Synthesis of 2b and 2d. The substituted biphenyls 4,4'-dimethylbiphenyl 2b and 4,4'-ditrifluoromethylbiphenyl 2d were similarly prepared. 2b: isolated yield 51% based on 1b, mp 119 °C (from CH₂Cl₂) (lit., 18 120.7-121.5 °C). Found: C, 91.60; H, 7.69%. C₁₄H₁₄ requires C, 92.30; H, 7.69%. 2d: isolated yield 69% based on 1d, mp 80 °C (from EtOH/H₂O) (lit., 19 93-94.5 °C). Found: C, 57.82; H, 2.90; F, 39.28. C₁₄H₈F₆ requires C, 57.93; H, 2.75; F, 39.31%. δH (CDCl₃; Me₄Si) 7.69 (8H, m, ArH) (lit., 20 7.67).

Experimental procedure for kinetic studies. Example: 44 mmol 1a, 45 mmol Zn; 125 mmol NaOH, 5% Pd/C, 1 g (1.0 mol% Pd relative to 1a), and 1.5 g PEG-400 (8.4 mol% relative to 1a) were mixed in water (50 ml total reaction volume) at 100 °C in an autoclave. Reaction progress was monitored by GC. The following parameters were studied: (i) initial substrate concentration, using xylene as the diluting organic solvent (3 experiments at 1.76 M, k_{obs} = 3.8 \times 10^{-2} \text{min}^{-1}, r^2 = 0.999 for 5 observations; 2.0 M, k_{obs} = 3.98 \times 10^{-2} \text{min}^{-1}, r^2 = 0.999 for 5 observations; and 2.5 M, k_{obs} = 4.3 \times 10^{-2} \text{min}^{-1}, r^2 = 0.997 for 5 observations); (ii) catalyst loading (5 experiments using 0.25 g of 5% w/v Pd, k_{obs} = 0.33 \times 10^{-2} \text{min}^{-1}, r^2 = 0.999 for 7 observations; 0.5 g 5% w/v Pd, k_{obs} = 0.75 \times 10^{-2} \text{min}^{-1}, r^2 = 0.973 for 7 observations; 0.75 g 5% Pd, k_{obs} = 1.46 \times 10^{-2} \text{min}^{-1}, r^2 = 0.88 for 7 observations; 1.0 g of 5% w/v Pd, k_{obs} = 3.67 \times 10^{-2} \text{min}^{-1}, r^2 = 0.996 for 6 observations); and 1.5 g of 5% w/v Pd, k_{obs} = 4.09 \times 10^{-2} \text{min}^{-1}, r^2 = 0.97 for 6 observations); (iii) Zn loading (4 experiments using 0.02 mol Zn, k_{obs} = 1.1 \times 10^{-2} \text{min}^{-1}, r^2 = 0.973 for 5 observations; 0.045 mol, k_{obs} = 3.8 \times 10^{-2} \text{min}^{-1}, r^2 = 0.999 for 5 observations; 0.05 mol, k_{obs} = 5.7 \times 10^{-2} \text{min}^{-1}, r^2 = 0.97 for 5 observations; and 0.06 mol, k_{obs} = 8.9 \times 10^{-2} \text{min}^{-1}, r^2 = 0.91 for 4 observations); and (iv) reaction temperature (4 experiments at 60 °C, k_{obs} = 1.47 \times 10^{-2} \text{min}^{-1}, r^2 = 0.993 for 7 observations; 80 °C, k_{obs} = 2.48 \times 10^{-2} \text{min}^{-1}, r^2 = 0.998 for 7 observations; 100 °C, k_{obs} = 3.67 \times 10^{-2} \text{min}^{-1}, r^2 = 0.996 for 7 observations; and 120 °C, k_{obs} = 8.22 \times 10^{-2} \text{min}^{-1}, r^2 = 0.986 for 7 observations).

References: