Supporting Information

For

Secondary Benzylolation with Benzyl Alcohols Catalyzed by A High-Valent Heterobimetallic Ir-Sn Complex

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General Methods:

All preparations and manipulations were performed under a dry, oxygen-free argon atmosphere using standard vacuum lines and Schlenk techniques. All solvents, used for the synthesis, were dried and distilled by standard methods and previously deoxygenated in the vacuum line. Pre-coated silica gel 60F₂₅₄ was used for thin layer chromatography and silica gel 60-120 mesh was used for column chromatography. [Ir(COD)(μ-Cl)]₂ was prepared according to the literature procedure.¹

¹H (200, 400 MHz), ¹³C (54.6, 100 MHz) NMR spectra were recorded on 200 MHz and 400 MHz Spectrometer. ¹H chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard (deuteriochloroform: δ 7.26 ppm). Data are reported as follows: chemical shifts, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet), coupling constant (Hz). ¹³C chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard (CDCl₃: δ 77.0 ppm and DMSO-d₆: δ 39.52 ppm). Melting points are uncorrected.

GC Analysis:

GC analysis was performed using a flame ionization detector using 6 ft x 1/8 inch x 2 mm SS 10% Silicone OV-1 packed column. *n*-Nonane was used as internal standard. The analytical conditions are as follows:

Injector temperature 180 °C

Detector temperature 230 °C

Career gas (N₂) flow 1.8 bar

Oven temperature program 60 °C-5 min-2 °C/min-80 °C-0 min-20 °C/min-200 °C-9 min.

General Procedure for Kinetic Study (vide Fig. 2)

The reaction was carried out in a 10-mL Schlenk flask using *o*-xylene (370 μL, 3.1 mmol), catalyst **1** (5.5 mg, 0.75 mol%), 1-phenylethanol **2** (75 μL, 0.62 mmol) in 1,2-dichloroethane (2.5 mL) against *n*-nonane (70 μL) as internal standard under argon at 80 °C. Known volume of aliquot was withdrawn periodically from the reaction mixture, filtered through a short pad of celite, diluted with toluene and organic layer was analyzed with GC.

The retention times are as follows:

n-Nonane.....10.140 min

Alcohol **2**.....17.427 min

Ether **3**.....23.473 min

Product **4**.....25.233 min

General Procedure for Benzylation Kinetics (vide Table 4, Fig. 3 & Chart S1)

The reaction was carried out in a 10-mL Schlenk flask using thiophene (5.0 mmol), catalyst **1** (1 mol%), *para* substituted 1-phenylethanol (0.5 mmol) in 1,2-dichloroethane (2 mL) against *n*-nonane (60 μ L) as internal standard under argon at 45 °C. Known volume of aliquot was withdrawn periodically from the reaction mixture, filtered through a short pad of celite, diluted with toluene and organic layer was analyzed with GC.

Chart S1. Products resulted from the reaction of *p*-R-C₆H₄-CH(Me)OH with thiophene

The retention times are as follows:

n-Nonane.....10.140 min

Product **34**.....23.780 min

Product **20**.....22.080 min

Product **35**.....22.647 min

Product **36**.....27.320 min

Product **37**.....24.966 min

Figure S1. Pseudo-first order rate plots (vide Table 4 in original manuscript)

Spectroscopic & Analytical Data of Products:

[6196-95-8]²

Colorless oil: TLC R_f = 0.30 (pet ether 60-80 °C)

¹H NMR (200 MHz, CDCl₃) δ = 1.62 (d, ³ J (H,H) = 7.2 Hz, 3H), 2.22 (s, 6H), 4.09 (q, ³ J (H,H) = 7.2 Hz, 1H), 6.95-7.08 (m, 3H); 7.17-7.29 (m, 5H).

¹³C NMR (54.6 MHz, CDCl₃) δ = 19.3, 19.8, 21.9, 44.4, 124.9, 125.9, 127.5, 128.3, 129.0, 129.6, 134.1, 136.4, 143.9, 146.7.

Anal. (C₁₆H₁₈) calcd, C: 91.37, H: 8.63; found, C: 91.15, H: 8.67.

[3717-68-8]³

Colorless oil: TLC R_f = 0.32 (pet ether 60-80 °C)

¹H NMR (200 MHz, CDCl₃) major-isomer, δ = 1.65 (d, ³ J (H,H) = 7.2 Hz, 3H), 2.33 (s, 3H), 4.14 (q, ³ J (H,H) = 7.2 Hz, 1H), 7.13-7.35 (m, 9H); minor-isomer, 2.26 (s, 3H).

¹³C NMR (54.6 MHz, CDCl₃) (major-isomer), δ = 20.9, 21.8, 44.3, 125.8, 127.4, 127.5, 128.2, 129.0, 135.4, 143.3, 146.5.

Anal. (C₁₅H₁₆) calcd, C: 91.78, H: 8.22; found, C: 91.45, H: 8.20.

[863093-07-6]²

Colorless oil: TLC R_f = 0.36 (pet ether 60-80 °C)

¹H NMR (200 MHz, CDCl₃) major-isomer, δ = 1.76 (d, ³ J (H,H) = 7.1 Hz, 3H), 2.67 (s, 3H), 4.91 (q, ³ J (H,H) = 7.1 Hz, 1H), 7.16-7.50 (m, 9H), 8.00-8.09 (m, 2H); minor-isomer, 2.61 (s, 3H).

¹³C NMR (54.6 MHz, CDCl₃) (major-isomer), δ = 19.4, 22.6, 40.4, 124.0, 124.4, 124.7, 125.1, 125.4, 125.8, 126.2, 127.5, 128.3, 131.7, 132.8, 133.0, 139.6, 146.8.

Anal. (C₁₉H₁₈) calcd, C: 92.64, H: 7.36; found, C: 93.54, H: 7.70.

[124494-12-8]⁴

Light yellow solid: mp 43-44 °C; TLC R_f = 0.13 (pet ether 60-80 °C)

¹H NMR (200 MHz, CDCl₃) δ = 2.77 (dd, ³J(H,H) = 7.9, 6.9 Hz, 2H), 3.75 (s, 3H), 3.95 (t, ³J(H,H) = 7.9 Hz, 1H), 4.90-5.06 (m, 2H), 5.60-5.81 (m, 1H), 6.75-6.83 (m, 2H), 7.10-7.31 (m, 7H).

¹³C NMR (54.6 MHz, CDCl₃) δ = 40.1, 50.4, 55.2, 113.8, 116.2, 126.1, 127.8, 128.4, 128.8, 136.6, 136.9, 144.9, 157.9.

Anal. (C₁₇H₁₈O) calcd, C: 85.67, H: 7.61; found, C: 85.64, H: 7.38.

[499194-65-9]⁴

Light yellow solid: TLC R_f = 0.20 (pet ether 60-80 °C)

¹H NMR (200 MHz, CDCl₃) δ = 2.78 (dd, ³J(H,H) = 7.9, 7.2 Hz, 2H), 3.77 (s, 3H), 4.49 (t, ³J(H,H) = 7.9 Hz, 1H), 4.90-5.06 (m, 2H), 5.64-5.84 (m, 1H), 6.81-6.95 (m, 2H), 7.10-7.27 (m, 7H).

¹³C NMR (54.6 MHz, CDCl₃) δ = 39.1, 43.3, 55.4, 110.7, 115.8, 120.5, 125.8, 127.1, 127.8, 128.1, 128.2, 133.0, 137.2, 144.4, 157.0.

Anal. (C₁₇H₁₈O) calcd, C: 85.67, H: 7.61; found, C: 85.54, H: 7.48.

Yellow solid: TLC R_f = 0.44 (pet ether/EtOAc = 9/1)

^1H NMR (200 MHz, CDCl_3) δ = 2.35 (s, 3H), 4.02 (s, 3H), 5.42 (d, $^3J(\text{H,H})$ = 9.0 Hz, 1H), 6.38 (d, $^3J(\text{H,H})$ = 9.0 Hz, 1H), 6.83 (d, $^3J(\text{H,H})$ = 8.1 Hz, 1H), 7.09 (d, $^3J(\text{H,H})$ = 8.1 Hz, 2H), 7.32 (d, $^3J(\text{H,H})$ = 8.1 Hz, 2H), 7.41-7.62 (m, 3H), 8.07 (d, $^3J(\text{H,H})$ = 8.0 Hz, 1H), 8.31 (d, $^3J(\text{H,H})$ = 8.0 Hz, 1H).

^{13}C NMR (54.6 MHz, CDCl_3) δ = 21.1, 48.6, 55.5, 56.8, 103.0, 122.7, 122.8, 124.3, 125.0, 126.0, 127.0, 128.3, 128.8, 129.2, 132.3, 137.1, 137.7, 154.9.

Anal. ($\text{C}_{20}\text{H}_{18}\text{Br}_2\text{O}$) calcd, C: 55.33, H: 4.18; found, C: 55.87, H: 4.04.

White Solid: mp 64-65 °C; TLC R_f = 0.26 (pet ether 60-80 °C)

^1H NMR (400 MHz, CDCl_3) δ = 1.76-1.86 (m, 2H), 2.05-2.23 (m, 2H), 2.85-3.01 (m, 2H), 3.96 (s, 3H), 4.86 (t, $^3J(\text{H,H})$ = 5.6 Hz, 1H), 6.67 (d, $^3J(\text{H,H})$ = 8.0 Hz, 1H), 6.81 (d, $^3J(\text{H,H})$ = 8.0 Hz, 1H), 6.87 (dd, $J(\text{H,H})$ = 7.8 Hz, 5.6 Hz, 1H), 7.03 (m, 1H), 7.13-7.20 (m, 2H), 7.46-7.58 (m, 2H), 8.07 (d, $^3J(\text{H,H})$ = 8.0 Hz, 1H), 8.34 (d, $^3J(\text{H,H})$ = 8.0 Hz, 1H).

^{13}C NMR (100 MHz, CDCl_3) δ = 20.4, 29.8, 31.0, 40.8, 55.4, 103.1, 122.7, 123.5, 124.7, 125.7, 125.8, 125.9, 126.3, 127.3, 128.9, 129.0, 130.3, 132.2, 135.1, 137.8, 139.8, 153.9.

ESI-MS: for $\text{C}_{21}\text{H}_{20}\text{O}$ [M], $[\text{M}+\text{H}]^+ = 289.15$.

Anal. ($\text{C}_{21}\text{H}_{20}\text{O}$) calcd, C: 87.46, H: 6.99; found, C: 86.96, H: 6.96.

[80355-66-4]⁵

Yellow viscous oil: TLC R_f = 0.52 (pet ether/EtOAc = 9/1)

^1H NMR (400 MHz, CDCl_3) δ = 1.69-2.19 (m, 4H), 2.23 (s, 3H), 2.54 (brs, 1H), 2.82-2.99 (m, 2H), 4.27 (t, $^3J(\text{H,H})$ = 7.4 Hz, 1H), 6.70 (d, $^3J(\text{H,H})$ = 8.0 Hz, 1H), 6.77 (s, 1H), 6.91-7.00 (m, 2H), 7.04-7.08 (m, 1H), 7.12-7.15 (m, 2H).

^{13}C NMR (100 MHz, CDCl_3) δ = 20.6, 21.8, 29.8, 30.8, 41.1, 116.1, 126.2, 126.3, 127.9, 129.3, 129.4, 129.9, 131.3, 132.3, 137.7, 138.1, 151.0.

Anal. ($\text{C}_{17}\text{H}_{18}\text{O}$) calcd, C: 85.67, H: 7.61; found, C: 85.83, H: 7.67.

[19353-89-0]⁶

White Solid: mp 65-67 °C; TLC R_f = 0.19 (pet ether 60-80 °C)

^1H NMR (400 MHz, CDCl_3) δ = 1.76-1.88 (m, 3H), 2.11-2.18 (m, 1H), 2.84-2.89 (m, 2H), 3.79 (s, 3H), 4.07 (t, $^3J(\text{H,H})$ = 6.8 Hz, 1H), 6.81-6.86 (m, 4H), 7.00-7.05 (m, 2H), 7.11-7.14 (m, 2H).

^{13}C NMR (100 MHz, CDCl_3) δ = 20.9, 29.7, 33.3, 44.5, 55.2, 113.5, 125.6, 125.8, 128.9, 129.6, 130.1, 137.5, 139.6, 139.7, 157.7.

Anal. ($\text{C}_{17}\text{H}_{18}\text{O}$) calcd, C: 85.67, H: 7.61; found, C: 85.03, H: 7.54.

Colorless oil: TLC R_f = 0.33 (pet ether/EtOAc = 9/1)

^1H NMR (200 MHz, CDCl_3) δ = 1.57 (d, $^3J(\text{H,H})$ = 7.1 Hz, 3H), 2.31 (s, 3H), 4.03 (q, $^3J(\text{H,H})$ = 7.1 Hz, 3H), 5.40 (br s, 1H), 6.89-7.16 (m, 7H).

^{13}C NMR (54.6 MHz, CDCl_3) δ = 20.8, 21.8, 43.2, 115.8, 119.4, 127.1, 127.4, 127.6, 129.0, 135.6, 139.9, 142.8, 149.2.

Anal. ($\text{C}_{15}\text{H}_{15}\text{ClO}$) calcd, C: 73.02, H: 6.13; found, C: 73.28, H: 6.07.

[158121-60-9]⁷

Colorless oil: TLC R_f = 0.52 (pet ether 60-80 °C)

^1H NMR (200 MHz, CDCl_3) δ = 1.71 (d, $^3J(\text{H,H})$ = 7.1 Hz, 3H), 4.35 (q, $^3J(\text{H,H})$ = 7.1 Hz, 1H), 6.79-6.95 (m, 3H), 7.13-7.32 (m, 5H); minor isomer, 1.64 (d, $^3J(\text{H,H})$ = 7.1 Hz, 3H), 4.20 (d, $^3J(\text{H,H})$ = 7.1 Hz, 1H).

^{13}C NMR (54.6 MHz, CDCl_3) (major isomer), δ = 23.3, 40.7, 119.8, 123.5, 123.6, 126.5, 127.2, 128.4, 146.0, 150.7.

Anal. ($\text{C}_{12}\text{H}_{12}\text{S}$) calcd, C: 76.55, H: 6.42; found, C: 77.05, H: 6.67.

Colorless oil: TLC R_f = 0.48 (pet ether 60-80 °C)

^1H NMR (200 MHz, CDCl_3) δ = 2.74-2.99 (m, 2H), 4.25 (t, $^3J(\text{H,H})$ = 7.7 Hz, 3H), 4.96-5.12 (m, 2H), 5.64-5.85 (m, 1H), 6.84-7.03 (m, 3H), 7.15-7.37 (m, 5H); minor isomer, 4.08 (t, $^3J(\text{H,H})$ = 7.7 Hz, 3H).

^{13}C NMR (54.6 MHz, CDCl_3) (major isomer) δ = 41.4, 46.7, 116.5, 123.4, 123.8, 126.3, 126.4, 127.6, 128.3, 136.0, 143.8, 148.6.

Anal. ($\text{C}_{14}\text{H}_{14}\text{S}$) calcd, C: 78.45, H: 6.58; found, C: 78.72, H: 6.52.

Yellow oil: TLC R_f = 0.66 (pet ether/EtOAc = 9/1)

^1H NMR (200 MHz, CDCl_3) δ = 1.64 (d, $^3J(\text{H,H})$ = 7.2 Hz, 3H), 2.41 (s, 3H), 4.23 (q, $^3J(\text{H,H})$ = 7.2 Hz, 1H), 6.56 (s, 2H), 7.08-7.32 (m, 4H); minor isomer, 1.57 (d, $^3J(\text{H,H})$ = 7.2 Hz, 3H), 2.31 (s, 3H).

^{13}C NMR (54.6 MHz, CDCl_3) (major + minor-isomer) δ = 15.1, 22.9, 40.1, 121.1, 123.2, 124.3, 126.7, 128.3, 128.3, 128.4, 128.6, 132.0, 138.1, 144.5, 147.5.

Anal. ($\text{C}_{13}\text{H}_{13}\text{ClS}$) calcd, C: 65.95, H: 5.53; found, C: 65.66, H: 5.61.

[99159-22-5]⁸

White Solid: mp 44-45 °C, TLC R_f = 0.26 (pet ether 60-80 °C)

^1H NMR (200 MHz, CDCl_3) δ = 1.74 (d, $^3J(\text{H,H})$ = 7.2 Hz, 3H), 4.45 (q, $^3J(\text{H,H})$ = 7.2 Hz, 1H), 7.04-7.33 (m, 8H), 7.53-7.58 (m, 1H), 7.82-7.86 (m, 1H).

^{13}C NMR (54.6 MHz, CDCl_3) δ = 22.4, 39.5, 121.4, 122.5, 122.8, 123.8, 124.1, 126.3, 127.4, 128.5, 138.6, 140.5, 140.7, 145.4.

Anal. ($\text{C}_{16}\text{H}_{14}\text{S}$) calcd, C: 80.63, H: 5.92; found, C: 80.83, H: 6.03.

Yellow oil: TLC R_f = 0.51 (pet ether/EtOAc = 9/1)

^1H NMR (200 MHz, CDCl_3) δ = 0.91 (d, $^3J(\text{H,H})$ = 6.8 Hz, 3H), 2.83-2.95 (m, 1H), 3.68 (d, $^3J(\text{H,H})$ = 9.6 Hz, 1H), 3.85 (s, 3H), 3.86 (s, 3H), 4.84-5.04 (m, 2H), 5.65-5.82 (m, 1H), 6.08-6.09 (m, 1H), 6.24-6.28 (m, 1H), 6.76-6.88 (m, 3H), 7.30-7.33 (m, 1H); minor isomer, 1.00 (d, $^3J(\text{H,H})$ = 6.7 Hz, 3H).

^{13}C NMR (54.6 MHz, CDCl_3) δ = 18.6, 42.0, 51.3, 55.8, 106.0, 109.9, 111.0, 111.6, 113.9, 120.5, 134.0, 141.0, 142.4, 147.7, 148.7, 156.8.

Anal. ($\text{C}_{17}\text{H}_{20}\text{O}_3$) calcd, C: 74.97, H: 7.40; found, C: 74.75, H: 7.49.

Yellow oil: TLC R_f = 0.52 (pet ether/EtOAc = 8/2)

^1H NMR (200 MHz, CDCl_3) δ = 0.90 (d, $^3J(\text{H,H})$ = 6.7 Hz, 6H), 2.79-2.94 (m, 2H), 3.63 (d, $^3J(\text{H,H})$ = 9.1 Hz, 2H), 3.78 (s, 6H), 3.84 (s, 6H), 4.82 (m, 4H), 5.64-5.82 (m, 2H), 5.92 (s, 2H), 6.71-6.82 (m, 6H); minor isomer, 0.97 (d, $^3J(\text{H,H})$ = 6.4 Hz, 6H), 3.62 (d, $^3J(\text{H,H})$ = 9.2 Hz, 2H).

^{13}C NMR (54.6 MHz, CDCl_3) (major isomer) δ = 18.5, 42.0, 51.4, 55.7, 55.8, 106.6, 110.9, 111.7, 113.8, 120.6, 134.5, 142.4, 147.6, 148.7, 155.3.

Anal. ($\text{C}_{30}\text{H}_{36}\text{O}_5$) calcd, C: 75.60, H: 7.61; found, C: 75.42, H: 7.66.

Yellow oil: TLC R_f = 0.23 (pet ether 60-80 °C)

^1H NMR (200 MHz, CDCl_3) δ = 1.57 (d, $^3J(\text{H,H})$ = 7.2 Hz, 3H), 2.20 (s, 3H), 2.22 (s, 3H), 4.14 (q, $^3J(\text{H,H})$ = 7.2 Hz, 1H), 5.84 (s, 1H), 6.77-6.79 (m, 1H), 6.88-6.92 (m, 1H), 7.12 (dd, $^3J(\text{H,H})$ = 1.3 Hz, 5.2 Hz, 1H).

^{13}C NMR (54.6 MHz, CDCl_3) δ = 11.4, 13.4, 22.8, 31.2, 105.4, 122.8, 123.0, 123.9, 126.4, 144.6, 149.3, 151.0.

Anal. ($\text{C}_{12}\text{H}_{14}\text{OS}$) calcd, C: 69.86, H: 6.84; found, C: 69.68, H: 6.90.

Yellow oil: TLC R_f = 0.58 (pet ether/EtOAc = 9/1)

^1H NMR (200 MHz, CDCl_3) δ = 1.67 (d, $^3J(\text{H,H})$ = 7.1 Hz, 3H), 4.23 (q, $^3J(\text{H,H})$ = 7.1 Hz, 1H), 6.43 (s, 1H), 7.10-7.52 (m, 8H).

^{13}C NMR (54.6 MHz, CDCl_3) δ = 20.2, 39.1, 102.2, 111.0, 120.5, 122.6, 123.6, 128.5, 128.7, 128.8, 132.5, 141.8, 154.9, 161.4.

Anal. (C₁₆H₁₃ClO) calcd, C: 74.85, H: 5.10; found, C: 74.91, H: 5.14.

[1146-47-0]⁹

White Solid: mp 95-97 °C; TLC R_f = 0.20 (pet ether/EtOAc = 8/2)

¹H NMR (200 MHz, CDCl₃) δ = 1.42 (d, ³J(H,H) = 6.8 Hz, 3H), 4.52 (quintet, ³J(H,H) = 6.7 Hz, 1H), 5.02 (br s, 1H), 7.05-7.19 (m, 5H), 7.37-7.48 (m, 3H), 7.69-7.78 (m, 2H).

¹³C NMR (54.6 MHz, CDCl₃) δ = 23.5, 53.7, 126.1, 127.0, 127.4, 128.5, 128.8, 132.3, 140.6, 141.8.

Anal. (C₁₄H₁₅NO₂S) calcd, C: 64.34, H: 5.79, N: 5.36; found, C: 64.48, H: 5.85, N: 5.40.

[93007-79-5]¹⁰

White Solid: mp 117-119 °C; TLC R_f = 0.20 (pet ether/EtOAc = 8/2)

¹H NMR (200 MHz, CDCl₃) δ = 1.68 (d, ³J(H,H) = 6.9 Hz, 3H), 2.34 (s, 3H), 5.30 (quintet, ³J(H,H) = 6.9 Hz, 1H), 6.33 (br s, 1H), 7.16 (d, ³J(H,H) = 8.0 Hz, 2H), 7.29 (d, ³J(H,H) = 8.0 Hz, 2H), 7.36-7.52 (m, 3H), 7.76 (d, ³J(H,H) = 8.0 Hz, 2H).

¹³C NMR (54.6 MHz, CDCl₃) δ = 21.0, 21.6, 49.0, 126.2, 126.9, 128.5, 129.4, 131.4, 134.6, 137.1, 140.1, 166.5.

Anal. (C₁₆H₁₇NO) calcd, C: 80.30, H: 7.16, N: 5.85; found, C: 80.45, H: 7.11, N: 5.67.

Colorless oil: TLC R_f = 0.16 (pet ether 60-80 °C)

¹H NMR (200 MHz, CDCl₃) δ = 0.90 (t, ³J(H,H) = 7.1 Hz, 3H), 1.42-1.68 (m, 2H), 1.56 (d, ³J(H,H) = 7.2 Hz, 3H), 2.21-2.33 (m, 2H), 3.94 (q, ³J(H,H) = 7.1 Hz, 1H), 7.20-7.39 (m, 5H).

¹³C NMR (54.6 MHz, CDCl₃) δ = 13.4, 22.5, 22.6, 33.2, 43.9, 126.8, 127.1, 128.3, 144.1.

Anal. (C₁₁H₁₆S) calcd, C: 73.27, H: 8.94; found, C: 73.51, H: 8.89.

[3299-05-6]¹¹

Colorless oil

¹H NMR (200 MHz, CDCl₃) δ = 1.19 (t, ³*J*(H,H) = 6.9 Hz, 3H), 1.44 (d, ³*J*(H,H) = 6.4 Hz, 3H), 3.36 (q, ³*J*(H,H) = 6.9 Hz, 2H), 4.41 (q, ³*J*(H,H) = 6.4 Hz, 1H), 7.26-7.40 (m, 5H).

¹³C NMR (54.6 MHz, CDCl₃) δ = 15.4, 24.2, 63.9, 77.7, 126.1, 127.3, 128.4, 144.2.

Anal. (C₁₀H₁₄O) calcd, C: 79.96, H: 9.39; found, C: 80.04, H: 9.42.

References:

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¹H and ¹³C NMR of 4

¹H and ¹³C NMR of 12

(Additional signals correspond to the minor isomer)

¹H and ¹³C NMR of 13

¹H and ¹³C NMR of 14

¹H and ¹³C NMR of 14A

¹H and ¹³C NMR of 15

[illegible]

¹H and ¹³C NMR of 17

(Additional signals correspond to the minor isomer)

¹H and ¹³C NMR of 18

¹H and ¹³C NMR of 19

¹H and ¹³C NMR of 20

(Additional signals correspond to the minor isomer)

¹H and ¹³C NMR of 21

(Additional signals correspond to the minor isomer)

¹H and ¹³C NMR of 22

¹H and ¹³C NMR of 23

Chemical structure: COc1ccc(cc1OC)C(C)C(c2ccoc2)C=C

¹H NMR spectrum (CDCl₃) showing peaks from 0.5 to 7.5 ppm. Integration values are provided below the baseline: 5.35, 2.35, 22.50, 5.88, 6.29, 6.92, 14.77, 3.27, 4.93, 9.90, 6.95, 6.02, 1.10, 4.41, 17.12.

13C NMR spectrum of 1,4-dichlorobenzene in CDCl₃. The spectrum shows peaks at 155.52, 148.74, 148.55, 147.55, 142.40, 141.88, 141.02, 141.00, 134.02, 133.78, 120.72, 120.47, 114.15, 113.67, 111.98, 111.86, 111.06, 110.83, 108.47, 108.40, 108.02, 77.54, 77.00, 76.37, 55.81, 51.28, 41.98, 41.55, 18.53, and 18.44 ppm. The x-axis is labeled PPM and ranges from 150 to 20.

¹H and ¹³C NMR of 25

(Additional signals correspond to the minor isomer)

¹H and ¹³C NMR of 26

¹H and ¹³C NMR of 27

¹H and ¹³C NMR of 28

¹H and ¹³C NMR of 29

^1H and ^{13}C NMR of 30

¹H and ¹³C NMR of 31