Shape-Selective Mesoporous Silicalite-Encapsulated Palladium Catalyst

**Significance:** Palladium nanoparticles encapsulated in mesoporous silicalite-1 (Pd@S1; pore size 5.3 × 5.6 Å, 1.7 wt% Pd) were prepared for use as a shape-selective catalyst. Reduction of nitrobenzene (1a) by NaBH₄, oxidation of benzyl alcohol (3a) under O₂, and the Suzuki–Miyaura coupling of iodobenzene (5a) with 4-methoxyphenylboronic acid proceeded in the presence of Pd@S1 to give the corresponding products 2a, 4a, and 6a in 93–94% yield. Under similar conditions, the reactions of substrates with larger molecular size (1b, 3b, and 5b) gave the corresponding products in less than 4% yield.

**Comment:** The selectivity of the catalysis was evaluated by using Pd/C as catalyst as a control instead of Pd@S1 under similar conditions. Reduction of 1a, the oxidation of 3a, and the Suzuki–Miyaura coupling of 5a with 4-methoxyphenylboronic acid proceeded in the presence of Pd/C to give the corresponding products 2a, 4a, and 6a in 2%, 80%, and 4% yield, respectively. In the coupling reaction of 5a with 4-methoxyphenylboronic acid, Pd@S1 was reused fourteen times without significant loss of its catalytic activity.

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SYNFACTS 2016, 12(11), 1207 Published online: 18.10.2016
DOI: 10.1055/s-0036-1589340; Reg-No.: Y14116SF