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 \((1\text{a})\) by NaBH₄, oxidation of benzyl alcohol \((3\text{a})\) under O₂, and the Suzuki–Miyaura coupling of iodobenzene \((5\text{a})\) with 4-methoxyphenylboronic acid proceeded in the presence of Pd@S1 to give the corresponding products \(2\text{a}, 4\text{a},\) and \(6\text{a}\) in 93–94% yield. Under similar conditions, the reactions of substrates with larger molecular size \((1\text{b}, 3\text{b},\) and \(5\text{b})\) gave the corresponding products in less than 4% yield.

**Comment:** The selectivity of the catalysis was evaluated by using Pd/C as a control instead of Pd@S1 under similar conditions. Reduction of \(1\text{a},\) \(3\text{a},\) the oxidation of \(3\text{a},\) and the Suzuki–Miyaura coupling of \(5\text{a},\) \(5\text{b}\) with 4-methoxyphenylboronic acid proceeded in the presence of Pd/C to give the corresponding products \(2\text{a}, 4\text{a},\) and \(6\text{a}\) in 55–99% yield. In the coupling reaction of \(5\text{a}\) with 4-methoxyphenylboronic acid, Pd@S1 was reused fourteen times without significant loss of its catalytic activity.