Supporting Information for:

A phosphine-free carbonylative cross-coupling reaction of aryl iodides with arylboronic acids catalyzed by immobilization of palladium in MCM-41

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The spectral data of carbonylative Suzuki cross-coupling products:

4-Methoxybenzophenone 3a. White solid, m.p. 59–60 °C, lit.¹ m.p. 61–62 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.85–7.82 (m, 2 H), 7.76–7.74 (m, 2 H), 7.58–7.45 (m, 3 H), 6.98–6.95 (m, 2 H), 3.88 (s, 3 H). ¹³C NMR (100 MHz, CDCl₃) δ 195.64, 163.24, 138.27, 132.60, 131.94, 130.13, 129.76, 128.21, 113.57, 55.52. IR (KBr) v (cm⁻¹) 1651, 1599, 1508, 1172, 1029, 701.

4-Acetylbenzophenone 3b. White solid, m.p. 83–84 °C, lit.² m.p. 83–84 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.07–8.05 (m, 2 H), 7.88–7.86 (m, 2 H), 7.82–7.80 (m, 2 H), 7.65–7.49 (m, 3 H), 2.68 (s, 3 H). ¹³C NMR (100 MHz, CDCl₃) δ 197.57, 195.98, 141.31, 139.54, 136.89, 133.03, 130.12, 130.06, 128.50, 128.18, 26.94. IR (KBr) v (cm⁻¹) 1693, 1661, 1579, 931, 699.

4-Nitrobenzophenone 3c. Yellow solid, m.p. 136–137 °C, lit.¹ m.p. 138–139 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.35 (d, J = 8.8 Hz, 2 H), 7.95 (d, J = 8.4 Hz, 2 H), 7.82–7.80 (m, 2 H), 7.66–7.51 (m, 3 H). ¹³C NMR (100 MHz, CDCl₃) δ 194.84, 149.82, 142.88, 136.27, 133.51, 130.73, 130.12, 128.71, 123.57. IR (KBr) v (cm⁻¹) 1652, 1595, 1515, 1358, 707.

3-Nitrobenzophenone 3d. Yellow solid, m.p. 95–96 °C, lit.³ m.p. 94–95 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.62 (s, 1H), 8.45 (d, J = 8.4 Hz, 1 H), 8.15 (d, J = 7.6 Hz, 1 H), 7.81 (d, J = 8.4 Hz, 2 H), 7.73–7.64 (m, 2 H), 7.54 (t, J = 7.6 Hz, 2 H). ¹³C NMR (100 MHz, CDCl₃) δ 194.20, 148.10, 139.07, 136.23, 135.47, 133.41, 130.02, 129.68, 128.76, 126.72, 124.73. IR (KBr) v (cm⁻¹) 3080, 1655, 1614, 1595, 1537, 1351, 705.

2-Methoxybenzophenone 3e.⁴ Oil. ¹H NMR (400 MHz, CDCl₃) δ 7.82–7.80 (m, 2 H), 7.56–7.52 (m, 1 H), 7.49–7.40 (m, 3 H), 7.37–7.35 (m, 1 H), 7.06–6.98 (m, 2 H), 3.71 (s, 3 H). ¹³C NMR (100 MHz, CDCl₃) δ 196.50, 157.36, 137.81, 132.95, 131.91, 129.84, 129.59, 128.85, 128.24, 120.50, 111.47, 55.61. IR (neat) v (cm⁻¹) 1667, 1599, 1581, 1244, 1023, 702.

4-Aminobenzophenone 3f. White solid, m.p. 120–121 °C, lit.¹ m.p. 121–123 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.74–7.71 (m, 4 H), 7.56–7.43 (m, 3 H), 6.68 (d, *J* = 8.8 Hz, 2 H), 4.17 (br, 2 H). ¹³C NMR (100 MHz, CDCl₃) δ 195.36, 150.91, 138.86, 132.97, 131.43, 129.54, 128.08, 127.47, 113.65. IR (KBr) v (cm⁻¹) 3340, 3226, 1640, 1629, 1591, 1275, 687.

2-Aminobenzophenone 3g. White solid, m.p. 109–111 °C, lit.⁵ m.p. 109–110 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.64–7.62 (m, 2 H), 7.54–7.43 (m, 4 H), 7.31–7.25 (m, 1H), 6.73 (d, *J* = 8.0 Hz, 1 H), 6.62–6.57 (m, 1H), 6.09 (br, 2 H). ¹³C NMR (100 MHz, CDCl₃) δ 199.13, 150.95, 140.11, 134.70, 134.16, 131.15, 129.21, 128.02, 118.17, 117.05, 115.60. IR (KBr) v (cm⁻¹) 3542, 3306, 1637, 1625, 1547, 1247, 689.

1-Benzoylnaphthalene 3h.⁶ Oil. ¹H NMR (400 MHz, CDCl₃) δ 8.10–8.08 (m, 1 H), 7.98 (d, J = 8.4 Hz, 1 H), 7.92–7.84 (m, 3 H), 7.59–7.42 (m, 7 H). ¹³C NMR (100 MHz, CDCl₃) δ 198.06, 138.34, 136.37, 133.75, 133.28, 131.31, 130.99, 130.45, 128.49, 128.45, 127.82, 127.30, 126.50, 125.72, 124.38. IR (neat) v (cm⁻¹) 1659, 1596, 1578, 1282, 1249, 775, 697.

2-Benzoylthiophene 3i. White solid, m.p. 54-55 °C, lit.⁶ m.p. 56-57 °C. ¹H NMR

(400 MHz, CDCl₃) δ 7.89–7.85 (m, 2 H), 7.72–7.71 (m, 1 H), 7.64–7.63 (m, 1 H), 7.61–7.56 (m, 1 H), 7.51–7.47 (m, 2 H), 7.18–7.14 (m, 1 H). ¹³C NMR (100 MHz, CDCl₃) δ 188.28, 143.63, 138.14, 134.93, 134.29, 132.31, 129.19, 128.45, 128.03. IR (KBr) v (cm⁻¹) 1634, 1598, 1577, 1514, 1286, 842, 716.

3-Benzoylpyridine 3j. White solid, m.p. 38-40 °C, lit.⁷ m.p. 39-41 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.02 (d, J = 1.2 Hz, 1 H), 8.87-8.86 (dd, J = 4.8, 1.8 Hz, 1 H), 8.17–8.14 (dd, J = 8.0, 1.8 Hz, 1 H), 7.80 (d, J = 8.0 Hz, 2 H), 7.78–7.35 (m, 4 H). ¹³C NMR (100 MHz, CDCl₃) δ 194.62, 152.03, 150.24, 138.01, 133.68, 133.61, 130.14, 129.03, 128.39, 123.87. IR (KBr) v (cm⁻¹) 1665, 1596, 1247, 687.

4-Chloro-4'-methylbenzophenone 3k. White solid, m.p. 127–129 °C, lit.⁶ m.p. 123–125 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.75 (d, J = 8.4 Hz, 2 H), 7.71 (d, J = 8.0 Hz, 2 H), 7.47 (d, J = 8.4 Hz, 2 H), 7.31 (d, J = 8.0 Hz, 2 H), 2.46 (s, 3 H). ¹³C NMR (100 MHz, CDCl₃) δ 195.22, 143.53, 138.60, 136.25, 134.56, 131.34, 130.17, 129.10, 128.56, 21.66. IR (KBr) v (cm⁻¹) 1645, 1607, 1585, 1287, 1088, 853, 749.

2-(4-Methylbenzoyl)thiophene 31. White solid, m.p. 74–75 °C, lit.⁶ m.p. 75–76 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.79 (d, J = 8.0 Hz, 2 H), 7.71–7.64 (m, 2 H), 7.30 (d, J = 8.0 Hz, 2 H), 7.17–7.14 (m, 1 H), 2.45 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 187.99, 143.08, 135.43, 134.52, 133.88, 129.45, 129.42, 129.12, 127.89, 21.66. IR (KBr) v (cm⁻¹) 1624, 1604, 1563, 1414, 1139, 860.

3-(Methoxycarbonyl)-4'-methylbenzophenone 3m. White solid, m.p. 103–105 °C, lit.⁸ m.p. 104–105 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.42 (s, 1 H), 8.25 (d, *J* = 7.6 Hz, 1 H), 7.99 (d, *J* = 7.6 Hz, 1 H), 7.72 (d, *J* = 7.6 Hz, 2 H), 7.58 (t, *J* = 7.6 Hz, 1 H), 7.30 (d, *J* = 8.0 Hz, 2 H), 3.94 (s, 3 H), 2.46 (s, 3 H). ¹³C NMR (100 MHz, CDCl₃) δ 195.56, 166.36, 143.75, 138.29, 134.33, 134.00, 132.99, 130.89, 130.31, 130.28, 129.19, 128.57, 52.40, 21.72. IR (KBr) v (cm⁻¹) 1722, 1659, 1605, 1437, 1317, 1243, 1155, 1082, 941, 735.

4-Methyl-4'-nitrobenzophenone 3n. Yellow solid, m.p. 120–122 °C, lit.⁹ m.p. 120–121 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.34–8.32 (m, 2 H), 7.93–7.90 (m, 2 H), 7.71 (d, *J* = 8.4 Hz, 2 H), 7.32 (d, *J* = 8.0 Hz, 2 H), 2.47 (s, 3 H). ¹³C NMR (100 MHz, CDCl₃) δ 194.53, 149.67, 144.60, 143.33, 133.63, 130.57, 130.34, 129.40, 123.50, 21.77. IR (KBr) v (cm⁻¹) 1652, 1600, 1520, 1353, 1315, 732.

4-Methoxy-4'-methylbenzophenone 30. White solid, m.p. 88–89 °C, lit.⁶ m.p. 85–87 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.83–7.81 (m, 2 H), 7.69 (d, *J* = 8.0 Hz, 2 H), 7.28 (d, *J* = 8.4 Hz, 2 H), 6.98–6.96 (m, 2 H), 3.90 (s, 3 H), 2.45 (s, 3 H). ¹³C NMR (100 MHz, CDCl₃) δ 195.39, 163.04, 142.63, 135.51, 132.45, 130.49, 130.02, 128.89, 113.49, 55.50, 21.64. IR (KBr) v (cm⁻¹) 1646, 1598, 1505, 1262, 1170, 849, 761.

4-Acetyl-4'-methylbenzophenone 3p. White solid, m.p. 109–111 °C, lit.¹⁰ m.p. 111–112 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.05 (d, J = 8.4 Hz, 2 H), 7.84 (d, J = 8.4 Hz, 2 H), 7.72 (d, J = 8.0 Hz, 2 H), 7.30 (d, J = 8.0 Hz, 2 H), 2.67 (s, 3 H), 2.45 (s, 3 H). ¹³C NMR (100 MHz, CDCl₃) δ 197.59, 195.70, 143.98, 141.75, 139.37, 134.23, 130.34, 129.92, 129.19, 128.13, 26.91, 21.73. IR (KBr) v (cm⁻¹) 1689, 1651, 1604, 1286, 858, 757.

4-Bromo-4'-methylbenzophenone 3q. White solid, m.p. 139–140 °C, lit.⁶ m.p. 123–125 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.70–7.61 (m, 6 H), 7.29 (d, *J* = 8.0 Hz, 2 H), 2.45 (s, 3 H). ¹³C NMR (100 MHz, CDCl₃) δ 195.36, 143.57, 136.69, 134.49, 131.54, 131.46, 130.18, 129.11, 127.18, 21.67. IR (KBr) ν (cm⁻¹) 1645, 1605, 1586, 1288, 748.

4-Methoxycarbonyl-4'-methylbenzophenone 3r. White solid, m.p. 125–126 °C, lit.¹¹ m.p. 127–128 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.16–8.13 (m, 2 H), 7.83–7.81 (m, 2 H), 7.72 (d, *J* = 8.4 Hz, 2 H), 7.30 (d, *J* = 8.0 Hz, 2 H), 3.97 (s, 3 H), 2.46 (s, 3 H). ¹³C NMR (100 MHz, CDCl₃) δ 195.83, 166.40, 143.94, 141.73, 134.26, 132.99, 130.36, 129.68, 129.47, 129.18, 52.49, 21.74. IR (KBr) v (cm⁻¹) 1717, 1646, 1606, 1276, 1110, 736.

4-Chloro-4'-nitrobenzophenone 3s. Yellow solid, m.p. 100–101 °C, lit.¹² m.p. 100–101 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.35 (d, J = 8.8 Hz, 2 H), 7.92 (d, J = 8.4 Hz, 2 H), 7.76 (d, J = 8.4 Hz, 2 H), 7.51 (d, J = 8.4 Hz, 2 H). ¹³C NMR (100 MHz, CDCl₃) δ 193.56, 149.94, 142.48, 140.12, 134.57, 131.47, 130.59, 129.09, 123.66. IR (KBr) v (cm⁻¹) 1668, 1584, 1520, 1349, 1271, 851, 738.

4-Chloro-4'-methoxybenzophenone 3t. White solid, m.p. 125–126 °C, lit.⁶ m.p. 116–118 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.81–7.78 (m, 2 H), 7.71–7.69 (m, 2 H), 7.46–7.43 (m, 2 H), 6.98–6.95 (m, 2 H), 3.89 (s, 3 H). ¹³C NMR (100 MHz, CDCl₃) δ 194.23, 163.40, 138.26, 136.58, 132.44, 131.15, 129.81, 128.52, 113.69, 55.52. IR (KBr) v (cm⁻¹) 1640, 1605, 1508, 1256, 1030, 853, 760.

4,4'-Dichlorobenzophenone 3u. White solid, m.p. 146–147 °C, lit.⁶ m.p. 146–147 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.73 (d, *J* = 8.4 Hz, 4 H), 7.47 (d, *J* = 8.4 Hz, 4 H). ¹³C NMR (100 MHz, CDCl₃) δ 194.29, 139.17, 135.49, 131.33, 128.78. IR (KBr) v (cm⁻¹) 1654, 1589, 1492, 1146, 1088, 852, 754.

4-Bromo-4'-chlorobenzophenone 3v. White solid, m.p. 146–148 °C, lit.¹³ m.p. 147–148 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.73 (d, J = 8.4 Hz, 2 H), 7.64 (s, 4 H), 7.47 (d, J = 8.8 Hz, 2 H). ¹³C NMR (100 MHz, CDCl₃) δ 194.38, 139.21, 135.97, 135.46, 131.76, 131.41, 131.32, 128.79, 127.78. IR (KBr) v (cm⁻¹) 1646, 1586, 1289, 855, 753.

4-Chloro-2'-(trifluoromethyl)benzophenone 3w.⁶ Oil. ¹H NMR (400 MHz, CDCl₃) δ 7.81–7.78 (m, 1 H), 7.72 (d, *J* = 8.8 Hz, 2 H), 7.64 (t, *J* = 4.4 Hz, 2 H), 7.44 (d, *J* = 8.4 Hz, 2 H), 7.38 (t, *J* = 4.4 Hz, 1 H). ¹³C NMR (100 MHz, CDCl₃) δ 194.34, 140.52, 137.80, 134.74, 131.51, 130.04, 128.95, 128.36, 127.96, 126.78 (q), 124.86, 122.14 IR (KBr) v (cm⁻¹) 1677, 1585, 1486, 1316, 1267, 1135, 930, 769.

2-(4-Chlorobenzoyl)thiophene 3x. White solid, m.p. 99–100 °C, lit.⁶ m.p. 93–95 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.83–7.80 (m, 2 H), 7.75–7.74 (m, 1 H), 7.63–7.62 (m,

1 H), 7.49–7.46 (m, 2 H), 7.18–7.16 (m, 1 H). ¹³C NMR (100 MHz, CDCl₃) δ 186.97, 143.20, 138.71, 136.38, 134.85, 134.62, 130.62, 128.79, 128.13. IR (KBr) ν (cm⁻¹) 1632, 1588, 1414, 1304, 853, 722.

4-Chloro-3'-cyanobenzophenone 3y. White solid, m.p. 142–143 °C, lit.¹⁴ m.p. 142–143 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.05 (s, 1 H), 8.00 (d, *J* = 7.6 Hz, 1 H), 7.88 (d, *J* = 7.6 Hz, 1 H), 7.74 (d, *J* = 8.0 Hz, 2 H), 7.67–7.63 (m, 1 H), 7.51 (d, *J* = 8.0 Hz, 2 H). ¹³C NMR (100 MHz, CDCl₃) δ 193.15, 139.92, 138.29, 135.54, 134.60, 133.68, 133.28, 131.37, 129.52, 129.08, 117.79, 113.05. IR (KBr) v (cm⁻¹) 2235, 1659, 1587, 1297, 1091, 850, 752.

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