Supporting Information

Polymer Supported *N*-Heterocyclic Carbene-Palladium Complex for Heterogeneous Suzuki Cross-Coupling Reaction

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1. General. The ¹H NMR spectra were recorded on 300 MHz spectrometer. The chemical shifts were measured in ppm, using TMS as an internal standard and CDCl₃ as the solvent. The GC-MS

spectra were recorded on a gas chromatography-mass spectrometer. The size and morphology of the beads were observed on a field emission scanning electron microscope (FE-SEM). The location of the ligand precursor on the beads was observed on a confocal laser scanning microscope (CLSM). The EDX spectra were recorded on a FE-SEM energy dispersive X-ray spectrometer. The amount of palladium immobilized on the beads was determined by means of an inductively coupled plasma-atomic emission spectrometer (ICP-AES). All of the reagents including aryl iodides, bromides and arylboronic acids were commercially available.

2. ^1H , ^{31}P NMR for the Polymerizable Ionic Liquid Monomer (1).

1-Methyl-3-(4-vinylbenzyl)imidazolium chloride, [MVBIM][Cl]. ^1H NMR (300 MHz, $\text{DMSO-}d_6$): δ (ppm) 3.83 (s, 3H), 5.31 (d, 1H), 5.38 (s, 2H), 5.89 (d, 1H), 6.72 (q, 1H), 7.39 (d, 2H), 7.50 (d, 2H), 7.69 (d, 1H), 7.76 (d, 1H), 9.16 (s, 1H).

1-Methyl-3-(4-vinylbenzyl)imidazolium hexafluorophosphate (1), [MVBIM][PF₆]. ¹H NMR (300 MHz, DMSO-d₆): δ (ppm) 3.83 (s, 3H), 5.31 (d, 1H), 5.38 (s, 2H), 5.89 (d, 1H), 6.72 (q, 1H), 7.39 (d, 2H), 7.50 (d, 2H), 7.69 (d, 1H), 7.76 (d, 1H), 9.16 (s, 1H). ESI-MS for C₁₃H₁₅N₂: m/z 199.0.

³¹P NMR (500 MHz, DMSO-d₆): δ (ppm) -143.8 (hept).

3. ^1H NMR (300 MHz) and GC-MS Data for the Biphenyls Obtained from Suzuki Reaction.

Biphenyl (3). ^1H NMR ($\text{DMSO}-d_6$): δ (ppm) 7.33 (q, 2H), 7.44 (q, 4H), 7.64 (d, 4H). GC-MS: m/z 154.

4-Hydroxybiphenyl (4). ^1H NMR (CDCl_3): δ (ppm) 4.82 (s, 1H), 6.89 (d, 2H), 7.29 (q, 1H), 7.42 (m, 4H), 7.55 (d, 2H). GC-MS: m/z 170.

4-Methoxybiphenyl (5). ^1H NMR (CDCl_3): δ (ppm) 3.85 (s, 3H), 6.97 (d, 2H), 7.31 (q, 1H), 7.42 (q, 2H), 7.52 (d, 2H), 7.57 (d, 2H). GC-MS: m/z 184.

4-Methylbiphenyl (6).² ^1H NMR (CDCl_3): δ (ppm) 2.40 (s, 3H), 7.24 (d, 2H), 7.32 (q, 1H), 7.43 (q, 2H), 7.48 (d, 2H), 7.59 (d, 2H). GC-MS: m/z 168.

4-Nitrobiphenyl (7).³ ^1H NMR (CDCl_3): δ (ppm) 7.50 (m, 3H), 7.63 (d, 2H), 7.76 (d, 2H), 8.32 (d, 2H). GC-MS: m/z 199.

4-Formylbiphenyl (8). ¹H NMR (DMSO): δ (ppm) 7.48 (m, 3H), 7.74 (d, 2H), 7.91 (d, 2H), 8.00 (d, 2H), 10.04 (s, 1H). GC-MS: m/z 182.

4-Acetylbiphenyl (9).⁵ ^1H NMR (CDCl_3): δ (ppm) 2.65 (s, 3H), 7.45 (m, 3H), 7.62 (d, 2H), 7.71 (d, 2H), 8.05 (d, 2H). GC-MS: m/z 196.

4-Cyanobiphenyl (10).⁶ ^1H NMR (CDCl_3): δ (ppm) 7.46 (m, 3H), 7.59 (d, 2H), 7.67 (d, 2H), 7.75 (d, 2H). GC-MS: m/z 179.

Biphenyl 4-Carboxylic Acid (11). ⁷ ¹H NMR (DMSO-d₆): δ (ppm) 7.42 (q, 1H), 7.50 (q, 2H), 7.72 (d, 2H), 7.81 (d, 2H), 8.03 (d, 2H). GC-MS: m/z 198.

2-Methylbiphenyl (12).⁸ ¹H NMR (CDCl₃): δ (ppm) 2.31 (s, 3H), 7.23 (m, 3H), 7.33 (m, 6H). GC-MS: m/z 168.

2-Methoxybiphenyl (13).⁶ ¹H NMR (CDCl₃): δ (ppm) 3.79 (s, 3H), 6.99 (m, 2H), 7.31 (m, 3H), 7.40 (m, 2H), 7.51 (d, 2H). GC-MS: m/z 184.

2-Phenylbenzonitrile (14).¹¹ ¹H NMR (CDCl₃): δ (ppm) 7.50 (m, 6H), 7.66 (q, 2H), 7.75 (d, 1H).

GC-MS: m/z 179.

2-Phenylnaphthalene (15).¹² ¹H NMR (CDCl₃): δ (ppm) 7.37 (q, 1H), 7.47 (m, 4H), 7.70 (m, 3H),

7.91 (m, 3H), 8.05 (s, 1H). GC-MS: m/z 204.

4-Methoxy-4'-methylbiphenyl (16).⁵ ¹H NMR (CDCl₃): δ (ppm) 2.38 (s, 3H), 3.85 (s, 3H), 6.95 (d, 2H), 7.24 (d, 2H), 7.43 (d, 2H), 7.53 (d, 2H). GC-MS: m/z 198.

4-Chloro-4'-methoxybiphenyl (17). ^{13}H NMR (CDCl_3): δ (ppm) 3.85 (s, 3H), 6.96 (d, 2H), 7.39 (d, 2H), 7.46 (d, 2H), 7.50 (d, 2H). GC-MS: m/z 218.

4-Acetyl-4'-methoxybiphenyl (18). ^8H NMR (CDCl_3): δ (ppm) 2.63 (s, 3H), 3.87 (s, 3H), 6.99 (d, 2H), 7.52 (d, 2H), 7.66 (d, 2H), 8.02 (d, 2H). GC-MS: m/z 266.

4-Methoxy-4'-trifluoromethylbiphenyl (19). ³ ¹H NMR (CDCl₃): δ (ppm) 3.86 (s, 3H), 6.99 (d, 2H), 7.53 (d, 2H), 7.62 (d, 2H), 7.69 (d, 2H). GC-MS: m/z 252.

4-Methoxy-4'-methylmercaptobiphenyl (20).⁹ ¹H NMR (CDCl₃): δ (ppm) 2.52 (s, 3H), 3.85 (s, 3H), 6.95 (d, 2H), 7.29 (d, 2H), 7.47 (d, 2H), 7.52 (d, 2H). GC-MS: m/z 230.

4, 4'-Dimethoxybiphenyl (21).¹⁰ ¹H NMR (CDCl₃): δ (ppm) 3.84 (s, 6H), 6.95 (d, 4H), 7.49 (d, 4H). GC-MS: m/z 214.

4. 200 MHz Solid-State ¹³C NMR.

Poly(1-methylimidazoliummethyl styrene)-*sg*-PS Resin.

^{13}C NMR (solid state); δ 41 (aliphatic polystyrene skeleton), 45 (C4), 128 (C2, C3, aromatic polystyrene skeleton), 146 (C1, aromatic polystyrene skeleton).

Polymer-Supported NHC Palladium Complex (2).

^{13}C NMR (solid state); δ 41 (aliphatic polystyrene skeleton), 45 (C4). 128 (C2, C3, aromatic polystyrene skeleton), 146 (C1, aromatic polystyrene skeleton).

5. IR Spectra.

Poly(1-methylimidazoliummethyl styrene)-sg-PS Resin

IR absorption bands (cm^{-1}) : 1157 cm^{-1} (the quaternary imidazolium).

Polymer-Supported NHC Palladium Complex (2).

IR absorption bands (cm^{-1}) : 1655 cm^{-1} (C=C).

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