Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2018

# Pronounced effect of pore dimension of silica support on Pd-catalyzed Suzuki coupling reaction under ambient conditions

Trisha Das,<sup>a</sup> Hiroshi Uyama<sup>b</sup>, Mahasweta Nandi<sup>\* a</sup>

<sup>a</sup>Integrated Science Education and Research Centre, Siksha Bhavana, Visva-Bharati University, Santiniketan 731 235, India

<sup>b</sup>Department of Applied Chemistry, Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka, 565 0871, Japan

Email: mahasweta.nandi@visva-bharati.ac.in



**Fig. s1.** FT-IR spectra of (a) calcined MCM-41, (b) 3-APTES functionalized MCM-41, (c) *tris*(4-formyl phenyl) amine loaded MCM-41, (d) 2-aminothiophenol grafted *tris*(4-formyl phenyl) amine MCM-41 and (e) **MCM-Pd** 



**Fig. s2.** FT-IR spectra of (a) calcined SBA-15, (b) 3-APTES functionalized SBA-15, (c) *tris*(4-formyl phenyl) amine loaded SBA-15, (d) 2-aminothiophenol grafted *tris*(4-formyl phenyl) amine SBA-15 and (e) **SBA-Pd** 



**Fig. s3.** Thermogravimetric analysis of (a) calcined MCM-41, (b) 3-APTES functionalized MCM-41 and (c) *tris*(4-formyl phenyl) amine loaded MCM-41



**Fig. s4.** Thermogravimetric analysis of (a) calcined SBA-15, (b) 3-APTES functionalized SBA-15 and (c) *tris*(4-formyl phenyl) amine loaded SBA-15



Fig. s5. TEM image of SBA-Pd after three reaction cycles



Fig. s6. Mechanism of Suzuki coupling reaction\*

\*(i) P. Veerakumar, P. Thanasekaran, K.-L. Lu, S.-B. Liu and S. Rajagopal, ACS Sustainable Chem. Eng., 2017, 5, 6357. (ii) C. Len, S. Bruniaux, F. Delbecq, V. S. Parmar, Catalysts, 2017, 7, 146 (1-23).

# <sup>1</sup>H NMR of *tris*(4-formyl phenyl) amine

**Tris(4-formyl phenyl)amine.** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 9.88 (s, 3H), 7.76-7.78 (d, 6H), 7.17–7.19 (d, 6H)



# <sup>1</sup>H NMR of Biphenyl

**Biphenyl.** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.39–7.43 (m, 2H), 7.48–7.53 (m, 4H), 7.65–7.68 (m, 4H)



#### <sup>1</sup>H NMR of 4-methyl-1,1'-biphenyl

**4-methyl-1,1'-biphenyl.** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 2.45 (s, 3H), 7.30–7.31 (d, 2H), 7.40 (m, 1H), 7.46-7.50 (t, 2H), 7.54-7.57(d, 2H), 7.63-7.65 (d, 2H)

F2 - Acquisition Parameters Date 2017622 Time 17.36 INSTRUM 5 20170622 INSTRUM 5 Pect PULPROG 22930 TD 22768 SOLVENT 0.13 NS 201768 SOLVENT 0.250957 HZ NS 0.250957 HZ MR 8223.685 HZ 1992294 HZ NS 1.992294 HZ NS 0.297.9 KC DM 6.50 UNSC DE 6.50 UNSC TD 0.0000 SC TD0 1 1.000000 SC usec usec K sec w - Processing parameters 16384 400.150097 MHz EM MHZ 0.30 Hz ANNEL fl ===== 400.1524711 M 1H 12.00000000 W Current Data Parameters NAME External 2017 EXPNO 99 PROCNO 1 1.00 BRUKER CHANNEL 0 0 F2 -SI SF WDW SSB CB GB PC SF01 NUC1 P1 PLW1 ĊH₃ mdd 0.5 1.0 1.5 2.0 3.00 3.0 3.5 4.0 4.5 5.0 5.5 6.0 .300 310 6.5 363 423 423 7.0 000 000 000 000 000 000 7.5 815 155 895 825 8.0 8.5 633 ₽89 159 823 0.6 9.5

# <sup>1</sup>H NMR of 2-methyl-1,1'-biphenyl

**2-methyl-1,1'-biphenyl.** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 2.338 (s, 3H), 7.26–7.32 (m, 4H), 7.37-7.41 (m, 3H), 7.45-7.49 (t, 2H)



## <sup>1</sup>H NMR of 4-methoxy-1,1'-biphenyl

**4-methoxy-1,1'-biphenyl.** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 3.85 (s, 3H), 6.97 (d, 2H), 7.28 (t, 1H), 7.36 (t, 2H), 7.52–7.56 (m, 4H)



# <sup>1</sup>H NMR of 4-chloro-1,1'-biphenyl

**4-chloro-1,1'-biphenyl.** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.26-7.46 (m, 5H), 7.51-7.61 (m, 4H)



# <sup>1</sup>H NMR of 4-acetyl-1,1'-biphenyl

**4-acetyl-1,1'-biphenyl.** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 2.64 (s, 3H), 7.40-7.49 (m, 3H), 7.61-7.64 (m, 2H), 7.67-7.70 (d, 2H), 8.05 (d, 2H)



#### <sup>1</sup>H NMR of 4-nitro-1,1'-biphenyl

**4-nitro-1,1'-biphenyl.** <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 8.30 (d, 2H), 7.72-7.75 (d, 2H), 7.62–7.64 (m, 2H), 7.47-7.52 (m, 2H), 7.44 (m, 1H)

- Processing parameters 15384 400.1500100 MHz EM usec 14.75 usec 12.0000000 W Ksec sec MHZ 0.30 Hz HZ 5 BB/ 2930 32768 CDC13 1.00 Current Data Parameters NAME External 2018 EXPNO 563 PROCNO 1 800 400.1524711 Ξ F2 - Acquisition Parame Date 20180204 Time 15.48 INSTRUM spect 1.00000 68 0 mm PABBO CHANNEL f1 5 0 0 PROBHD TDULFROG SOLVENT NS SOLVENT NS SWH SSWH SSWH AC DD DM DM DM DD DD DD TD DD TDD F2 -SF WDW SSB LLB CGB SFO1 NUC1 P1 PLW1 NO<sub>2</sub> mdd 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0 6.5 529 463 7.0 L05 - L L05 8.0 1.92 8.5 0.6 9.5

#### <sup>1</sup>H NMR of 1,1'-biphenyl-4-carboxylic acid

**4-COOH substituted biphenyl.** <sup>1</sup>H NMR (DMSO-d<sub>6</sub>) δ 13.07 (s, 1H), 8.07-8.12 (d, 2H), 7.85-7.87 (d, 2H), 7.81 (m, 1H), 7.72 (m, 1H), 7.52-7.58 (t, 2H), 7.38 (t, 1H)

