

Electronic Supplementary Material (ESI) for Dalton Transactions

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Supplementary Information

Synthesis and Characterization of Dinuclear NHC–Palladium Complexes and Their Applications in the Hiyama Reactions of Aryltrialkoxysilanes with Aryl Chlorides

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1. Characterization data for the products

4-Methoxybiphenyl

¹H NMR (400 MHz, CDCl₃): δ = 7.59–7.55 (4H, m), 7.44 (2H, t, *J* = 7.6 Hz), 7.33 (1H, t, *J* = 7.6 Hz), 7.01 (2H, d, *J* = 8.8 Hz), 3.87 (3H, s). ¹³C NMR (100 MHz, CDCl₃): δ = 159.1, 140.8, 133.7, 128.7, 128.1, 126.7, 126.6, 114.2, 55.3.

3-Methoxybiphenyl

¹H NMR (400 MHz, CDCl₃): δ = 7.52 (2H, d, *J* = 7.2 Hz), 7.40 (2H, t, *J* = 7.2 Hz), 7.32–7.29 (3H, m), 7.04–6.96 (2H, m), 3.78 (3H, s). ¹³C NMR (100 MHz, CDCl₃): δ = 156.4, 138.5, 130.8, 130.6, 129.5, 128.6, 127.9, 126.9, 120.8, 111.1, 55.5.

2-Methoxybiphenyl

¹H NMR (400 MHz, CDCl₃): δ = 7.58–7.56 (2H, m), 7.43–7.39 (2H, m), 7.35–7.31 (2H, m), 7.17–7.12 (2H, m), 6.87 (1H, dd, *J* = 8.4 and 2.4 Hz), 3.82 (3H, s). ¹³C NMR

(100 MHz, CDCl₃): δ = 159.9, 142.7, 141.0, 129.7, 128.7, 127.4, 127.1, 119.6, 112.8, 112.6, 55.2.

4-Nitrobiphenyl

¹H NMR (400 MHz, CDCl₃): δ = 8.30 (2H, d, J = 8.8 Hz), 7.74 (2H, d, J = 8.8 Hz), 7.65–7.62 (2H, m), 7.53–7.49 (2H, m), 7.47–7.44 (1H, m). ¹³C NMR (100 MHz, CDCl₃): δ = 147.6, 147.0, 138.7, 129.1, 128.9, 127.8, 127.4, 124.1.

3-Nitrobiphenyl

¹H NMR (400 MHz, CDCl₃): δ = 8.46 (1H, s), 8.22–8.20 (1H, m), 7.93 (1H, d, J = 8.0 Hz), 7.65–7.62 (3H, m), 7.53–7.49 (2H, m), 7.46–7.43 (1H, m). ¹³C NMR (100 MHz, CDCl₃): δ = 148.7, 142.8, 138.6, 132.9, 129.6, 129.1, 128.5, 127.1, 122.0, 121.9.

1,1'-Biphenyl-4-carbonitrile

¹H NMR (400 MHz, CDCl₃): δ = 7.74–7.67 (4H, m), 7.59 (2H, d, J = 8.0 Hz), 7.50–7.41 (3H, m). ¹³C NMR (100 MHz, CDCl₃): δ = 145.6, 139.1, 132.6, 129.1, 128.6, 127.7, 127.2, 118.9, 110.9.

1-(4-Biphenyl)ethanone

¹H NMR (400 MHz, CDCl₃): δ = 8.03 (2H, d, J = 8.4 Hz), 7.68 (2H, d, J = 8.4 Hz), 7.62 (2H, d, J = 7.6 Hz), 7.48–7.45 (2 H, m), 7.40 (1H, t, J = 7.6 Hz), 2.63 (3H, s). ¹³C NMR (100 MHz, CDCl₃): δ = 197.7, 145.7, 139.8, 135.8, 128.9, 128.9, 128.2, 127.2, 127.1, 26.7.

4-(Ethoxycarbonyl)-1,1'-biphenyl

¹H NMR (400 MHz, CDCl₃): δ = 8.07 (2H, d, J = 8.4 Hz), 7.62–7.57 (4H, m), 7.44–7.40 (2H, m), 7.35 (1H, t, J = 7.6 Hz), 4.36 (2H, q, J = 7.2 Hz), 1.37 (3H, t, J = 7.2 Hz). ¹³C NMR (100 MHz, CDCl₃): δ = 166.5, 145.5, 140.1, 130.1, 129.2, 128.9, 128.1, 127.3, 127.0, 61.0, 14.4.

4-Fluoro-1,1'-biphenyl

^1H NMR (400 MHz, CDCl_3): $\delta = 7.49\text{--}7.46$ (4H, m), 7.38–7.34 (2H, m), 7.27 (1H, t, $J = 7.6$ Hz), 7.08–7.03 (2H, m). ^{13}C NMR (100 MHz, CDCl_3): $\delta = 162.5$ (d, $^1J_{\text{CF}} = 244.7$ Hz), 140.3, 137.4 ($^4J_{\text{CF}} = 3.3$ Hz), 128.8, 128.7 ($^3J_{\text{CF}} = 8.0$ Hz), 127.2, 127.0, 115.6 ($^2J_{\text{CF}} = 21.3$ Hz).

Biphenyl

^1H NMR (400 MHz, CDCl_3): $\delta = 7.49$ (4H, d, $J = 8.0$ Hz), 7.35–7.32 (4H, m), 7.26–7.22 (2H, m). ^{13}C NMR (100 MHz, CDCl_3): $\delta = 141.2, 128.7, 127.2, 127.2$.

4-Methylbiphenyl

^1H NMR (400 MHz, CDCl_3): $\delta = 7.46$ (2H, d, $J = 7.6$ Hz), 7.38 (2H, d, $J = 8.0$ Hz), 7.32–7.29 (2H, m), 7.20 (1H, t, $J = 7.6$ Hz), 7.13 (2H, d, $J = 7.6$ Hz), 2.28 (3H, s). ^{13}C NMR (100 MHz, CDCl_3): $\delta = 141.1, 138.3, 137.0, 129.5, 128.7, 127.0, 126.9, 21.1$.

2-Phenylpyridine

^1H NMR (400 MHz, CDCl_3): $\delta = 8.60\text{--}8.58$ (1H, m), 7.90 (2H, d, $J = 7.2$ Hz), 7.59–7.58 (2H, m), 7.39–7.35 (2H, m), 7.32–7.28 (1H, m), 7.10–7.07 (1H, m). ^{13}C NMR (100 MHz, CDCl_3): $\delta = 157.3, 149.5, 139.2, 136.6, 128.8, 128.6, 126.8, 121.9, 120.4$.

3-Phenylpyridine

^1H NMR (400 MHz, CDCl_3): $\delta = 8.75$ (1H, s), 8.50–8.49 (1H, m), 7.78–7.76 (1H, m), 7.48 (2H, d, $J = 7.2$ Hz), 7.40–7.36 (2H, t, $J = 7.2$ Hz), 7.32–7.27 (2H, m). ^{13}C NMR (100 MHz, CDCl_3): $\delta = 148.4, 148.3, 137.8, 136.6, 134.3, 129.0, 128.1, 127.1, 123.5$.

2. ^1H NMR and ^{13}C NMR spectra































