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Generation uniform and small particle size of palladium onto the *SH*-decorated SBA-15 pore-walls: SBA-15/$(SH)_X$Pd-NP_Y as a recoverable nanocatalyst for Suzuki-Miyaura coupling reaction in air and water

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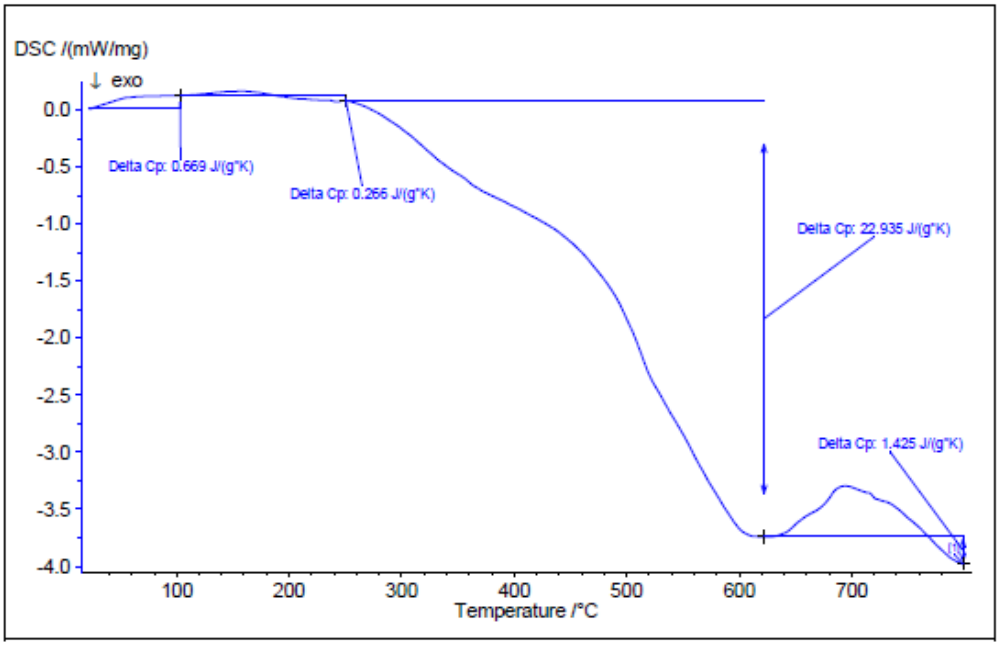
General procedure for recovery study:

The recycling possibility and ability of the SBA-15/$(SH)_X$Pd-NP_Y catalyst, the model reactions (example **3a**) were studied. During this study, when the reaction was completed (GC), the catalyst was easily separated from the product by filtration. The solid catalyst was washed with water and then dichloromethane and diethyl ether (×3) to remove residual product and dried under vacuum at 60 ^oC and reused in a subsequent reaction.

SBA-15/$(SH)_X$Pd-NP_Y: After preparation of the SBA-15/H.$PdCl_2$ (Cat. A_1), this palladium loaded pre-catalyst (1 g) will react with 0.2 mmol of $NaBH_4$ in 10 mL methanol during 2 h. After that, the new solid Pd(0)@SBA-15/SO_3H pre-catalyst was filtered, and then dried under vacuum. Atomic absorption spectroscopy analysis using residual contents in solvents of residual solutions showed 93% Pd-loading.



Synthesis of biaryls 3: In a test tube equipped with a magnetic stirrer bar, the aryl halides **1** (1 mmol), was mixed with boronic acid **2** (1.2 mmol), K_2CO_3 (3 mmol), and the Pd-catalyst **(**0.5 mol% Pd ($Pd(AN)_2(Cl)_2$@SBA-15/SO_3H or Pd-NPs@SBA-15/SO_3H) in 3 mL of 1:1 mixture of DMF:H_2O, in air. The reaction mixture was than heated to 80 °C. After completion of the reaction, the reaction was cooled to room temperature, the catalyst was removed by filtration. The catalyst was then washed with Et_2O (3 × 8 mL). The organic layer was separated and dried over anhydrous $MgSO_4$. The solvent was evaporated under reduced pressure to give the corresponding biaryl compounds. The ^1H and ^{13}C NMR spectroscopic data of known compounds were found to be identical with those reported in the *literature* [12].

4-Methylbiphenyl: ^1H NMR: 7.28-7.63 (9 H), 2.44 (3 H). ^{13}C NMR: 141.18, 138.38, 137.03, 129.50, 128.73, 127.23, 127.18, 127.00, 21.11.

Biphenyl: ^1H NMR: 7.62-7.65 (4 H), 7.46-7.50 (4 H), 7.38-7.40 (2 H). ^{13}C NMR: 141.25, 128.77, 127.27, 127.19.

1-Biphenyl-4-yl-ethanone: ^{1}H NMR: 8.03-8.06 (2 H), 7.63-7.78 (4 H), 7.41-7.50 (3 H), 2.65 (3 H). ^{13}C NMR: 197.83, 145.80, 139.87, 135.85, 128.95, 128.92, 128.23 127.27, 127.23, 26.65.

4-Methoxybiphenyl: ^{1}H NMR: 7.57-7.61 (4 H), 7.44-7.48 (2 H), 7.32-7.37 (1 H), 7.01-7.04 (2 H), 3.88 (3 H).

2-Methoxylbiphenyl: ^{1}H NMR: 7.62 (2 H), 7.50 (2 H), 7.41-7.43 (3 H), 7.05-7.14 (2 H), 3.88 (3 H).

2-Methyl-biphenyl: ^{1}H NMR: 7.26-8.46 (9 H), 1.26 (3 H). ^{13}C NMR: 142.87, 138.66, 133.04, 129.71, 129.16, 128.54, 127.95, 127.15, 122.02, 121.95, 29.69.

3-Methyl-4'-methoxy-biphenyl: ^{1}H NMR: 6.99-7.57 (8 H), 3.87 (3 H), 2.45 (3 H).

3-Methyl-2'-methoxy-biphenyl: ^{1}H NMR: 7.00-7.36 (8 H), 3.84 (3 H), 2.44 (3 H).

1-[4-(3-methylphenyl)phenyl]-1-ethanone: ^{1}H NMR: 2.45 (3 H), 2.65 (3 H), 7.22-8.04 (8 H). ^{13}C NMR: 197.82, 145.94, 139.85, 138.60, 135.86, 128.98, 128.86, 128.02, 127.22, 124.38, 26.66, 21.52.

1-Nitro-3-phenylbenzene: ^{1}H NMR: 7.25-8.44 (9 H). ^{13}C NMR: 148.71, 142.85, 138.65, 133.03, 129.69, 129.15, 128.52, 127.14, 122.01, 121.94.

3-Phenylbenzaldehyde: ^{1}H NMR: 7.26-8.12 (9 H), 10.10 (1 H). ^{13}C NMR: 192.38, 142.16, 136.91, 135.57, 133.07, 129.50, 129.01, 128.64, 128.20, 128.02, 127.14.

2-Phenylbenzaldehyde: ^{1}H NMR: 6.87-8.01 (9 H), 9.97 (1 H). ^{13}C NMR: 192.44, 145.92, 137.70, 133.56, 130.75, 130.07, 129.51, 128.40, 128.10, 127.75, 127.53.