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# Alkyl scandium complexes coordinated by dianionic O,N,N- and O,N,O-ligands derived from Schiff bases

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## Experimental Section

All air- and/or moisture-sensitive reactions were performed under inert atmosphere using standard Schlenk-type vessels or in a dry-box filled with nitrogen. THF, toluene and hexane were purified by distillation from sodium/triglyme benzophenone ketyl and stored over $CaH_2$. Benzene-$d_6$ was dried over sodium/benzophenone ketyl and condensed *in vacuo* prior to use. $Sc(CH_2SiMe_3)_3(THF)_2$[S1] and ligands **1a**–**c**[S2,S3] were prepared according to previously published procedures. $Ph_2PH$ was donated by Synor Ltd. and was vacuum-distilled over $CaH_2$ and then degassed by freeze-pump-thaw methods. $^1H$ and $^{13}C\{^1H\}$ NMR spectra were recorded on a Bruker Avance III-400 spectrometer (400.13 and 100.61 MHz for $^1H$ and $^{13}C$, respectively). Chemical shifts are reported in ppm relative to TMS and peaks are referenced to the chemical shifts of residual solvent resonances ($^1H$ and $^{13}C$). The C, H, N elemental analyses are conducted in the microanalytical laboratory of IMOC. The scandium content was determined by direct complexometric titration with the disodium salt of EDTA (ethylenediaminetetraacetic acid), using xylenol orange indicator.[S4]

**Synthesis of 2a**. A bright-orange solution of **1a** (0.1231 g, 0.50 mmol) in toluene (5 ml) was added to a pale-yellow solution of $Sc(CH_2SiMe_3)_3(THF)_2$ (0.2254 g, 0.50 mmol) in toluene (10 mL) at 0 °C. The reaction mixture gradually turned red and was stirred for *ca*. 1.5 h. The volatiles were removed in vacuum, the resulting deep-red residue was dissolved in a toluene-hexane mixture (1:3 vol) and was stored at –20 °C to afford dark-red crystals of **2a**. The mother liquor was decanted, the crystals were washed with cold hexane and dried in vacuum for 10 min. Complex **2a** was isolated in 59% yield (0.1708 g). Anal. Calc. for $C_{64}H_{98}N_4O_2Sc_2Si_4$ (1342.01): C, 67.81; H, 8.56; N, 4.17, Sc, 6.70. Found: C, 69.39; H, 8.23; N, 4.29; Sc, 7.02. **$^1$H NMR** (400 MHz, benzene-$d_6$, 20 °C, TMS): δ = 0.01 (s, 18H, $CHCH_2Si\mathit{Me}_3$), 0.06 (s, 2H, $ScC\mathit{H}_2SiMe_3$), 0.16 (s, 2H, $ScC\mathit{H}_2SiMe_3$), 0.29 (s, 18H, $ScCH_2Si\mathit{Me}_3$), 0.75 (br s, 2H, $CHC\mathit{H}_2SiMe_3$), 1.08 (br s, 2H, $CHC\mathit{H}_2SiMe_3$), 1.43 (s, 18H, $C(C\mathit{H}_3)_3$), 1.85 (s, 18H, $C(C\mathit{H}_3)_3$), 4.93 (dd, 2H, $^3J_{HH}$ = 12.1 Hz, $^3J_{HH}$ = 2.7 Hz, $C\mathit{H}CH_2SiMe_3$), 6.67 (d, $^3J_{HH}$ = 8.8 Hz, 2H, Ar), 6.78 (d, $^3J_{HH}$ = 8.6 Hz, 2H, Ar), 6.89 (d, $^3J_{HH}$ = 8.6 Hz, 2H, Ar), 7.26 (s, 2H, Ar), 7.42 (s, 2H, Ar), 7.50 (t, $^3J_{HH}$ = 8.6 Hz, 2H, Ar), 7.64 (d, $^3J_{HH}$ = 8.6 Hz, 2H, Ar), 9.27 (s, 2H, Ar) ppm. **$^{13}$C NMR** (101 MHz, benzene-$d_6$): δ = −1.3 (s, $CHCH_2Si(\mathit{C}H_3)_3$), 1.0 (s, $ScCH_2Si(\mathit{C}H_3)_3$), 24.1 (s, $CH\mathit{C}H_2SiMe_3$), 30.3 (s, $C(\mathit{C}H_3)_3$), 31.2 (s, $\mathit{C}(CH_3)_3$), 31.9 (s, $C(\mathit{C}H_3)_3$), 34.0 (s, $Sc\mathit{C}H_2SiMe_3$), 35.5 (s, $\mathit{C}(CH_3)_3$), 60.3 (s, $\mathit{C}HCH_2SiMe_3$), 102.4 (*C*H, Ar), 107.3 (*C*H, Ar), 120.3 (*C*, Ar), 121.7 (*C*, Ar), 123.7 (*C*H, Ar), 125.3 (*C*, Ar), 129.0 (*C*, Ar), 130.8 (*C*, Ar), 131.2 (*C*H, Ar), 134.2 (*C*, Ar), 136.1 (*C*, Ar), 137.5 (*C*, Ar), 138.8 (*C*H, Ar), 142.9 (*C*, Ar), 146.1 (*C*H, Ar), 153.7 (C, Ar), 158.6 (C, Ar) ppm.

**Synthesis of 2b**. A yellow solution of **1b** (0.1196 g, 0.50 mmol) in toluene (5 ml) was added to a pale-yellow solution of $Sc(CH_2SiMe_3)_3(THF)_2$ (0.2254 g, 0.50 mmol) in toluene (10 mL) at 0 °C. The reaction mixture gradually turning brownish-yellow was stirred for *ca*. 1.5 h. The volatiles were removed in vacuum and the resulting brownish-yellow residue was dissolved in hexane (7 ml) and was stored at –20 °C to afford yellow crystals of **2b**. The mother liquor was decanted, the crystals were washed with cold hexane and dried in vacuum for 10 min. Complex **2b** was isolated in 56% yield (0.1601 g). Anal. Calc. for $C_{62}H_{104}N_2O_4Sc_2Si_4$ (1229.92): C, 65.11; H, 9.17; N, 2.45; Sc, 7.86. Found: C, 64.89; H, 8.96; N, 2.67; Sc, 7.80%. **$^1$H NMR** (400 MHz, benzene-$d_6$, 20 °C, TMS): δ = −0.22 (s, 18H, $ScCH_2Si\mathit{Me}_3$), −0.13 (s, 18H, $CHCH_2Si\mathit{Me}_3$), −0.04 (s, 4H, $ScC\mathit{H}_2SiMe_3$), 0.69 (dd, $^2J_{HH}$ = 14.8, $^3J_{HH}$ = 11.7 Hz, 2H, $CHC\mathit{H}_2SiMe_3$), 0.88 (br d, $^2J_{HH}$ = 14.8 Hz, 2H, $CHC\mathit{H}_2SiMe_3$), 1.34 (s, 18H, $C(C\mathit{H}_3)_3$), 1.81 (s, 18H, $C(C\mathit{H}_3)_3$), 2.23 (s, 6H, $C\mathit{H}_3$), 3.68 (s, 6H, $OC\mathit{H}_3$), 4.78 (br. s, 2H, $C\mathit{H}CH_2SiMe_3$), 6.26 (d, $^3J_{HH}$ = 8.1 Hz, 2H, Ar), 6.34 (d, $^3J_{HH}$ = 8.1 Hz, 2H, Ar), 6.40 (s, 2H, Ar), 7.32 (s, 2H, Ar), 7.54 (s, 2H, Ar) ppm. **$^{13}$C NMR** (101 MHz, benzene-$d_6$): δ = −1.1 (s, $CHCH_2Si(\mathit{C}H_3)_3$), 2.6 (s, $ScCH_2Si(\mathit{C}H_3)_3$), 21.2 (s, $\mathit{C}H_3$), 24.6 (s, $CH\mathit{C}H_2SiMe_3$), 31.3 (s, $C(\mathit{C}H_3)_3$), 34.1 (s, $\mathit{C}(CH_3)_3$), 34.4 (s, $C(\mathit{C}H_3)_3$), 36.5 (s, $\mathit{C}(CH_3)_3$), 38.9 (s, $Sc\mathit{C}H_2SiMe_3$), 57.0 (s, $O\mathit{C}H_3$), 61.0 (s, $\mathit{C}HCH_2SiMe_3$), 108.5 (*C*H, Ar), 109.2 (*C*H, Ar), 113.3 (*C*H, Ar), 125.3 (*C*H, Ar), 128.2 (*C*, Ar), 129.0 (*C*, Ar), 134.3 (*C*, Ar), 136.6 (*C*, Ar), 138.0 (*C*, Ar), 143.9 (*C*, Ar), 146.3 (*C*, Ar), 151.0 (*C*, Ar) ppm.

**Synthesis of 2c**. A yellow solution of **1c** (0.1437 g, 0.50 mmol) in toluene (5 ml) was added to a pale-yellow solution of $Sc(CH_2SiMe_3)_3(THF)_2$ (0.2254 g, 0.50 mmol) in toluene (10 ml) at 0 °C. The mixture darkening slightly was stirred at the same temperature for *ca*. 1.5 h. The volatiles were removed in vacuum, and the brownish-yellow residue was dissolved in a toluene-hexane mixture (1:1 v/v). The resulting solution was stored at –18 °C to afford microcrystalline yellow powder. The mother liquor was decanted, and the precipitate was washed twice with cold hexane and dried in vacuum for 10 min. Complex **2c** was isolated in 65% yield (0.2015 g). Anal. Calc. for $C_{74}H_{112}N_2O_4Sc_2Si_4$ (1263.97): C, 70.32; H, 8.93; N, 2.22; Sc, 7.11. Found: C, 70.00; H, 8.56; N, 2.06; Sc, 7.01 %. **$^1$H NMR** (400 MHz, benzene-$d_6$, 20 °C, TMS): δ = −0.21 (s, 2H, $ScC\mathit{H}_2SiMe_3$), −0.23 (s, 2H, $ScC\mathit{H}_2SiMe_3$), 0.02 (s, 18H, $CHCH_2Si\mathit{Me}_3$), 0.41 (s, 18H, $ScCH_2Si\mathit{Me}_3$), 0.71 (d, $^3J_{HH}$ = 11.9 Hz, 2H, $CHC\mathit{H}_2SiMe_3$), 1.08 (br s, 2H, $CHC\mathit{H}_2SiMe_3$), 1.45 (s, 18H, $C(C\mathit{H}_3)_3$), 1.72 (s, 18H, $C(C\mathit{H}_3)_3$), 4.95 (dd, $^3J_{HH}$ = 11.9 Hz, $^3J_{HH}$ = 3.6 Hz, 2H, $C\mathit{H}CH_2SiMe_3$), 6.39 (d, $^3J_{HH}$ = 7.7 Hz, 4H, Ar), 6.79 (dd, $^3J_{HH}$ = 7.8 Hz, $^3J_{HH}$ = 6.5 Hz, 2H, Ar), 6.86 (dd, $^3J_{HH}$ = 7.8 Hz, $^3J_{HH}$ = 6.5 Hz, 4H, Ar), 6.96 (d, $^3J_{HH}$ = 7.7 Hz, 4H, Ar), 7.01 (s, 2H, Ar), 7.07 (t, $^3J_{HH}$ = 8.4 Hz, 2H, Ar), 7.38 (d, $^3J_{HH}$ = 8.4 Hz, 2H, Ar), 7.46 (d, $^3J_{HH}$ = 8.1 Hz, 2H, Ar) ppm. **$^{13}$C NMR** (101 MHz, benzene-$d_6$): δ = −1.4 (s, $CHCH_2Si(\mathit{C}H_3)_3$), 3.5 (s, $ScCH_2Si(\mathit{C}H_3)_3$), 26.4 (s, $CH\mathit{C}H_2SiMe_3$), 30.2 (s, $C(\mathit{C}H_3)_3$), 31.6 (s, $\mathit{C}(CH_3)_3$), 31.9 (s, $C(\mathit{C}H_3)_3$), 34.0 (s,

Sc*C*H$_2$SiMe$_3$), 35.4 (s, *C*(CH$_3$)$_3$), 60.6 (s, *C*HCH$_2$SiMe$_3$), 108.0 (*C*H, Ar), 111.1 (*C*H, Ar), 112.2 (*C*H, Ar), 121.6 (*C*H, Ar), 123.0 (*C*H, Ar), 124.2 (*C*H, Ar), 125.3 (*C*H, Ar), 125.9 (*C*H, Ar), 126.3 (*C*H, Ar), 128.9 (*C*H, Ar), 129.8 (*C*H, Ar), 135.4 (*C*, Ar), 135.8 (*C*, Ar), 138.1 (*C*, Ar), 145.3 (*C*, Ar), 150.4 (*C*, Ar), 153.2 (*C*, Ar), 158.1 (*C*, Ar) ppm.

**Catalytic tests for hydrophosphination reactions**. All procedures for hydrophosphination tests were similar, and a typical procedure is given below. In a nitrogen dry box, the desired compound **2a**–**c** (10 μmol) was loaded in an NMR tube, then substrates (desired alkene or alkyne, 0.5 mmol; 50 equiv. and phosphine 0.5 mmol, 50 equiv.) were added at ambient temperature. The NMR tube was capped and placed for 48 h in a preheated to 70 °C oil bath.

After the specified reaction time, $CDCl_3$ was added to the reaction mixture, and the $^1H$ and $^{31}P\{^1H\}$ NMR spectra were recorded. Conversion was determined by integrating the remaining substrates and the newly formed addition product in the $^1H$ spectra as well as the remaining and newly formed phosphines in the $^{31}P\{^1H\}$.

**Catalytic tests for dehydrocoupling reactions**. In typical catalytic experiments of silylation of anisole the rare-earth complex in $C_6D_6$ was loaded into the ampule equipped with magnet stirrer in a glove-box. Anisole and hydrosilane were then added, and the reaction was started after heating the ampule at 80 ºC. After the specified reaction time, the $^1H$, $^{13}C$ and $^{29}Si$ NMR spectra were recorded. Conversion was determined by integrating the remaining hydrosilane and newly formed silylation product in the $^1H$ NMR spectra. The data for 2-MeO-$C_6H_4$-$SiH_2Ph$[S5,S6], 2-MeO$C_6H_4$-SiHMePh[S5] and 2-MeO$C_6H_4$-$SiHPh_2$[S6] are already reported.

**Table S1**. Selected distances (Å) and angles (deg) for **2a** and **2b**.

| | **2a** | **2b** |
|---|---|---|
| $Sc–C_{alkyl}$ | 2.223(6) | 2.219(3) |
| | 2.230(6) | 2.201(4) |
| $Sc–O_{phenoxide}$ | 2.084(4) | 2.064(2) |
| | 2.098(4) | 2.086(2) |
| | 2.210(4) | 2.087(2) |
| | 2.156(4) | 2.101(2) |
| $Sc–N_{amido}$ | 2.070(5) | 2.030(3) |
| | 2.081(5) | 2.045(3) |
| $Sc–O_{OMe}$ | | 2.181(2) |
| | | 2.182(2) |
| $Sc–N_{quin}$ | 2.292(5) | |
| | 2.309(5) | |
| $C_{CH}–N_{amido}$ | 1.462(7) | 1.457(4) |
| | 1.468(7) | 1.471(4) |
| $N_{amido}–Sc–N_{quin}$ | 74.2(2) | |
| | 75.1(2) | |
| $N_{amido}–Sc–C_{alkyl}$ | 120.2(2) | |
| | 109.9(2) | |
| $O_{OMe}–Sc–N_{amido}$ | | 75.3(2) |
| | | 74.9(2) |
| $O_{Ome}–Sc–C_{alkyl}$ | | 95.9(2) |
| | | 100.6(2) |
| $Sc–O_{phenoxide}–Sc$ | 101.6(2) | 100.79(9) |
| | 102.4(2) | 101.1(2) |

The $Sc_2O_2$-cores in **2a** and **2b** are nearly planar, the dihedral angles between OScO planes are 169.2(2)° and 164.0(2)°, respectively. In **2a**, the Sc-$O_{phenoxide}$ bond lengths fall into the wide range of 2.084(4)-2.156(4) Å and are somewhat longer than in **2b** ((2.064(2)-2.101(2) Å)). The Sc-$O_{phenoxide}$ lengths in **2a** and **2b** are expectedly longer compared to the typical Sc–$O_{phenoxide}$ lengths in five-coordinate scandium compounds with terminal phenolate ligands [$CH_3C$(2,6-$iPr_2C_6H_3N$)C(R)C($CH_3$)(N($CH_2$)$_n$$CH_2PPh_2$]Sc($CH_2SiMe_3$)O-(2,6-$tBu_2C_6H_3$) (1.946(2) Å)[S7], LScO[2,6-$tBu_2C_6H_3$]$_2$ (L = N($SiMe_2R$)$_2$, R = 2-methylfuryl) (1.934(2) Å)[S8], [2-$Bu^t$-$OC_6H_3$CH=N-dipp]$_2$Sc($CH_2SiMe_3$) (2.001(2) and 2.001(2) Å)[S9] and [2-$Bu^t$-$OC_6H_3$CH=N-Mes]Sc($CH_2SiMe_3$)$_2$(THF) (1.993(2) Å).[S10] For **2b**, the Sc–$O_{OMe}$ distances (2.181(2), 2.182(2) Å) are comparable with the Sc–O coordination bonds in previously reported complex [LSc{($Bu^tC_6H_3O$)CH($CH_2SiMe_3$)NPh}(THF)] (L = N-phenyl-*ortho*-tert-butylsalicylaldiminate) (2.207(2) Å).[S11]

The Sc–$N_{amido}$ distances in **2a** (2.070(5), 2.081(5) Å) are slightly longer than in **2b** (2.030(3), 2.045(3) Å) and are in good agreement with distances in five-coordinate scandium amido complexes incorporating different types of ancillary ligands: Sc($N_2^{TMS}N_{py}$)Cl(THF) ($N_2^{TMS}N_{py}$ = MeC(2-$C_5H_4N$)($CH_2NSiMe_3$)$_2$) (2.024(2)–2.025(2) Å),[S12] [LSc$CH_2SiMe_3$)$_2$] (L = N($SiMe_2R$)$_2$, R = 2-methylfuryl) (2.093(2) Å)[S8], anilidopyridyl-pyrrolide [$C_4H_3N$-$C_6H_3N$-C($Pr^i$-$C_6H_4$)-Ndipp]ScN($SiHMe_2$)$_2$ (2.059(3) and 2.075(3) Å),[S13] [LSc{($Bu^tC_6H_3O$)CH($CH_2SiMe_3$)NPh}(THF)] (L = N-phenyl-*ortho*-tert-butylsalicylaldiminate) (2.080(2) Å).[S11] The Sc–$N_{quin}$ distances in **2a** fall into rather narrow range of 2.292(5)-2.309(5) Å and are comparable with Sc–N coordination bond distances in other pentacoordinate scandium species [$C_4H_3N$-$C_6H_3N$-C($Pr^i$-$C_6H_4$)-Ndipp]ScN($SiHMe_2$)$_2$] (2.211(3) and 2.243(3) Å),[S13] [LSc{($Bu^tC_6H_3O$)CH($CH_2SiMe_3$)NPh}(THF)] (L = N-phenyl-*ortho*- tert-butylsalicylaldiminate) (2.288(2) Å),[S11] [Sc(MeC(2-$C_5H_4N$)($CH_2NSiMe_3$)$_2$)Cl(THF)] (2.288(2) Å).[S12] Finally, the lengths of former "imino" C–N bonds in **2a** (1.462(7), 1.468(7) Å) and **2b** (1.457(4), 1.471(4) Å) are indicative of their single character (1.47 Å).[S14] The Sc–C bonds in **2a** (2.223(6), 2.230(6) Å) and **2b** (2.201(4), 2.219(3) Å) have similar lengths and are in a close agreement with Sc-C distances measured in five-coordinate alkyl complexes [(2-$Bu^t$-$OC_6H_3$CH=N-Mes)Sc($CH_2SiMe_3$)$_2$(THF)] (2.236(2) and 2.246(2) Å)S[10], LSc($CH_2SiMe_3$)$_2$THF (L = 2-(2,6-$Me_2$PhN)- phenyl-4-(S)-Me-oxazoline) (2.243(2) and 2.239(2) Å,[S15] LSc($CH_2SiMe_3$)$_2$ (L = N($SiMe_2R$)$_2$, R = 2-methylfuryl) (2.214(2) and 2.232(2) Å)[S8].

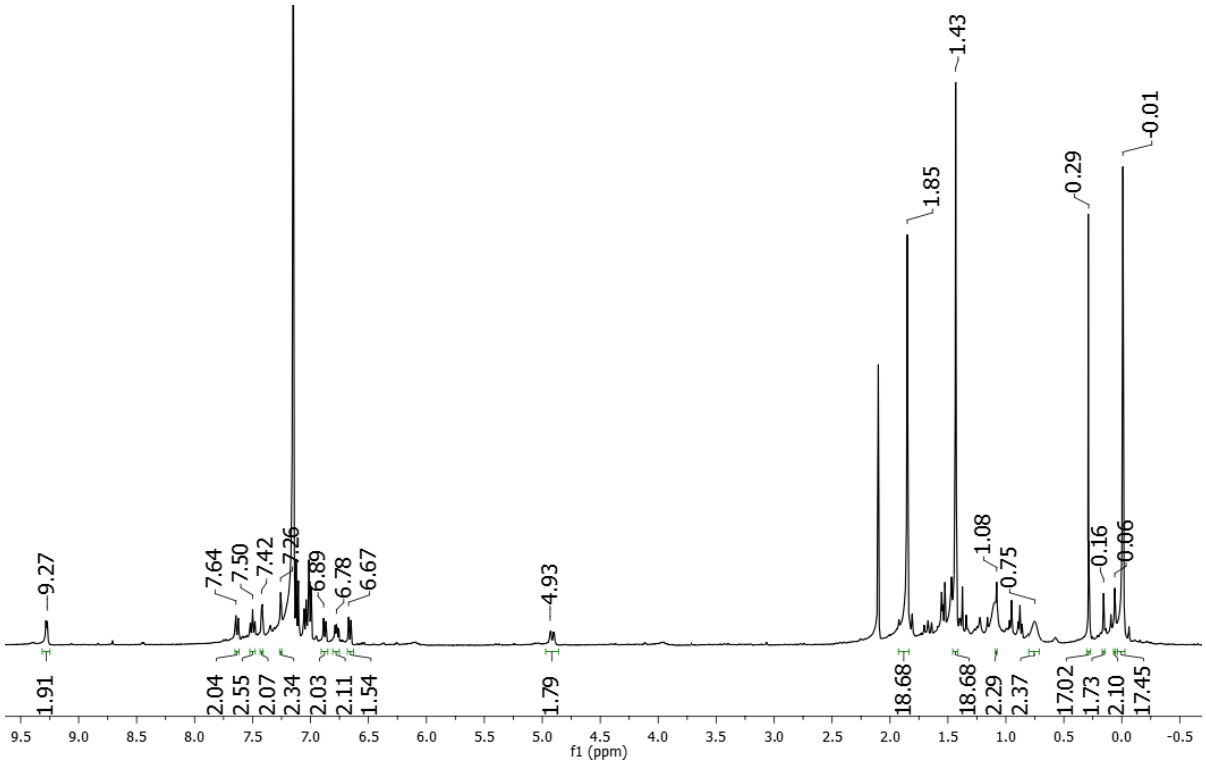


**Figure S1**. $^{1}$H NMR spectrum of complex **2a** (400 MHz, 293 K, benzene-$d_6$)

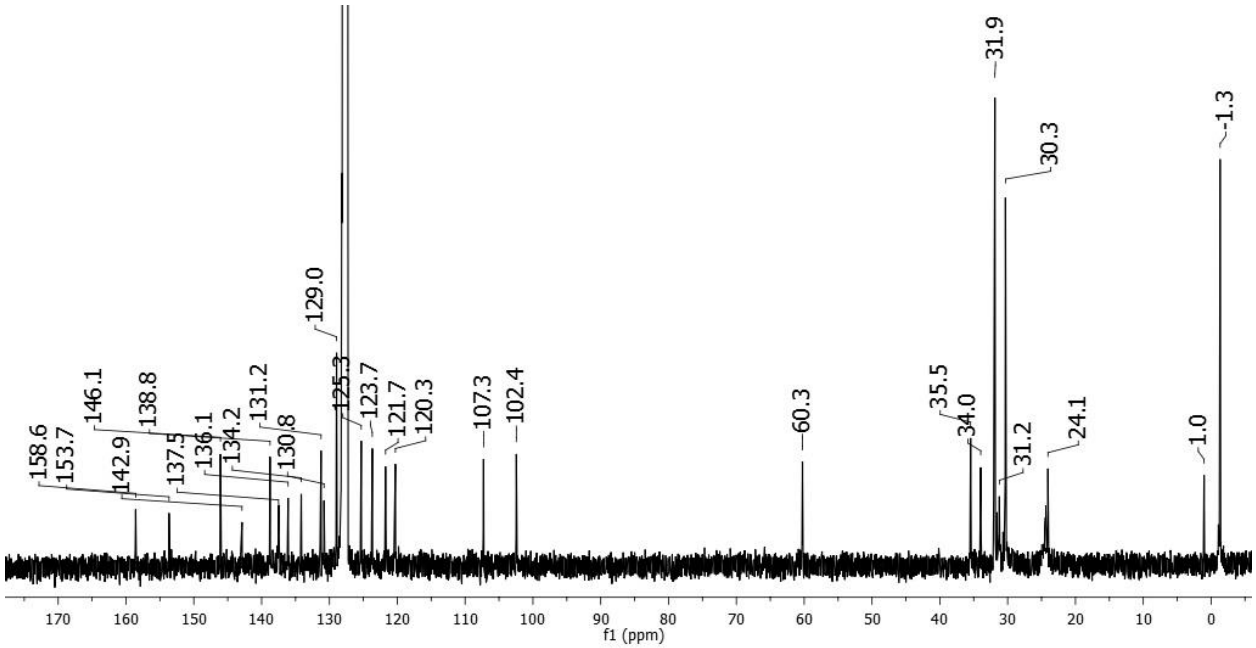


**Figure S2**. $^{13}$C NMR spectrum of complex **2a** (100 MHz, 293 K, benzene-$d_6$)

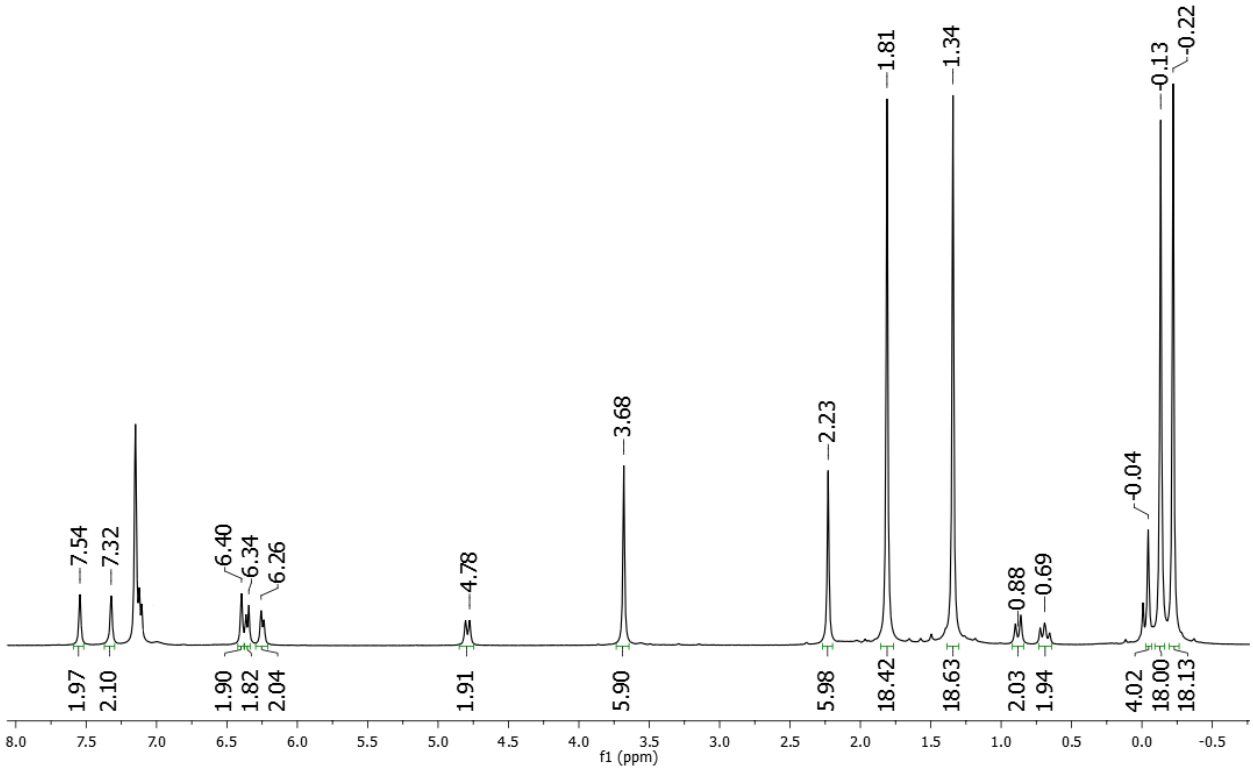


**Figure S3**. $^{1}$H NMR spectrum of complex **2b** (400 MHz, 293 K, benzene-$d_6$)

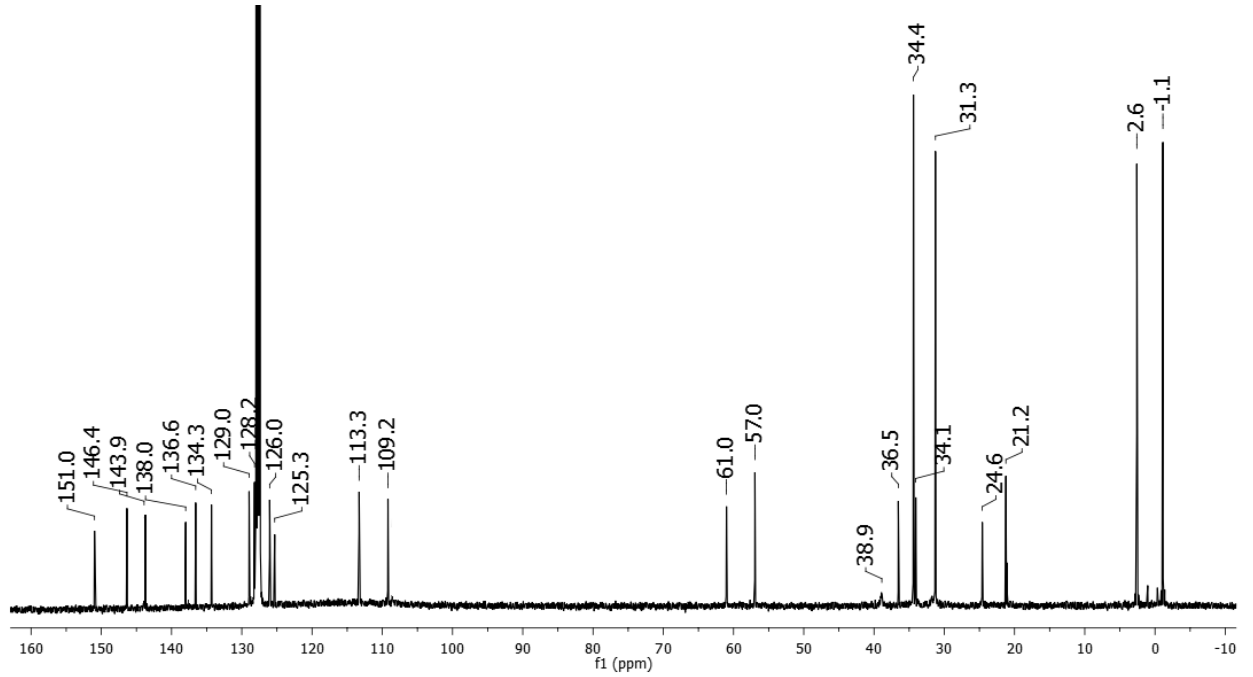


**Figure S4**. $^{13}$C NMR spectrum of complex **2b** (100 MHz, 293 K, benzene-$d_6$)

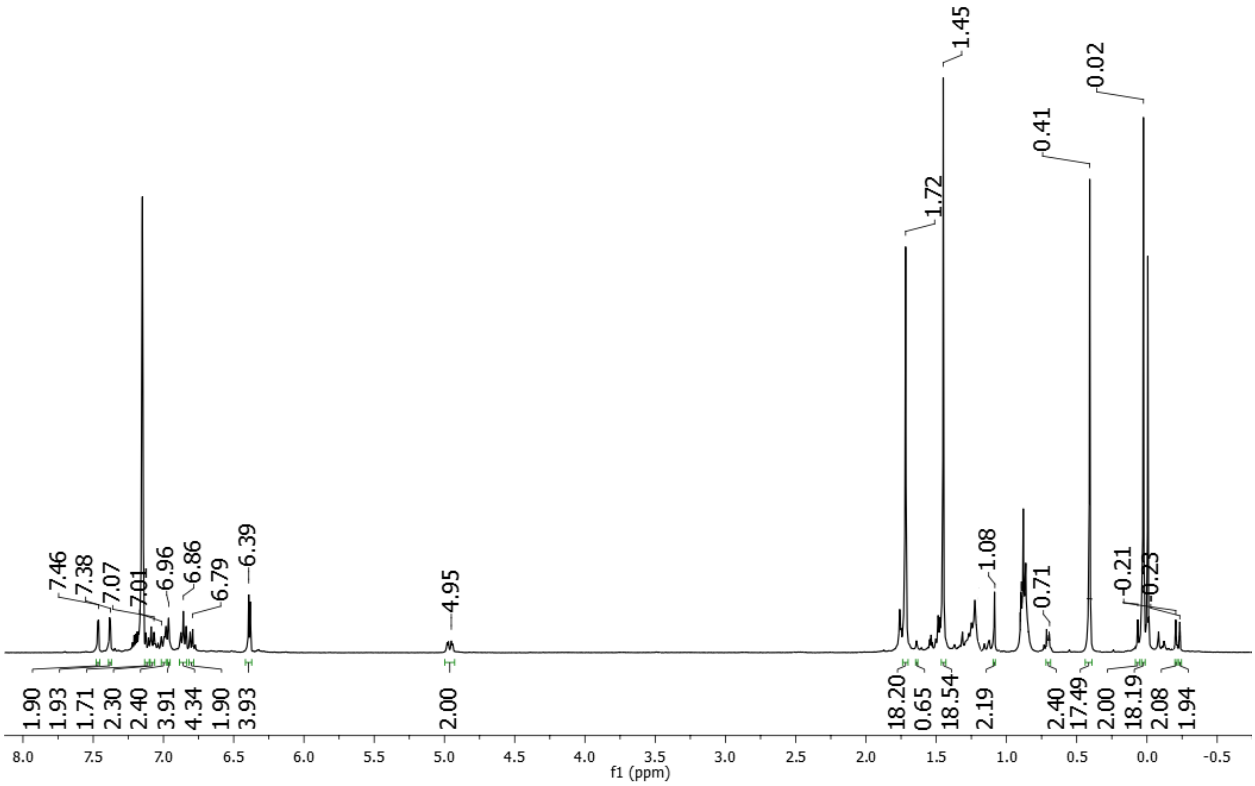


**Figure S5**. [1]H NMR spectrum of complex **2c** (400 MHz, 293 K, benzene-$d_6$)

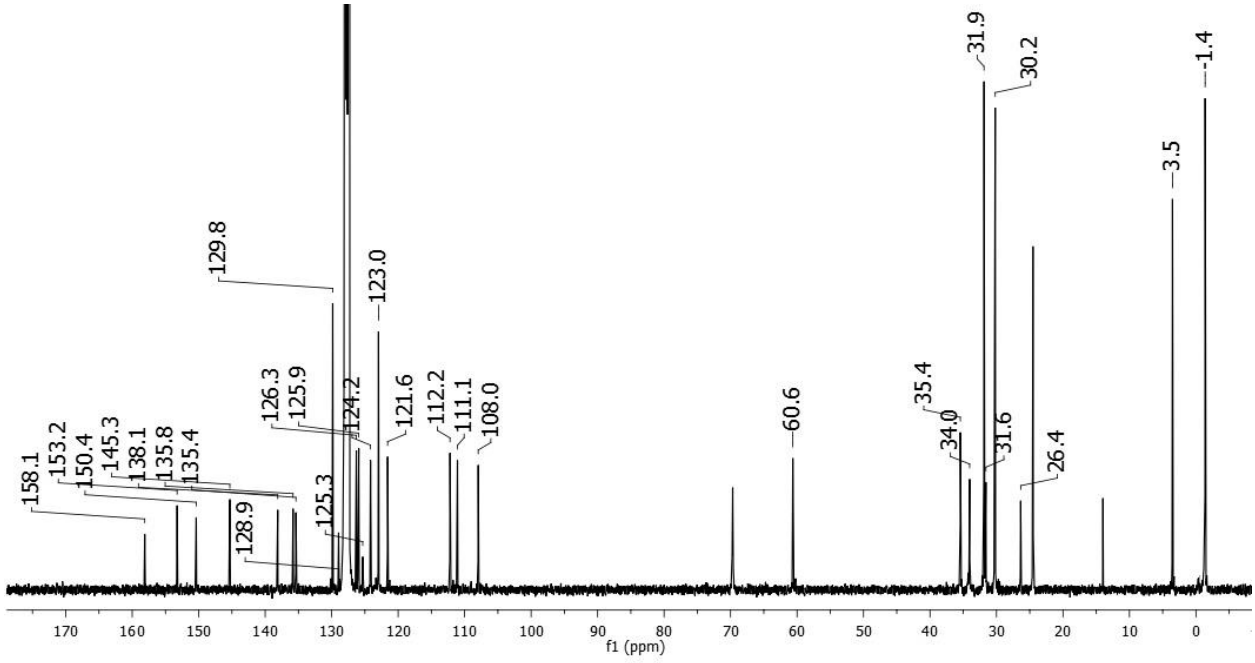


**Figure S6**. [13]C NMR spectrum of complex **2c** (100 MHz, 293 K, benzene-$d_6$)

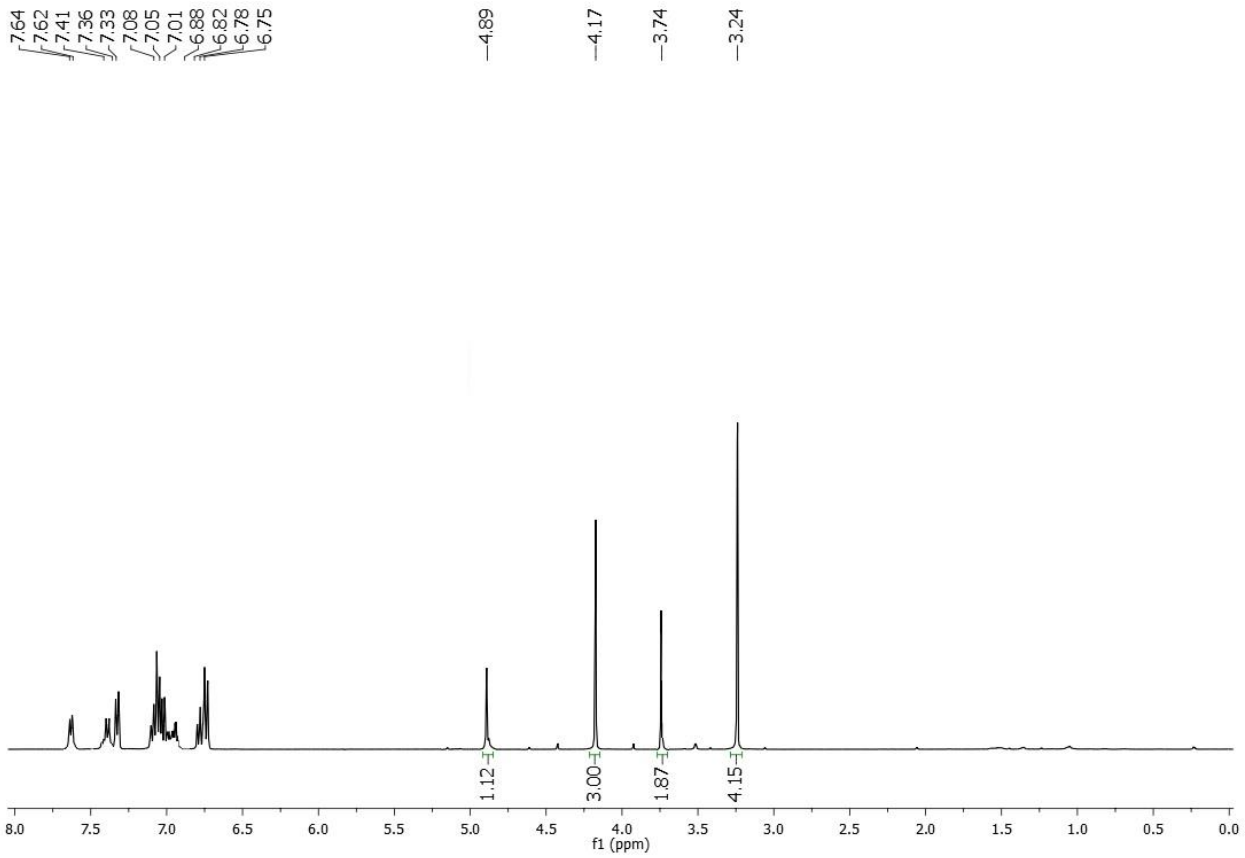


**Figure S7**. $^{1}$H NMR spectrum of the catalytic reaction of anisole with $PhSiH_3$ promoted by complex **2a** (400 MHz, 293 K, benzene-$d_6$).

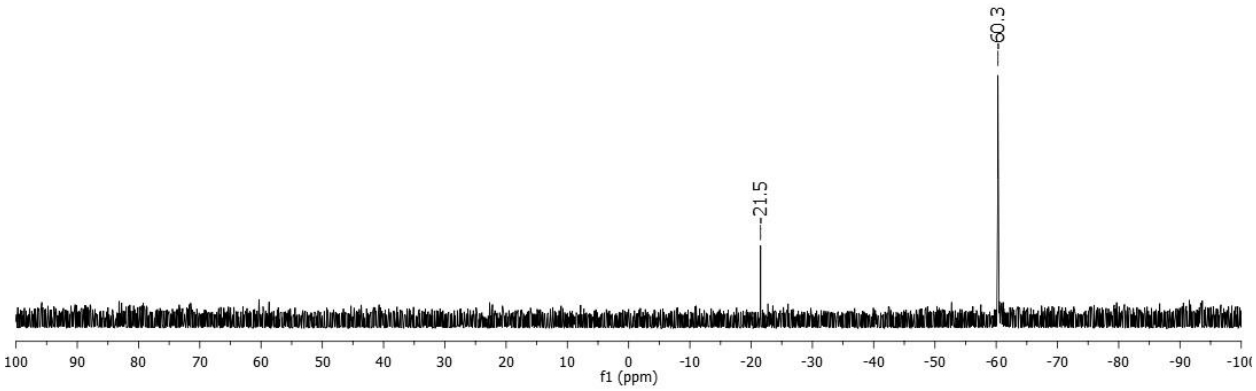


**Figure S8**. $^{29}$Si NMR spectrum of the catalytic reaction of anisole with $PhSiH_3$ promoted by complex **2a** (79 MHz, 293 K, benzene-$d_6$).

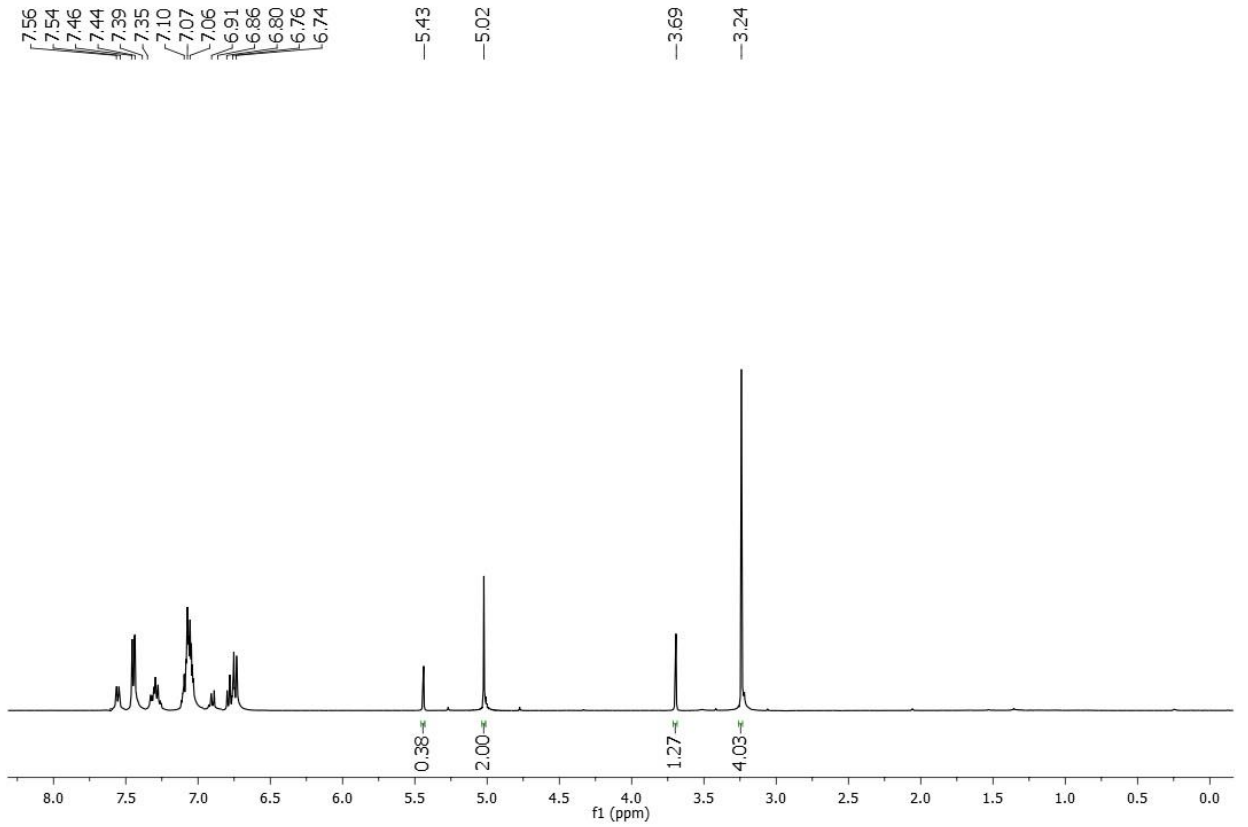


**Figure S9**. $^{1}$H NMR spectrum of the catalytic reaction of anisole with $Ph_2SiH_2$ promoted by complex **2a** (400 MHz, 293 K, benzene-$d_6$).

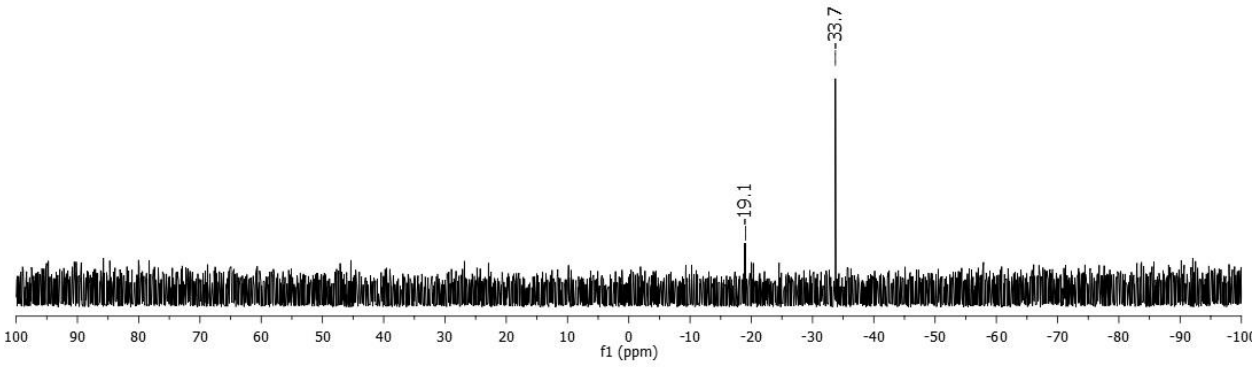


**Figure S10**. $^{29}$Si NMR spectrum of the catalytic reaction of anisole with $Ph_2SiH_2$ promoted by complex **2a** (79 MHz, 293 K, benzene-$d_6$).

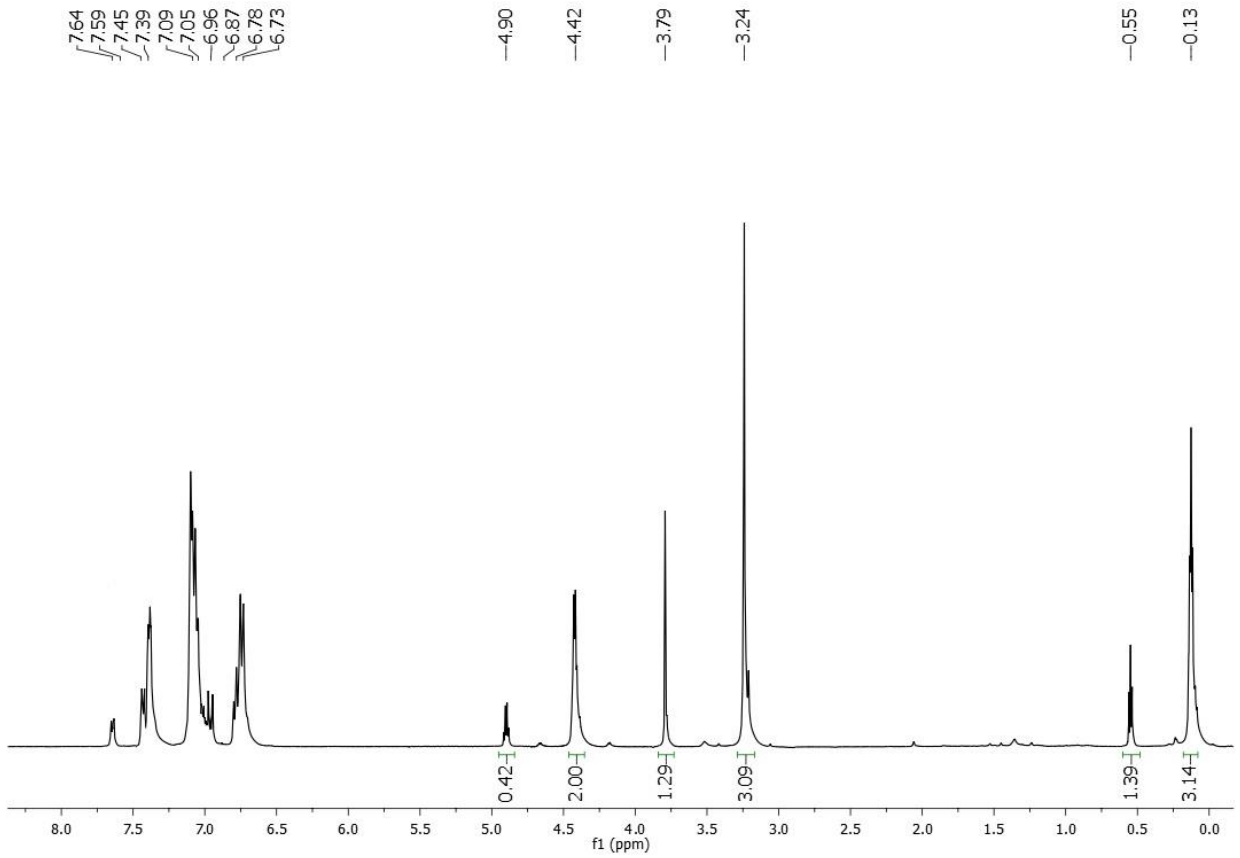


**Figure S11**. $^{1}$H NMR spectrum of the catalytic reaction of anisole with $PhMeSiH_2$ promoted by complex **2a** (400 MHz, 293 K, benzene-$d_6$).

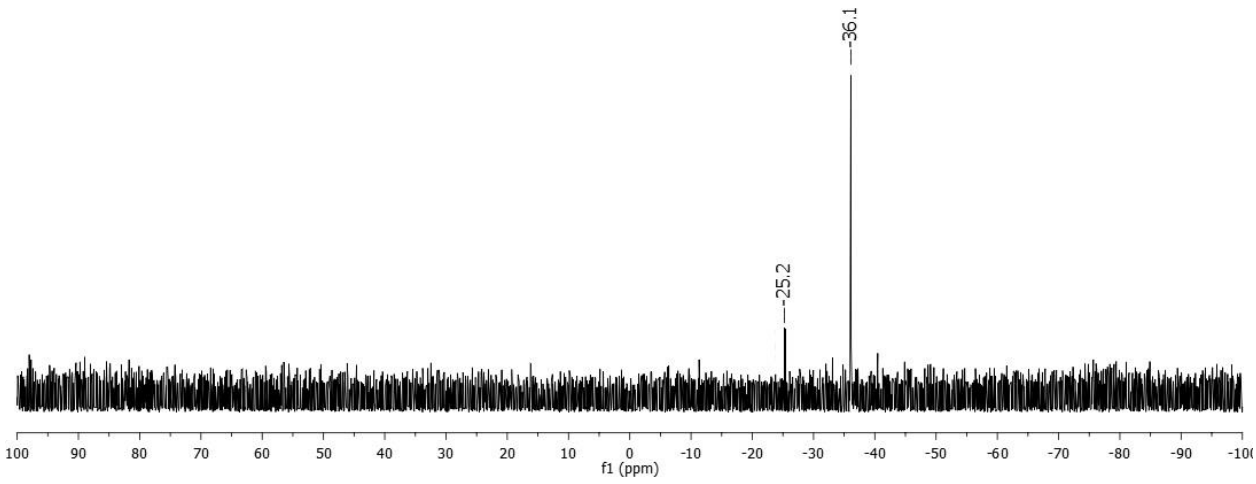


**Figure S12**. $^{29}$Si NMR spectrum of the catalytic reaction of anisole with $Ph_2SiH_2$ promoted by complex **2a** (79 MHz, 293 K, benzene-$d_6$).

## References


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