Supporting Information

Polyvinylpyridine-supported Palladium nanoparticles: an efficient catalyst for Suzuki-Miyaura coupling reactions

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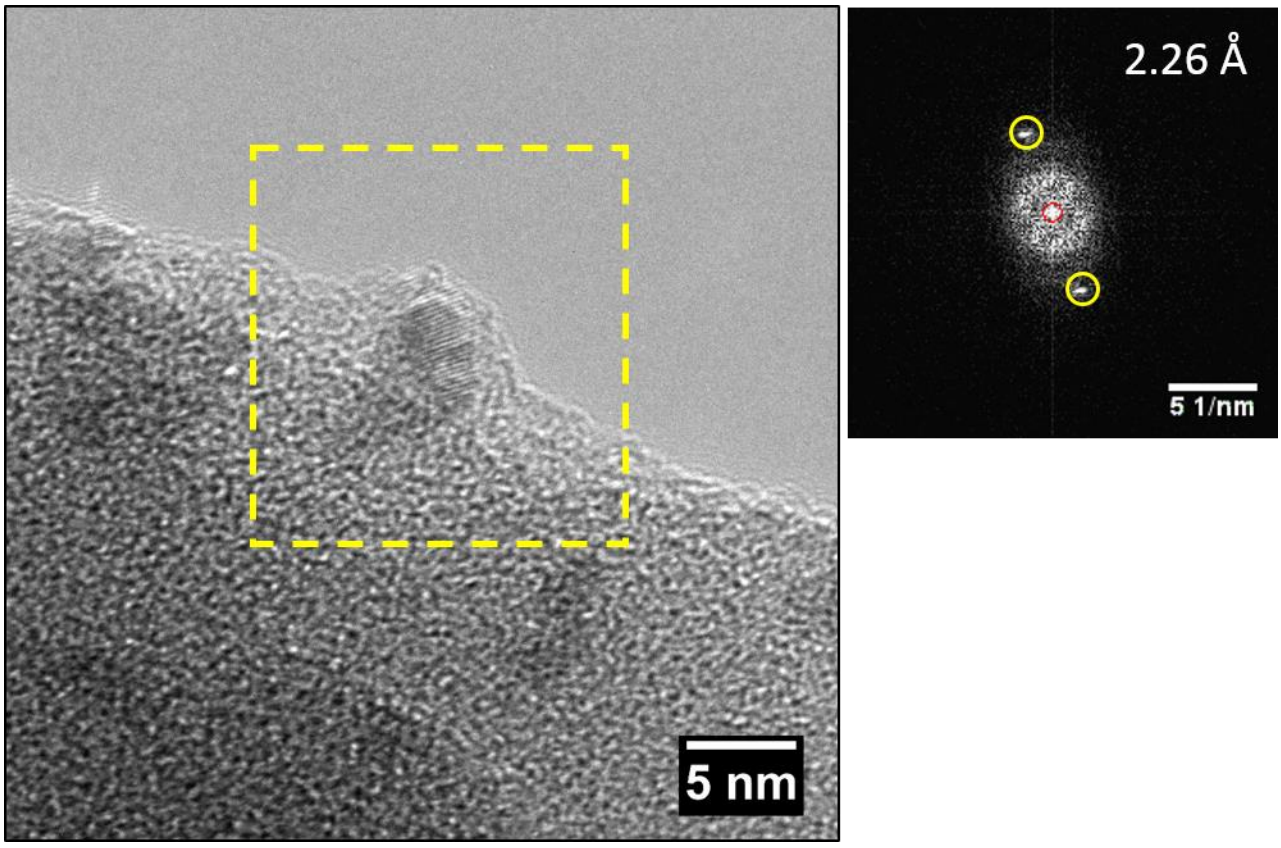
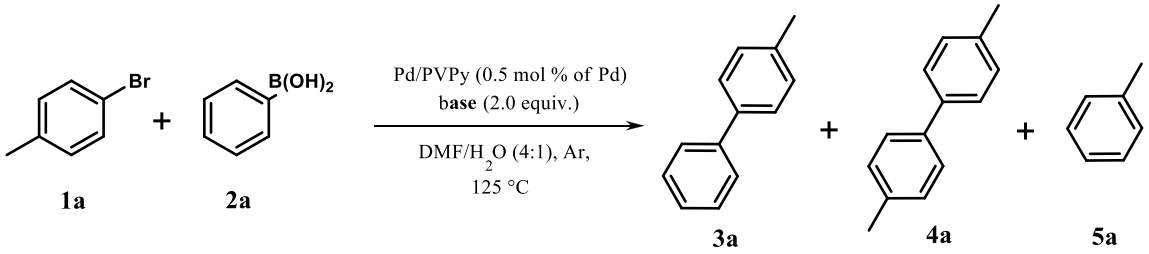


Figure 1S. High resolution TEM micrograph (800000X) of Pd/PVPy and FFT pattern taken from the yellow squared area.

Table 1S. Optimization reaction conditions



1a **2a** **3a** **4a** **5a**

Entry	*Pd/PVPy catalyst (Pd mol %)*	*Base*	*Solvent*	*Conversion (%)*[b]	*Selectivity (%)* ***3a*** */ [**4a**+**5a**]*[b]
1	0.5	Na_2CO_3	DMA/H_2O (4:1)	18	72 / 28
2	0.5	$NaHCO_3$	DMA/H_2O (4:1)	traces	-
3	0.5	NaOH	DMA/H_2O (4:1)	10	11 / 89
4	0.5	KF	DMA/H_2O (4:1)	99.9	1 / 99
5	0.5	K_3PO_4	DMA/H_2O (4:1)	64	99.9 / 0.1
6	0.5	K_3PO_4	H_2O	27	99.9 / 0.1
7	0.5	K_3PO_4	*i*PrOH/H_2O (1:1)	25	99.9 / 0.1
8	0.5	K_3PO_4	EtOH	5	-
9	0.5	K_3PO_4	EtOH/H_2O (1:1)	11	99.9 / 0.1
10	0.5	K_3PO_4	NMP/H_2O (4:1)	12	99.9 / 0.1
11	0.5	K_3PO_4	1,2-dioxane/H_2O (4:1)	10	99.9 / 0.1
12	0.5	K_3PO_4	DMA/H_2O (9:1)	30	99.9 / 0.1
13	0.5	K_3PO_4	DMA/H_2O (1:1)	35	99.9 / 0.1

a) Reaction conditions: 1.00 mmol of 1a, 1.25 mmol of 2a, 2 mmol of Base, catalyst Pd/PVPy (0.5 mol. %), solvent (4 mL), T = 120°C, Argon atmosphere, t = 7 h.

b) Evaluated by GC.

Isolation and characterization of Suzuki-Miyaura products:

*4-Methylbiphenyl (**3a**)*. Purified by MPLC on silica gel, using hexane as eluent. White solid (GLC purity: 99%). Mp: 43-46°C (Lit. Mp 44-46°C). GC-MS (EI) m/z %: 169 (14), 168 (100), 167 (69), 166 (8), 165 (28), 153 (16), 152 (22), 115 (6), 83 (6).

4-Nitrobiphenyl (**3b**). Purified by MPLC on silica gel, using a mixture of hexane and AcOEt (95:5) as eluant. White solid (GLC purity: 99%). Mp: 110-113°C (Lit. Mp 112-114 °C). GC-MS (EI) m/z %: 200 (14), 199 (100), 169 (29), 153 (26), 152 (89), 151 (26), 141 (25), 115 (11), 76 (8).

Biphenyl (**3c**). Purified by MPLC on silica gel, using hexane as eluent. White solid (GLC purity: 99%). Mp: 69-70°C (Lit. Mp 68-70°C). GC-MS (EI) m/z %: 155 (13), 154 (100), 153 (40), 152 (28), 151 (8), 128 (5), 115 (4), 77 (4), 76 (9).

4-Methoxybiphenyl (**3d**). Purified by MPLC on silica gel, using a mixture of hexane and AcOEt (97:3) as eluant. White solid (GLC purity: 98%). Mp: 87-89°C (Lit. Mp 88-90°C). GC-MS (EI) m/z %: 185 (15), 184 (100), 170 (6), 169 (46), 152 (5), 142 (5), 141 (39), 139 (10), 115 (25).

4-Chlorobiphenyl (**3e**). Purified by MPLC on silica gel, using hexane as eluent. White solid (GLC purity: 99%). Mp: 74-77°C (Lit. Mp 75-77°C). GC-MS (EI) m/z %: 190 (33), 189 (13), 188 (100), 153 (17), 152 (43), 151 (12), 150 (5), 76 (11), 75 (4). The spectral properties of this compound were in agreement with those previously reported.29

Ethyl biphenyl-4-carboxylate (**3f**). Purified by MPLC on silica gel, using a mixture of hexane and AcOEt (93:7) as eluent. White solid (GLC purity: 99.9%). Mp: 46-49°C (Lit. Mp 47-50°C). GC-MS (EI) m/z %: 227 (10), 226 (61), 198 (31), 182 (18), 181 (100), 153 (26), 152 (50), 151 (13), 76 (6).

4-Acetylbiphenyl (**3g**). Purified by MPLC on silica gel, using a mixture of hexane and AcOEt (90:10) as eluent. White solid (GLC purity: 98%). Mp: 117-119°C (Lit. Mp 118-120°C). GC-MS (EI) m/z %: 197 (8), 196 (53), 182 (14), 181 (100), 153 (32), 152 (52), 151 (14), 126 (4), 76 (11).

2-Phenylthiophene (**3h**). Purified by MPLC on silica gel, using hexane as eluent. White solid (GLC purity: 94%). Mp: 33-37°C (Lit. Mp 34-35°C). GC-MS (EI) m/z %: 161 (12), 160 (100), 159 (7), 134 (4), 128 (10), 116 (8), 115 (28), 102 (4), 89 (5).

4-Methyl-4'-methoxybiphenyl (**3i**). Purified by MPLC on silica gel, using a mixture of hexane and CH_2Cl_2(90:10) as eluent. White solid (GLC purity: 97%). Mp: 109-112 °C (Lit. Mp 109-110°C). GC-MS (EI) m/z %: 199 (16), 198 (100), 184 (7), 183 (50), 155 (25), 154 (6), 153 (9), 152 (10), 128 (8).

2-Methoxybiphenyl (**3l**). Purified by MPLC on silica gel, using a mixture of hexane and AcOEt (98:2) as eluent. White solid (GLC purity: 96%). Mp: 28-31 °C (Lit. Mp 30-33°C). GC-MS (EI) m/z %: 185 (15), 184 (100), 183 (21), 169 (53), 168 (15), 152 (9), 141 (33), 139 (15), 115 (30).

2,4'-Dimethoxybiphenyl (**3m**). Purified by MPLC on silica gel, using a mixture of hexane and AcOEt (98:2) as eluent. White solid (GLC purity: 94%). Mp: 68-72 °C (Lit.27 Mp 69-70°C). GC-MS (EI) m/z %: 215 (15), 214 (100), 199 (20), 185 (6), 184 (22), 171 (13), 168 (13), 128 (9), 115 (6). The spectral properties of this compound were in agreement with those previously reported.28

2-Methyl-2'-methoxybiphenyl (**3n**). Purified by MPLC on silica gel, using a mixture of hexane and CH_2Cl_2 (90:10) as eluent. White solid (GLC purity: 99%). Mp: 41-43°C (Lit. Mp 42-44°C). GC-MS (EI) m/z %: 199 (16), 198 (100), 197 (12), 183 (35), 168 (29), 167 (36), 165 (42), 153 (15), 152 (18).

4-Aminobiphenyl (**3o**). Purified by MPLC on silica gel, using a mixture of hexane and AcOEt (75:25) as eluant. White solid (GLC purity: 94%). Mp: 48-51°C (Lit. Mp 50-52°C). GC-MS (EI) m/z %: 170 (13), 169 (100), 168 (21), 167 (12), 141 (7), 139 (4), 115 (6), 84 (5), 83 (5).

3-Aminobiphenyl (**3p**). Purified by MPLC on silica gel, using a mixture of hexane and AcOEt (75:25) as eluent. White solid(GLC purity: 97%). Mp: 27-29°C (Lit. Mp 29-30°C). GC-MS (EI) m/z %: 170 (14), 169 (100), 168 (25), 167 (16), 152 (4), 141 (9), 139 (5), 115 (7), 83 (5).

4-Hydroxybiphenyl (**3q**). Purified by MPLC on silica gel, using a mixture of hexane and AcOEt (75:25) as eluent. White solid (GLC purity: 93%). Mp: 53-57°C (Lit. Mp 56-58°C). GC-MS (EI) m/z %: 171 (14), 170 (100), 152 (3), 142 (3), 141 (17), 139 (6), 115 (13), 85 (5), 63 (3).