
H	6.374034	0.739094	1.940393
H	6.349616	-0.995148	2.316505
H	4.838765	-0.058830	2.308465
H	6.906515	-0.670395	-1.428817
H	7.686687	-1.211887	0.074508
H	7.448441	0.519844	-0.236724

Intermediate **14c**

92

scf done: -2538.86958903

C	-3.893558591	3.527511239	0.647204569
C	-3.672951950	2.274513651	0.082965046
C	-2.842432027	1.341479216	0.715805636
C	-3.289051758	3.869363465	1.855358926
C	-2.474026419	2.946134473	2.503268660
C	-2.258498538	1.692727826	1.938098369
C	-6.343100340	-1.365298515	-0.442043447
C	-6.222364744	-2.592175942	-1.087271242
C	-4.959689022	-3.087681960	-1.409353934
C	-5.205265378	-0.627404835	-0.121851296
C	-3.936868178	-1.107596381	-0.457010172
C	-3.825841747	-2.349560877	-1.094700909
Sn	0.266132060	-1.456886396	-0.382336697
P	-2.373286163	-0.272204602	-0.023872517
N	-1.316648966	-0.169610967	-1.252988163
N	-1.450945738	-1.126687293	1.001508097
C	-1.443139108	0.215104261	-2.671643617
C	-2.446698020	1.353496106	-2.873896606
C	-1.873363448	-0.989626592	-3.526566335

C	-0.064897387	0.688057976	-3.152701250
C	-1.847578706	-3.429716948	1.785806467
C	-3.143572799	-1.568899546	2.814325383
C	-0.680516351	-1.742293428	3.219977247
C	-1.793404640	-1.943913056	2.182425153
O	1.470122737	0.078917878	0.281969794
C	1.008365184	1.304105619	0.733827463
C	1.727342950	1.645265867	2.044322450
C	2.338263387	2.520107020	-1.036870853
C	1.168625650	2.421319538	-0.281776350
C	0.128397475	3.324970780	-0.501523411
C	2.457185498	3.505483013	-2.012690932
C	1.411420498	4.400743895	-2.239696974
C	0.247537376	4.311804931	-1.478501197
B	3.758560887	-0.828123407	-1.573827914
O	3.839207679	-2.079170978	-1.031548841
O	4.701914353	0.036689388	-1.094873103
C	4.767556506	-2.010181278	0.077858188
C	5.609331658	-0.725654721	-0.264417021
C	5.571449517	-3.302935130	0.118499120
C	3.932489884	-1.869232237	1.350619542
C	5.996567352	0.116687127	0.942308257
C	6.842408050	-1.018205357	-1.121669769
F	1.542560231	0.682648347	2.972675261
F	3.056747384	1.798126523	1.904243524
F	1.250065926	2.792068411	2.580508923
H	-4.537856920	4.238398048	0.138700812
H	-4.150841136	2.035399658	-0.860332469
H	-3.454747703	4.850453083	2.289834299
H	-1.992001434	3.200120473	3.441948107
H	-1.610613404	0.984184832	2.442941218
H	-7.324141262	-0.981151515	-0.179664962
H	-7.110695497	-3.165868079	-1.334088878
H	-4.858825610	-4.048787981	-1.903917800
H	-5.312357367	0.314264613	0.406214726
H	-2.841394682	-2.738880195	-1.341551427
H	-1.844085799	-0.733625465	-4.591917378
H	-2.891744047	-1.307794703	-3.284587473

H	-1.196567280	-1.836982503	-3.364483706
H	-0.103252490	0.940533101	-4.218252777
H	0.691179570	-0.097963598	-3.030181751
H	0.266025394	1.566635017	-2.596450078
H	-2.067518786	-4.057061129	2.657341312
H	-0.889755514	-3.760634562	1.367218597
H	-2.626899553	-3.599900742	1.035625499
H	-3.292033152	-2.152995911	3.728846757
H	-3.977363363	-1.791582831	2.141284149
H	-0.829945268	-2.402861378	4.081610639
H	-0.654926325	-0.708385231	3.577098003
H	0.302674475	-1.961875038	2.787446372
H	-2.462893990	1.655458832	-3.926850355
H	-2.170699437	2.224513320	-2.271329212
H	-3.462352347	1.031723469	-2.611812261
H	-3.190539094	-0.510217718	3.085215180
H	3.143113547	1.811440553	-0.873316536
H	-0.787340413	3.246692981	0.078272689
H	3.367774219	3.569714740	-2.600804348
H	1.503162268	5.163716522	-3.007121509
H	-0.571549372	5.004423344	-1.649371349
H	-0.048400466	1.264850047	1.020211806
H	2.977025832	-0.532457241	-2.419674522
H	4.904408081	-4.137579532	0.350901726
H	6.338563652	-3.251322444	0.898406622
H	6.054985371	-3.510146841	-0.837915838
H	3.259009523	-2.729344500	1.420675787
H	3.319446844	-0.965306522	1.324772235
H	4.566573245	-1.854715748	2.242358195
H	6.559795781	0.993662456	0.611040042
H	6.631503445	-0.462229301	1.621615762
H	5.117389816	0.462527488	1.486102152
H	6.583107721	-1.609305332	-2.005093850
H	7.606469786	-1.555502091	-0.552000065
H	7.267130272	-0.070215643	-1.462684588

Transition state **TS-15a**

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scf done: -2201.886129

C	-3.598708	2.984512	2.278418
C	-3.432326	2.013786	1.295502
C	-2.448900	1.026639	1.425964
C	-2.788657	2.978556	3.412365
C	-1.815272	1.994682	3.560039
C	-1.647481	1.028853	2.571982
H	-4.363919	3.745546	2.158707
H	-4.075399	2.036095	0.422396
H	-2.917357	3.738230	4.177422
H	-1.176361	1.983478	4.437893
H	-0.872294	0.277513	2.675507
C	-6.043585	-1.420987	-0.000083
C	-6.030533	-2.284705	-1.090872
C	-4.845953	-2.498563	-1.793823
C	-4.877796	-0.762201	0.385805
C	-3.690009	-0.954219	-0.325061
C	-3.685484	-1.838427	-1.411160
H	-6.961874	-1.260631	0.556612
H	-6.940178	-2.796866	-1.389632
H	-4.826727	-3.181066	-2.637861
H	-4.896890	-0.110381	1.253356
H	-2.760909	-2.012368	-1.955332
Sn	0.416945	-1.121407	-1.057031
P	-2.081903	-0.211861	0.125678
N	-1.242482	0.341869	-1.146108
N	-1.002577	-1.303915	0.657427
C	-1.566064	1.225329	-2.282390
C	-2.497555	2.370254	-1.874900
C	-2.222614	0.433316	-3.426133
C	-0.247129	1.819519	-2.795260
C	-1.491109	-3.730093	0.683765
C	-2.284986	-2.315822	2.576987
C	0.164090	-2.692048	2.249598
H	-2.351976	1.072300	-4.307135
H	-3.207479	0.053994	-3.137175
H	-1.594431	-0.417837	-3.715166

H	-0.433922	2.460490	-3.663812
H	0.448786	1.032526	-3.114565
H	0.243563	2.411613	-2.021616
H	-1.532065	-4.626804	1.313122
H	-0.720784	-3.889418	-0.079947
H	-2.456345	-3.622314	0.178852
H	-2.357798	-3.230234	3.175691
H	-3.260835	-2.152912	2.108422
H	0.119258	-3.557332	2.920766
H	0.431504	-1.805876	2.836130
H	0.967882	-2.867217	1.526655
H	-2.625925	3.065548	-2.711618
H	-2.085797	2.925349	-1.027398
H	-3.491625	1.987501	-1.613624
C	-1.173504	-2.483157	1.528403
H	-2.084834	-1.486052	3.259545
O	1.839337	0.085947	-0.167456
C	1.688851	1.069115	0.831599
H	2.595455	1.050413	1.453407
C	2.482402	3.038700	-0.546614
C	1.506732	2.470231	0.280460
C	0.367060	3.218089	0.580163
C	2.301595	4.309386	-1.084958
C	1.149147	5.041679	-0.794531
C	0.186005	4.495007	0.048567
H	3.384299	2.477794	-0.766346
H	-0.399491	2.796401	1.220624
H	3.063625	4.730531	-1.734360
H	1.007743	6.030711	-1.220467
H	-0.715040	5.053463	0.287173
H	0.837213	0.821640	1.476629
B	3.718300	-0.182320	-1.078058
O	3.947042	-1.549698	-0.968872
O	4.520080	0.534636	-0.191915
C	4.702488	-1.776572	0.229387
C	5.403263	-0.386471	0.461365
C	5.665423	-2.933587	-0.015338
C	3.725318	-2.160968	1.343612

C	5.545162	0.013703	1.925403
C	6.760765	-0.270751	-0.239332
H	3.322595	0.284057	-2.105406
H	5.098015	-3.856484	-0.166147
H	6.327567	-3.076218	0.845868
H	6.274559	-2.764399	-0.904916
H	3.180783	-3.055061	1.025193
H	2.994959	-1.369491	1.524745
H	4.247193	-2.393050	2.277442
H	6.020980	0.996315	1.991382
H	6.169000	-0.706197	2.466630
H	4.573449	0.074706	2.419534
H	6.677190	-0.536142	-1.297011
H	7.517300	-0.909482	0.227234
H	7.097038	0.768006	-0.177569

Transition state **TS-15b**

92

scf done: -2241.199246

C	-3.962448	3.251303	1.425024
C	-3.674195	2.115240	0.675317
C	-2.672135	1.226796	1.081121
C	-3.256670	3.512046	2.597880
C	-2.269354	2.626999	3.021794
C	-1.980732	1.493536	2.267838
H	-4.738705	3.933608	1.092260
H	-4.235618	1.928834	-0.233985
H	-3.478231	4.401827	3.179394
H	-1.715170	2.821357	3.934935
H	-1.198421	0.815117	2.591530
C	-6.027145	-1.625966	-0.170282
C	-5.891365	-2.638262	-1.115439
C	-4.648467	-2.884170	-1.696418
C	-4.925856	-0.851598	0.189004
C	-3.679313	-1.078945	-0.400912
C	-3.551021	-2.111727	-1.337791
H	-6.990344	-1.439915	0.295004

H	-6.750977	-3.239879	-1.395282
H	-4.534546	-3.678176	-2.427975
H	-5.040556	-0.080993	0.944773
H	-2.581031	-2.311390	-1.785533
Sn	0.446753	-1.260345	-0.742652
P	-2.143489	-0.203856	0.065019
N	-1.187916	0.165668	-1.192016
N	-1.098091	-1.150733	0.870752
C	-1.382232	0.855355	-2.480711
C	-2.332615	2.050828	-2.365302
C	-1.933815	-0.111880	-3.542096
C	-0.005494	1.356513	-2.943671
C	-1.474715	-3.551304	1.316913
C	-2.543259	-1.861684	2.805770
C	-0.059351	-2.129177	2.821382
H	-1.970204	0.376655	-4.522478
H	-2.946890	-0.442182	-3.291975
H	-1.292113	-0.996752	-3.628557
H	-0.094908	1.863347	-3.910778
H	0.698875	0.524713	-3.076277
H	0.427775	2.051413	-2.221036
H	-1.584855	-4.311608	2.098946
H	-0.599856	-3.816733	0.711399
H	-2.359902	-3.589401	0.673127
H	-2.623126	-2.625338	3.587010
H	-3.467743	-1.893562	2.220616
H	-0.129770	-2.881105	3.615665
H	0.069294	-1.143808	3.282974
H	0.841433	-2.342613	2.233939
H	-2.361199	2.596802	-3.314589
H	-2.007968	2.741439	-1.582055
H	-3.354665	1.716785	-2.151838
C	-1.311640	-2.150689	1.933146
H	-2.477002	-0.887601	3.297436
O	1.766238	0.138049	0.063835
C	1.370732	1.211134	0.905784
C	2.189519	1.194864	2.196032
H	2.066751	0.230866	2.701425

H	1.851868	1.989501	2.870671
H	3.249749	1.342989	1.978014
C	2.629006	3.099627	-0.268571
C	1.430705	2.568531	0.219793
C	0.264027	3.325448	0.089531
C	2.645791	4.339234	-0.902834
C	1.471112	5.079103	-1.042804
C	0.278446	4.571203	-0.535303
H	3.552034	2.539549	-0.159855
H	-0.673019	2.927238	0.464946
H	3.582011	4.730552	-1.290347
H	1.488980	6.044679	-1.539647
H	-0.644624	5.136124	-0.631886
H	0.323399	1.047291	1.173615
B	3.519652	-0.009461	-0.943661
O	3.620463	-1.397471	-1.085700
O	4.483143	0.460088	-0.043613
C	4.453746	-1.893843	-0.030328
C	5.328950	-0.636544	0.325490
C	5.240644	-3.088485	-0.558018
C	3.560523	-2.350046	1.128419
C	5.693232	-0.514220	1.800840
C	6.596427	-0.533637	-0.529024
H	3.136264	0.654587	-1.860238
H	4.550935	-3.908646	-0.778088
H	5.963330	-3.437848	0.187723
H	5.773507	-2.840799	-1.477745
H	2.858196	-3.102066	0.752379
H	2.985071	-1.513743	1.529001
H	4.146987	-2.803475	1.933839
H	6.274008	0.399482	1.958021
H	6.302297	-1.366885	2.121178
H	4.804175	-0.462655	2.432077
H	6.358433	-0.618523	-1.593102
H	7.326723	-1.306159	-0.267860
H	7.052831	0.446097	-0.361927

Transition state **TS-15c**

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scf done: -2538.86147622

C	-3.678702479	3.578678083	0.958053776
C	-3.529355675	2.338431380	0.346539288
C	-2.629039793	1.395229073	0.857121047
C	-2.932843066	3.893980366	2.092923764
C	-2.047401085	2.959018986	2.620108376
C	-1.901267481	1.717998901	2.007518883
C	-6.269624060	-1.203941213	-0.035705681
C	-6.260022461	-2.336455803	-0.844287055
C	-5.059692367	-2.795368147	-1.384329561
C	-5.083708282	-0.522534617	0.227738010
C	-3.878129938	-0.963468547	-0.325400609
C	-3.877608651	-2.113445587	-1.124078270
Sn	0.231830996	-1.536126418	-0.642288716
P	-2.260477289	-0.192113195	0.021671962
N	-1.294920668	-0.074389689	-1.280238879
N	-1.278982856	-1.111028755	0.939573174
C	-1.462435288	0.452690746	-2.649547265
C	-2.339132412	1.707434078	-2.686531731
C	-2.082501988	-0.609154362	-3.573572678
C	-0.064526851	0.802022979	-3.179210816
C	-1.891851612	-3.419181510	1.593375257
C	-2.779038824	-1.506415834	2.924742366
C	-0.339157892	-2.023545426	2.977091376
C	-1.586860464	-1.993363361	2.086040145
O	1.661135388	-0.013812346	-0.091568714
C	1.296848634	1.185115503	0.537243081
C	2.008467485	1.345866061	1.893243310
C	2.632403152	2.846876675	-0.879748126
C	1.426080441	2.452046724	-0.294246044
C	0.293429227	3.249419094	-0.470790073
C	2.684605468	4.000420346	-1.657744321
C	1.544539433	4.780649599	-1.847312493
C	0.347404214	4.406948088	-1.242519137
B	3.151940394	-0.305089772	-1.125932178
O	3.184115615	-1.719896721	-1.186180255

O	4.253144105	0.155679279	-0.378676227
C	4.122031332	-2.188125479	-0.209827212
C	5.088517718	-0.957611542	-0.056064936
C	4.783692033	-3.452511581	-0.748430345
C	3.372245479	-2.530090605	1.084083274
C	5.654470668	-0.771708868	1.347431129
C	6.233004588	-0.972792106	-1.075977774
F	1.367391765	2.294829777	2.622881390
F	1.949640651	0.207698706	2.616759119
F	3.292301138	1.707265647	1.834148231
H	-4.378780276	4.300172171	0.547676949
H	-4.118000448	2.113744212	-0.536345210
H	-3.044164560	4.865797073	2.563934914
H	-1.456016233	3.195038993	3.498837931
H	-1.198266557	0.998799452	2.414184766
H	-7.200048568	-0.850291367	0.397810579
H	-7.185839266	-2.865654780	-1.048577317
H	-5.044857033	-3.684782596	-2.006661060
H	-5.101415487	0.343203202	0.881887245
H	-2.942247160	-2.477937995	-1.540540627
H	-2.086782850	-0.254826337	-4.610613085
H	-3.115696781	-0.831817502	-3.289768825
H	-1.503590812	-1.539791403	-3.537335944
H	-0.134221439	1.188210511	-4.201961391
H	0.585228962	-0.082426189	-3.209112921
H	0.422836321	1.553351659	-2.554504324
H	-2.078618750	-4.090171268	2.439603021
H	-1.047136225	-3.826368331	1.024896430
H	-2.776425203	-3.428772320	0.948142693
H	-2.920464711	-2.180243991	3.776470613
H	-3.709202728	-1.508811958	2.347891106
H	-0.473056541	-2.730500117	3.803643778
H	-0.134268704	-1.033627363	3.394107421
H	0.546186670	-2.333635374	2.408725040
H	-2.350373989	2.124681094	-3.699197827
H	-1.960647437	2.474465324	-2.005571453
H	-3.376172988	1.467376933	-2.422777145
H	-2.616847571	-0.499856702	3.319983678

H	3.526863495	2.251556265	-0.733190725
H	-0.644865226	2.958902927	-0.010130864
H	3.623955430	4.289714601	-2.118869291
H	1.592328053	5.677892782	-2.457364641
H	-0.547299762	5.008431245	-1.373758166
H	0.246223823	1.102718617	0.826313399
H	2.802578787	0.281494606	-2.115062932
H	4.036910074	-4.248332833	-0.827540746
H	5.576680114	-3.792696577	-0.072940597
H	5.210390235	-3.289438470	-1.739656449
H	2.605114293	-3.278646943	0.856090623
H	2.887078971	-1.650352618	1.509236130
H	4.045684665	-2.955868727	1.834792896
H	6.307227325	0.105978537	1.363960597
H	6.246423829	-1.644954161	1.644695737
H	4.862620000	-0.613998771	2.081321431
H	5.847168197	-1.108266488	-2.090498477
H	6.960826167	-1.762785088	-0.863990691
H	6.746016395	-0.007858724	-1.034830045

Intermediate **16a**

89

scf done: -2201.898964

C	-2.117322	-0.220283	4.232315
C	-2.482019	-0.077619	2.897767
C	-1.605547	-0.465549	1.877914
C	-0.866953	-0.742413	4.556247
C	0.012313	-1.121857	3.544257
C	-0.350043	-0.990559	2.205613
H	-2.805800	0.081020	5.015929
H	-3.449048	0.355117	2.654785
H	-0.578300	-0.853802	5.597372
H	0.989750	-1.522708	3.794709
H	0.346957	-1.293443	1.424888
C	-5.859170	-1.437907	0.373555
C	-6.433260	-0.819031	-0.733134
C	-5.670642	0.036821	-1.526638

C	-4.524368	-1.200052	0.690999
C	-3.756425	-0.335511	-0.093948
C	-4.339209	0.273297	-1.210694
H	-6.448332	-2.110553	0.989269
H	-7.473971	-1.006071	-0.980158
H	-6.113815	0.513311	-2.395666
H	-4.081908	-1.702058	1.545939
H	-3.733523	0.921242	-1.837751
Sn	0.085125	0.565417	-1.778298
P	-1.961487	-0.121993	0.128885
N	-1.410100	1.335424	-0.346153
N	-1.105322	-1.039095	-0.910637
C	-1.635507	2.686957	0.200787
C	-1.110372	2.839568	1.637304
C	-3.125499	3.060707	0.184122
C	-0.879195	3.663201	-0.711026
C	-2.607256	-2.571745	-2.187764
C	-1.467984	-3.350821	-0.078039
C	-0.146030	-2.924806	-2.135546
H	-3.260963	4.071391	0.585556
H	-3.721094	2.376944	0.799366
H	-3.527206	3.040566	-0.833652
H	-1.052323	4.695910	-0.390675
H	-1.220438	3.566943	-1.748732
H	0.202041	3.487719	-0.676247
H	-2.668478	-3.579710	-2.613548
H	-2.565279	-1.852730	-3.013914
H	-3.527497	-2.393163	-1.626374
H	-1.639702	-4.387942	-0.388140
H	-2.307559	-3.056040	0.562730
H	-0.324187	-3.950956	-2.476234
H	0.765873	-2.903699	-1.535493
H	-0.001879	-2.302334	-3.028166
H	-1.083102	3.898397	1.919404
H	-0.100362	2.437342	1.720046
H	-1.741598	2.314263	2.358594
C	-1.346962	-2.446116	-1.312056
H	-0.546400	-3.311405	0.510030

O	1.678995	0.340165	-0.197065
C	2.187610	1.110516	0.874475
H	3.106820	0.627036	1.221478
C	2.988098	2.778027	-0.841078
C	2.505671	2.522898	0.445096
C	2.341569	3.589101	1.330777
C	3.266914	4.082169	-1.243047
C	3.081844	5.144768	-0.359211
C	2.627491	4.893578	0.933949
H	3.146770	1.946937	-1.521936
H	1.969589	3.402059	2.335053
H	3.634879	4.267669	-2.247666
H	3.294026	6.161734	-0.674802
H	2.485628	5.713214	1.632083
H	1.466795	1.107700	1.700704
B	2.392815	-0.916391	-0.650734
O	2.067840	-2.082340	0.162742
O	3.821780	-0.752945	-0.572679
C	3.266056	-2.670593	0.646178
C	4.370792	-2.026092	-0.271881
C	3.155879	-4.190110	0.526371
C	3.427398	-2.302769	2.126355
C	5.723914	-1.836076	0.404801
C	4.557870	-2.794565	-1.588474
H	1.936544	-1.038497	-1.807390
H	2.376482	-4.555753	1.202695
H	4.099580	-4.677636	0.796966
H	2.885892	-4.486409	-0.489326
H	2.537213	-2.646104	2.662231
H	3.514017	-1.221317	2.262321
H	4.302885	-2.781344	2.577486
H	6.434328	-1.407683	-0.308552
H	6.126130	-2.793326	0.755748
H	5.647386	-1.153198	1.254180
H	3.597976	-2.960769	-2.086628
H	5.046342	-3.762259	-1.434251
H	5.181931	-2.190728	-2.253485

Intermediate **16b**

92

scf done: -2241.205274

C	-2.216299	-0.121747	4.237541
C	-2.564249	0.051550	2.901855
C	-1.715139	-0.398531	1.884248
C	-1.013387	-0.744090	4.567394
C	-0.160674	-1.185779	3.558787
C	-0.504710	-1.014734	2.220229
H	-2.884645	0.226963	5.019035
H	-3.501543	0.545129	2.656512
H	-0.744004	-0.885026	5.610056
H	0.779667	-1.670381	3.806615
H	0.176584	-1.359253	1.445786
C	-5.971210	-1.343071	0.390910
C	-6.513772	-0.817621	-0.777757
C	-5.721772	-0.046987	-1.628008
C	-4.639860	-1.093319	0.716103
C	-3.842668	-0.311581	-0.124176
C	-4.393872	0.197673	-1.305650
H	-6.581349	-1.953492	1.049576
H	-7.552012	-1.012124	-1.029419
H	-6.139115	0.355963	-2.545669
H	-4.223677	-1.523235	1.621844
H	-3.766295	0.774777	-1.977986
Sn	0.084644	0.485604	-1.744132
P	-2.050542	-0.083546	0.122499
N	-1.476725	1.348645	-0.390613
N	-1.176335	-1.052837	-0.854538
C	-1.791632	2.740956	-0.017127
C	-3.263777	3.088584	-0.291928
C	-0.916504	3.643975	-0.897274
C	-1.498433	3.048100	1.459597
C	-2.606197	-2.575709	-2.216385
C	-1.726368	-3.323619	0.015586
C	-0.177190	-3.024472	-1.898143
H	-1.114304	4.698493	-0.677210

H	-1.129345	3.474824	-1.959492
H	0.149624	3.466367	-0.719854
H	-1.652793	4.114935	1.658415
H	-0.466588	2.802342	1.714849
H	-2.154628	2.484076	2.127769
H	-2.668579	-3.594820	-2.614931
H	-2.456149	-1.887505	-3.056216
H	-3.566016	-2.341615	-1.748960
H	-1.920259	-4.358999	-0.286581
H	-2.610338	-2.969262	0.557265
H	-0.349420	-4.067992	-2.185360
H	0.673412	-2.977759	-1.215284
H	0.069880	-2.466402	-2.810540
H	-3.451021	4.139747	-0.045650
H	-3.944206	2.476870	0.309955
H	-3.509693	2.938887	-1.347548
C	-1.434668	-2.465065	-1.223579
H	-0.872755	-3.318272	0.699254
O	1.554126	0.348554	-0.031453
C	1.850350	1.266469	1.015489
C	2.792070	0.692462	2.066636
H	2.374509	-0.224955	2.483804
H	2.910820	1.425300	2.870601
H	3.768225	0.480965	1.626184
C	3.110941	2.581917	-0.752538
C	2.392131	2.564188	0.444121
C	2.190659	3.763738	1.131616
C	3.592149	3.785138	-1.265573
C	3.372115	4.980681	-0.584461
C	2.675705	4.965780	0.623448
H	3.305232	1.647770	-1.270814
H	1.637942	3.760699	2.068385
H	4.144129	3.785633	-2.200807
H	3.744440	5.916811	-0.989386
H	2.502249	5.891598	1.163916
H	0.890571	1.470976	1.502343
B	2.295858	-0.884526	-0.455678
O	2.076398	-2.041613	0.394444

O	3.723019	-0.723406	-0.560478
C	3.291658	-2.771217	0.520011
C	4.270041	-2.031787	-0.482924
C	3.030032	-4.238059	0.170629
C	3.754128	-2.704862	1.980799
C	5.713867	-1.934386	-0.000068
C	4.254743	-2.649490	-1.890567
H	1.751019	-1.059601	-1.586003
H	2.338231	-4.665584	0.903692
H	3.958060	-4.820666	0.194926
H	2.577482	-4.343781	-0.817193
H	2.928628	-3.034606	2.620477
H	4.028985	-1.691752	2.275194
H	4.611230	-3.361970	2.162072
H	6.313372	-1.410103	-0.750215
H	6.146065	-2.930109	0.149782
H	5.785089	-1.376749	0.936090
H	3.236945	-2.738590	-2.280477
H	4.723522	-3.638596	-1.907521
H	4.813315	-1.989771	-2.560872

Intermediate **16c**

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scf done: -2538.85898452

C	-3.096334195	-1.281665789	3.885576845
C	-3.273416684	-0.692867036	2.637567491
C	-2.299969520	-0.842669033	1.642906695
C	-1.939343787	-2.010393695	4.150668593
C	-0.965247344	-2.154295220	3.165259218
C	-1.138442240	-1.576669367	1.910970608
C	-6.407584208	-0.368112716	-0.475538079
C	-6.706670709	0.732947722	-1.273232401
C	-5.708082542	1.650003705	-1.596236628
C	-5.112295726	-0.553752795	0.000067191
C	-4.106354215	0.364592288	-0.315287081
C	-4.415299448	1.464275691	-1.122363319
Sn	-0.083762848	1.010443902	-1.460824441

P	-2.350399628	0.096488138	0.092233990
N	-1.503210053	1.483670430	0.179624265
N	-1.536010068	-0.577530522	-1.151171783
C	-1.507131995	2.504534320	1.240944756
C	-2.927770296	3.013573145	1.532395895
C	-0.681128826	3.686187217	0.714526457
C	-0.892480252	1.984165524	2.555610685
C	-3.090942527	-1.323397545	-2.956038185
C	-2.371798043	-2.910681699	-1.129431165
C	-0.748534424	-2.153865137	-2.844453187
C	-1.950943225	-1.718712163	-1.999886515
O	1.512037477	0.270193277	0.100222463
C	2.304132360	1.197791319	0.794137480
C	3.085252879	0.569760113	1.960096379
C	3.898989445	1.642847951	-1.159517878
C	3.165649799	2.110983908	-0.066506765
C	3.199260793	3.473315704	0.244549228
C	4.642104213	2.532947896	-1.930451883
C	4.670089019	3.890913929	-1.618192484
C	3.949414626	4.360543075	-0.522947457
B	1.870224979	-1.001558443	-0.694816619
O	1.227665917	-2.181443371	-0.168032356
O	3.268690885	-1.284546555	-0.773105001
C	2.197457293	-3.208927264	0.012590758
C	3.409579668	-2.698727382	-0.849655397
C	1.602325397	-4.533520421	-0.462423721
C	2.530926424	-3.317886973	1.502769905
C	4.780687356	-3.087334296	-0.308693973
C	3.302981306	-3.111773103	-2.324464494
F	3.485444223	1.560029491	2.793724687
F	4.179842115	-0.116104160	1.623138024
F	2.291409394	-0.245435736	2.679236756
H	-3.856509280	-1.163005631	4.651773314
H	-4.165671528	-0.101974439	2.451736759
H	-1.794397640	-2.461848008	5.127755727
H	-0.054594583	-2.706861341	3.375713033
H	-0.363899994	-1.688338377	1.153245379
H	-7.180506538	-1.088822170	-0.226934790

H	-7.716154896	0.875111758	-1.647188383
H	-5.937551099	2.507113899	-2.221989077
H	-4.887278637	-1.426689265	0.605360565
H	-3.630250684	2.167694246	-1.385679968
H	-0.659133447	4.498330658	1.449073018
H	-1.111992222	4.073103368	-0.216008541
H	0.355994998	3.399288995	0.507542351
H	-0.636414417	2.820208371	3.217228977
H	0.008611177	1.397167290	2.365895788
H	-1.585591381	1.333260367	3.095442478
H	-3.272961354	-2.128240413	-3.677505909
H	-2.818518265	-0.419738742	-3.513694555
H	-4.029275907	-1.128920531	-2.431049325
H	-2.648544861	-3.761048331	-1.763002505
H	-3.238981290	-2.671224958	-0.503354404
H	-1.036901683	-2.992316914	-3.488349866
H	0.071916840	-2.464293695	-2.195755973
H	-0.399461507	-1.342572532	-3.496145982
H	-2.898460812	3.773311034	2.321403019
H	-3.582164354	2.204991938	1.875896634
H	-3.379668583	3.459682855	0.641200268
H	-1.545746755	-3.210928982	-0.477635316
H	3.895993689	0.583701398	-1.393552757
H	2.638150814	3.845830530	1.097864424
H	5.205545011	2.158900981	-2.779887380
H	5.251857952	4.578437594	-2.224684487
H	3.964743270	5.416027321	-0.269180776
H	1.600331871	1.845063221	1.326636240
H	1.355313527	-0.701685098	-1.809765893
H	0.776949848	-4.820661963	0.197138894
H	2.352600602	-5.331678042	-0.436124604
H	1.208930495	-4.455263408	-1.478139255
H	1.601845190	-3.497078365	2.051948023
H	2.977473468	-2.397894417	1.879633095
H	3.212827352	-4.150650230	1.704662673
H	5.559986696	-2.706746361	-0.975775045
H	4.881994736	-4.176907977	-0.251534631
H	4.947218400	-2.663451957	0.682900749

H	2.325331968	-2.853255136	-2.741515592
H	3.468340493	-4.185306630	-2.459854577
H	4.064328348	-2.569350728	-2.892595440

Intermediate **17a**

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scf done: -2201.895179

C	-2.700641	-2.173234	3.639493
C	-2.881413	-1.275326	2.591207
C	-2.007661	-1.281476	1.498594
C	-1.638671	-3.073292	3.609456
C	-0.751275	-3.067763	2.535582
C	-0.932248	-2.177729	1.483303
C	-6.162930	0.288076	0.020236
C	-6.317271	1.575369	-0.486482
C	-5.195393	2.362765	-0.739307
C	-4.889381	-0.213044	0.277273
C	-3.759392	0.574712	0.036848
C	-3.924256	1.863543	-0.481798
Sn	0.202751	0.765160	-1.477307
P	-2.055783	-0.063080	0.149599
N	-0.952558	1.122416	0.336340
N	-1.523140	-0.627342	-1.269732
C	-0.635946	1.930945	1.531393
C	0.352974	1.183757	2.439346
C	-1.896687	2.281974	2.336004
C	-0.011760	3.237962	1.027599
C	-3.218090	-0.828228	-3.064297
C	-2.750786	-2.769604	-1.534749
C	-1.024597	-2.026215	-3.171849
C	-2.140427	-1.546022	-2.233116
O	2.373029	0.538220	-0.189661
C	3.552625	1.077892	0.372634
C	3.321058	3.213070	-0.930758
C	3.493414	2.581356	0.305242
C	3.562585	3.360976	1.459087
C	3.200573	4.596860	-1.006950

C	3.263586	5.369636	0.154050
C	3.452265	4.749515	1.386159
B	2.285847	-0.900573	-0.400539
O	2.207910	-1.733710	0.775714
O	3.310278	-1.443787	-1.245708
C	3.208268	-2.742386	0.683806
C	3.497847	-2.797331	-0.857470
C	2.667852	-4.043747	1.269592
C	4.429113	-2.291094	1.494631
C	4.912348	-3.232949	-1.221926
C	2.480331	-3.668247	-1.608775
H	-3.387730	-2.164630	4.480246
H	-3.700665	-0.563940	2.636443
H	-1.496499	-3.772891	4.428008
H	0.094130	-3.747470	2.518933
H	-0.210867	-2.157647	0.671359
H	-7.034338	-0.330221	0.213341
H	-7.310806	1.965341	-0.686153
H	-5.312317	3.364770	-1.140780
H	-4.782229	-1.223537	0.660344
H	-3.044611	2.468465	-0.685520
H	-1.620198	2.909812	3.190057
H	-2.384622	1.387028	2.735899
H	-2.621948	2.832359	1.729147
H	0.265416	3.884549	1.867149
H	-0.720392	3.779862	0.390383
H	0.899736	3.049896	0.452328
H	-3.602870	-1.486654	-3.852096
H	-2.794230	0.065069	-3.536999
H	-4.061296	-0.514077	-2.441338
H	-3.172241	-3.458800	-2.275086
H	-3.559023	-2.481579	-0.853324
H	-1.416421	-2.740360	-3.904345
H	-0.222854	-2.510605	-2.605316
H	-0.590002	-1.186977	-3.729808
H	0.683819	1.831481	3.260753
H	1.224482	0.859874	1.866479
H	-0.111297	0.291367	2.872087

H	-1.992718	-3.304542	-0.953937
H	4.420190	0.700672	-0.185218
H	3.263128	2.608095	-1.831670
H	3.681669	2.876684	2.424942
H	3.057191	5.075122	-1.971298
H	3.165241	6.449355	0.095008
H	3.500072	5.343824	2.293891
H	3.651797	0.750245	1.416712
H	1.115098	-0.967162	-1.008478
H	2.514870	-3.923867	2.346927
H	3.375347	-4.866312	1.115741
H	1.712351	-4.314755	0.814119
H	4.103384	-2.047731	2.510493
H	4.882471	-1.397373	1.057757
H	5.192580	-3.074096	1.551658
H	5.017506	-3.280079	-2.309988
H	5.130368	-4.225982	-0.812829
H	5.651756	-2.524897	-0.841738
H	1.455666	-3.420994	-1.313772
H	2.644381	-4.735758	-1.429094
H	2.581528	-3.475465	-2.680704

Intermediate **17b**

92

scf done: -2241.206742

C	-2.620948	-1.516806	4.037227
C	-2.918602	-0.773834	2.898383
C	-2.181212	-0.956984	1.724299
C	-1.580363	-2.441028	4.011089
C	-0.831316	-2.616352	2.849216
C	-1.125513	-1.876617	1.709701
C	-6.465278	0.479062	0.524331
C	-6.670480	1.709276	-0.094613
C	-5.580726	2.452984	-0.543151
C	-5.172440	-0.007726	0.697673
C	-4.073264	0.736024	0.256784
C	-4.290047	1.966797	-0.371183

Sn	-0.352472	0.719444	-1.738817
P	-2.369592	0.087206	0.249332
N	-1.248154	1.270315	0.177085
N	-2.003962	-0.653310	-1.141127
C	-0.757701	2.141373	1.266009
C	0.159331	1.372738	2.233443
C	-1.922133	2.766453	2.047813
C	0.043196	3.266181	0.600434
C	-3.900430	-1.021816	-2.695382
C	-3.261801	-2.788444	-1.019794
C	-1.738049	-2.260276	-2.919406
C	-2.736144	-1.660152	-1.918460
O	2.096769	0.936164	-0.813697
C	3.301484	1.517173	-1.288028
C	5.684877	1.606362	-0.462954
C	4.320809	1.667138	-0.173398
C	3.917158	1.879824	1.145104
C	6.633767	1.748963	0.547308
C	6.223568	1.956334	1.863390
C	4.862284	2.023338	2.157199
B	2.006936	-0.507641	-0.667111
O	2.122035	-1.082554	0.642175
O	2.821260	-1.263360	-1.561563
C	3.049231	-2.165331	0.579610
C	3.051101	-2.527719	-0.949330
C	2.563966	-3.291702	1.486451
C	4.410994	-1.668052	1.075385
C	4.367467	-3.094379	-1.466940
C	1.896557	-3.464369	-1.333560
C	2.979194	2.868970	-1.920205
H	-3.196981	-1.367672	4.945361
H	-3.718262	-0.040222	2.936524
H	-1.344206	-3.017705	4.900554
H	-0.005128	-3.319292	2.836426
H	-0.511466	-1.981339	0.818894
H	-7.312305	-0.105502	0.870371
H	-7.679050	2.088270	-0.229940
H	-5.737386	3.411092	-1.029196

H	-5.026332	-0.973570	1.172318
H	-3.435773	2.535857	-0.727678
H	-1.530654	3.411382	2.842259
H	-2.546656	2.003079	2.524708
H	-2.560111	3.372967	1.397169
H	0.391520	3.985498	1.349798
H	-0.573465	3.801126	-0.131978
H	0.920555	2.854936	0.094256
H	-4.373975	-1.755951	-3.357944
H	-3.532537	-0.191439	-3.308802
H	-4.665993	-0.630414	-2.018526
H	-3.760659	-3.554421	-1.623985
H	-3.991197	-2.416539	-0.291694
H	-2.213444	-3.049950	-3.511429
H	-0.874933	-2.686396	-2.397330
H	-1.374362	-1.497861	-3.620052
H	0.685390	2.075502	2.892135
H	0.899172	0.781590	1.686344
H	-0.410858	0.687693	2.868325
H	-2.441602	-3.259553	-0.468540
H	6.006611	1.424025	-1.486107
H	2.857634	1.892228	1.375453
H	7.691785	1.685225	0.310346
H	6.960287	2.057377	2.654742
H	4.534616	2.174847	3.181736
H	3.727567	0.857621	-2.053756
H	0.703134	-0.717854	-0.999031
H	2.566307	-2.948322	2.525660
H	3.221757	-4.164830	1.410825
H	1.548055	-3.598926	1.228955
H	4.281213	-1.220801	2.064905
H	4.816649	-0.897042	0.416972
H	5.136772	-2.484847	1.151641
H	5.177917	-2.372633	-1.346234
H	4.273918	-3.326886	-2.532088
H	4.631423	-4.015402	-0.935311
H	0.945387	-3.101196	-0.931345
H	2.060049	-4.484474	-0.971739

H	1.814831	-3.489630	-2.424211
H	2.594046	3.567288	-1.170814
H	2.232788	2.750311	-2.712115
H	3.883856	3.305237	-2.354118

Intermediate **17c**

92

scf done: -2538.86938519

C	3.163334400	2.708812406	3.293512943
C	3.342345894	1.610544664	2.457788490
C	2.558439882	1.462852644	1.308949552
C	2.194485017	3.661079271	2.990119443
C	1.398694780	3.510889451	1.855873238
C	1.574585574	2.415547227	1.018024569
C	6.656141132	-0.640364247	0.562445363
C	6.744842469	-2.022620435	0.419292927
C	5.585204150	-2.785828181	0.299315744
C	5.410025555	-0.020809803	0.585900663
C	4.241066905	-0.780573091	0.471744466
C	4.340366122	-2.167638561	0.322369596
Sn	0.458979560	-1.155064700	-1.319557254
P	2.590061706	-0.033632963	0.281979696
N	1.384321460	-1.068519464	0.650259963
N	2.201480531	0.205312696	-1.273428149
C	0.862116446	-1.456213383	1.977012178
C	0.085815540	-0.303325211	2.638719589
C	1.996909662	-1.912136252	2.904925921
C	-0.090314513	-2.633174285	1.743024946
C	4.038506014	-0.147300049	-2.903706686
C	3.604875916	2.138194290	-1.939339511
C	1.956207420	1.105153075	-3.497011001
C	2.961276005	0.814188091	-2.373516995
O	-2.122872907	-0.729374878	-0.391310156
C	-3.445485465	-1.149507495	-0.544783620
C	-5.678318188	-0.819000274	0.594094979
C	-4.290716767	-0.926284491	0.698793702
C	-3.684986392	-0.783366997	1.944933172

C	-6.453121159	-0.571256864	1.724090395
C	-5.843160422	-0.426544982	2.969186916
C	-4.457866980	-0.534812444	3.076067361
B	-1.780735962	0.649794780	-0.741316524
O	-1.809514841	1.643462173	0.294530569
O	-2.495010552	1.160603533	-1.868151150
C	-2.608056105	2.737393356	-0.152636725
C	-2.566972776	2.574193502	-1.713912358
C	-2.001984707	4.040761948	0.356498638
C	-4.018905282	2.576381686	0.422773670
C	-3.802427898	3.090381430	-2.440879534
C	-1.306603642	3.190090373	-2.337084190
C	-3.408390353	-2.628576700	-0.942194886
F	-4.649687764	-3.098534999	-1.181019647
F	-2.694547699	-2.816089967	-2.067773807
F	-2.863267895	-3.412318317	0.006422692
H	3.775119592	2.815102988	4.184042077
H	4.085398023	0.862312104	2.716604167
H	2.049614950	4.515770173	3.644166292
H	0.626003633	4.239365966	1.634030132
H	0.919715770	2.274205606	0.162036016
H	7.557917691	-0.042406016	0.652061499
H	7.717239762	-2.505215074	0.398945027
H	5.652311149	-3.863238871	0.183899666
H	5.354479644	1.059049820	0.687693738
H	3.432545055	-2.755727942	0.219555752
H	1.587848517	-2.196692813	3.880517839
H	2.726587255	-1.112341770	3.075217487
H	2.525829069	-2.775249641	2.488601472
H	-0.488154755	-3.002775622	2.694418590
H	0.427956606	-3.460772859	1.243865888
H	-0.940641413	-2.329144191	1.125389920
H	4.526247581	0.270226399	-3.792180296
H	3.584086076	-1.105938093	-3.178717433
H	4.809147537	-0.340904670	-2.151369670
H	4.122939241	2.603433754	-2.785248293
H	4.343046642	1.985875104	-1.144265902
H	2.452133932	1.595766391	-4.341587134

H	1.152667656	1.756115177	-3.137975540
H	1.506301452	0.178369496	-3.875728464
H	-0.481234393	-0.679438259	3.499518247
H	-0.611608663	0.157378496	1.932158087
H	0.757306051	0.480031801	3.002937185
H	2.846615902	2.836312402	-1.570101831
H	-6.155066130	-0.916862320	-0.377452923
H	-2.605819337	-0.836868734	2.016307512
H	-7.530847218	-0.479808852	1.629654278
H	-6.444303800	-0.223734314	3.850462337
H	-3.974748276	-0.414629932	4.041156883
H	-3.911914387	-0.633720160	-1.394729498
H	-0.489624920	0.527407922	-1.050447884
H	-2.047567495	4.061780790	1.449733320
H	-2.554863720	4.905240413	-0.027654417
H	-0.957020674	4.136996580	0.054392936
H	-3.943531416	2.445459740	1.505962646
H	-4.513852653	1.690627020	0.019500775
H	-4.643163667	3.451920188	0.214888561
H	-4.699622387	2.556177629	-2.121596823
H	-3.683753225	2.942788043	-3.518436996
H	-3.945691919	4.160444857	-2.254171262
H	-0.405874201	2.871933185	-1.802207816
H	-1.343030244	4.284106870	-2.336627431
H	-1.224814293	2.844659074	-3.371866440

Hydroboration product **5a**

36

scf done: -757.313407

B	-1.364555	-0.670109	0.047839
O	-1.022056	0.581726	-0.397069
O	-0.311050	-1.558907	0.043993
C	0.413343	0.592588	-0.542060
C	0.744644	-0.934052	-0.714522
C	0.993269	1.190183	0.741370
C	0.780410	1.458409	-1.738346
C	0.601274	-1.421596	-2.158064

C	2.087104	-1.363807	-0.142183
H	0.558781	2.181536	0.893740
H	2.080810	1.291722	0.679475
H	0.748198	0.574405	1.611822
H	0.517728	2.499747	-1.533536
H	0.246690	1.144424	-2.637143
H	1.857466	1.408125	-1.930923
H	0.630943	-2.514382	-2.163996
H	1.411630	-1.045552	-2.789651
H	-0.354775	-1.111782	-2.590723
H	2.142154	-1.176671	0.931918
H	2.903580	-0.826309	-0.635813
H	2.233342	-2.434549	-0.309000
O	-2.621422	-0.985470	0.448204
C	-2.958535	-2.364411	0.595781
H	-2.228301	-2.867888	1.238918
H	-3.928941	-2.378320	1.099319
C	-3.992308	-2.646587	-1.682979
C	-3.041443	-3.058081	-0.743892
C	-2.153280	-4.079684	-1.081358
C	-4.054529	-3.248001	-2.936370
C	-3.167446	-4.274258	-3.263632
C	-2.218118	-4.690448	-2.333206
H	-4.677201	-1.841986	-1.429101
H	-1.396339	-4.385683	-0.364679
H	-4.795793	-2.919462	-3.658562
H	-3.216864	-4.746270	-4.240224
H	-1.522031	-5.485169	-2.584491

Hydroboration product **3d**

39

scf done: -796.625481

B	-1.157421	-1.013547	0.208774
O	-0.726287	0.264874	-0.039613
O	-0.188140	-1.969208	-0.003791
C	0.690979	0.182065	-0.297722
C	0.863417	-1.315897	-0.743091

C	1.412284	0.503066	1.012476
C	1.056776	1.204115	-1.364160
C	0.565116	-1.541392	-2.227613
C	2.198323	-1.941863	-0.369692
H	1.081670	1.484066	1.363935
H	2.497405	0.529633	0.875091
H	1.175864	-0.232769	1.786720
H	0.914440	2.214335	-0.970726
H	0.432240	1.093884	-2.252359
H	2.107127	1.095060	-1.654856
H	0.485874	-2.616623	-2.409578
H	1.357419	-1.132613	-2.861787
H	-0.387207	-1.086669	-2.516928
H	2.351397	-1.943351	0.710975
H	3.021475	-1.395579	-0.842281
H	2.230514	-2.976818	-0.721176
O	-2.426789	-1.292331	0.601145
C	-2.900306	-2.635086	0.456477
C	-4.298071	-2.684201	1.056387
H	-2.238794	-3.308706	1.015781
H	-4.962185	-1.997735	0.522815
H	-4.267109	-2.390147	2.108931
H	-4.708089	-3.695104	0.978072
C	-3.413298	-2.203435	-1.981913
C	-2.881759	-3.049032	-1.004106
C	-2.326558	-4.267755	-1.391712
C	-3.388071	-2.572524	-3.324092
C	-2.835456	-3.795471	-3.703869
C	-2.306126	-4.643807	-2.733676
H	-3.830123	-1.244030	-1.688033
H	-1.886283	-4.918506	-0.640638
H	-3.801506	-1.905566	-4.074753
H	-2.815663	-4.084617	-4.750170
H	-1.867074	-5.594049	-3.022657

Hydroboration product **3j**

39

scf done: -1094.28428984

B	0.917133275	-0.831956956	0.187569491
O	1.945591177	-1.030176256	1.065127312
O	1.254717858	-0.083036869	-0.912253633
C	3.134248970	-0.513400669	0.422916871
C	2.537593695	0.511466416	-0.609764482
C	3.837213856	-1.694808656	-0.246690954
C	4.032785758	0.105225512	1.482949622
C	2.254246701	1.885098149	0.001670032
C	3.331297117	0.657009378	-1.898292643
O	-0.335975961	-1.321891803	0.408072804
C	-1.387886578	-0.816869130	-0.381786363
C	-2.598031148	-1.711476996	-0.095830419
C	-1.557151673	1.146985962	1.199778300
C	-1.671151856	0.645107790	-0.097964193
C	-2.018555927	1.502716770	-1.140464675
C	-1.786378921	2.497521200	1.447932520
C	-2.135352260	3.352683329	0.403663188
C	-2.254538272	2.852122978	-0.891366244
F	-2.984695300	-1.667930735	1.186647492
F	-2.334106046	-2.993377417	-0.397110877
F	-3.644362898	-1.327575207	-0.852937220
H	4.043833434	-2.456442005	0.509483566
H	4.784374677	-1.388999416	-0.700521433
H	3.208731744	-2.145118116	-1.020678640
H	4.395582921	-0.674462985	2.157989786
H	3.496210742	0.845898901	2.078405216
H	4.899195285	0.586321126	1.017119221
H	1.643113614	2.463272315	-0.696409796
H	3.181290318	2.432813744	0.194953687
H	1.696845257	1.797795898	0.939231029
H	3.406591125	-0.291833408	-2.432278735
H	4.341218155	1.022470169	-1.685081192
H	2.838055252	1.380177173	-2.553369006
H	-1.170785332	-0.945384733	-1.449160496
H	-1.280369226	0.479660859	2.009956399
H	-2.097577458	1.115400302	-2.152510343

H	-1.692723672	2.883001853	2.458486464
H	-2.312424045	4.405933216	0.598062515
H	-2.523052366	3.513777318	-1.708995410

Tin(II) chloride **1**

53

scf done: -1693.57531047

P	-0.52860204	0.09006101	0.01201700
Cl	3.49009527	0.63803605	-0.56198004
N	0.50306204	0.03382500	1.28895910
N	0.36092303	-0.84526506	-1.00027708
C	0.61203304	0.90995207	2.48507819
C	-0.82960606	1.78023113	-0.63747105
C	0.15664901	2.32775918	-1.47625511
H	1.02508808	1.73222113	-1.74161213
C	-3.33906526	-0.34772803	-0.33299103
H	-3.31939125	0.39124103	-1.12728308
C	-1.92068815	2.57720420	-0.25310302
H	-2.68312520	2.18443317	0.41191903
C	0.00617500	-1.55650112	-2.25195817
C	-2.23709717	-1.60706112	1.41258211
H	-1.34022110	-1.83917114	1.97855515
C	-2.03400715	3.89108830	-0.71560005
H	-2.88322422	4.49700934	-0.41248603
C	-2.17651117	-0.63250205	0.40231403
C	1.32988810	-1.87630114	-2.97503423
H	1.89597614	-0.96210307	-3.17623124
H	1.13284009	-2.38572218	-3.92437330
H	1.96035615	-2.54273519	-2.37353718
C	-0.75761806	1.12529109	3.16043224
H	-1.46058411	1.63438413	2.49323019
H	-0.63957005	1.75416013	4.04974431
H	-1.20539909	0.17675301	3.47104726
C	0.04073300	3.64036628	-1.93536415
H	0.81251306	4.05293531	-2.57862220
C	-0.73284706	-2.87800622	-1.94538615
H	-0.13252001	-3.50492727	-1.27708810

H	-0.91756107	-3.44276226	-2.86698122
H	-1.69615513	-2.69308320	-1.46218911
C	-4.58529035	-1.97768015	0.95524907
H	-5.51597441	-2.49496419	1.17020009
C	1.23428509	2.27996417	2.13516716
H	2.18807517	2.15180016	1.61632712
H	1.40734811	2.86074922	3.04922623
H	0.57378804	2.86371722	1.48854612
C	1.53743012	0.18385601	3.48119826
H	1.14398609	-0.80732506	3.73148929
H	1.63058213	0.76241806	4.40620334
H	2.54702319	0.06314700	3.07092823
C	-0.85717907	-0.68504205	-3.18554524
H	-1.81946114	-0.43323903	-2.72979821
H	-1.06811108	-1.22757009	-4.11370731
H	-0.34428603	0.24575102	-3.44228626
C	-4.53571535	-1.01512708	-0.05634800
H	-5.42652139	-0.78239906	-0.63286305
C	-1.05642408	4.42284434	-1.56109312
H	-1.14496909	5.44448241	-1.91975315
C	-3.43157326	-2.27383817	1.68814513
H	-3.46190427	-3.02288723	2.47433819
Sn	2.05499016	-1.21852810	0.34711103