REVISED
7/16Supplementary material
for

New Palladium-Carbene Catalysts for Heck Reaction of Aryl Chlorides in Ionic Liquids

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Standard reaction conditions: 1 mmol aryl chloride, 1.5 mmol olefin, 1.2 mmol sodium acetate, catalyst and 2 g tetrabutylammonium bromide were stirred under argon at 140 °C for 24 h in a schlenk tube. After cooling the internal standard (diethyleneglycol di-n-butylether) was added, the mixture was diluted with 5 ml water and extracted with 3 x 5 ml ether. The combined organic layers were dried over sodium sulfate. The conversion and the yield were determined by gas chromatography. The products were isolated by column chromatography (SiO₂, ethyl acetate/hexane mixtures).

***E*-Stilbene**

Data are in accordance with the data of a commercially available sample.

***E-p*-Nitrostilbene**

¹H NMR (400 MHz, CDCl₃, 23 °C): δ = 7.14 (d, ³J(H,H) = 16.2 Hz, 1H), 7.25-7.42 (m, 4H), 7.55 (d, ³J(H,H) = 7.4 Hz, 2H), 7.63 (d, ³J(H,H) = 8.7 Hz, 2H), 8.22 (d, ³J(H,H) = 8.7 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃, 23 °C): δ = 123.1, 125.2, 125.8, 126.0, 127.8, 127.9, 132.3, 135.1, 142.8, 145.7; MS (70 eV): *m/z* 225 [*M*⁺], 178.

***E-p*-Acetylstilbene**

¹H NMR (360 MHz, CDCl₃, 23 °C): δ = 2.56 (s, 3H), 7.09 (d, ³J(H,H) = 16.4 Hz, 1H), 7.19 (d, ³J(H,H) = 16.3 Hz, 1H), 7.34 (m, 3H), 7.51 (d, ³J(H,H) = 7.3 Hz, 2H), 7.54 (d, ³J(H,H) = 8.2 Hz, 2H), 7.92 (d, ³J(H,H) = 8.2 Hz, 2H); ¹³C NMR (90.6 MHz, CDCl₃, 23 °C): δ = 26.5, 126.4, 126.8, 127.4, 128.3, 128.7, 128.8, 131.4, 135.9, 136.7, 141.9, 197.3; MS (70 eV): *m/z* 222 [*M*⁺], 207, 178, 152, 89.

***E-p*-(Trifluoromethyl)stilbene**

¹H NMR (360 MHz, CDCl₃, 23 °C): δ = 7.11 (d, ³J(H,H) = 16.4 Hz, 1H), 7.19 (d, ³J(H,H) = 16.4 Hz, 1H), 7.31 (m, 1H), 7.39 (m, 2H), 7.54 (d, ³J(H,H) = 7.3 Hz, 2H), 7.60 (m, 4H); ¹³C NMR (90.6 MHz, CDCl₃, 23 °C): δ = 124.2 (q, ¹J(C,F) = 272 Hz), 125.6 (q, ³J(C,F) = 3.8 Hz), 126.5, 126.8, 128.8, 129.2 (q, ²J(C,F) = 32.3 Hz), 127.1, 128.3, 131.2, 136.6, 140.8; MS (70 eV): *m/z* 248 [*M*⁺], 179, 152, 89, 76.

***E-o*-Cyanostilbene**

Data are in accordance with literature (A. Zapf, M. Beller, *Chem. Eur. J.* **2001**, *7*, 2908).

***E-p*-Methylstilbene**

Data are in accordance with literature (G. Bellucci, R. Bianchini, C. Chiappe, R. S. Brown, H. Slebocka-Tilk, *J. Am. Chem. Soc.* **1991**, *113*, 8012).

2-Ethylhexyl *o*-cyanocinnamate

¹H NMR (400 MHz, CDCl₃, 23 °C): δ = 0.90 (m, 6H), 1.32 (m, 9H), 4.13 (m, 2H), 6.59 (d, ³J(H,H) = 16.1 Hz, 1H), 7.45 (dd, ³J(H,H) = 7.6 Hz, ⁴J(H,H) = 1.0 Hz, 1H), 7.60 (dd, ³J(H,H) = 7.7 Hz, ⁴J(H,H) = 1.0 Hz, 1H), 7.70 (m, 2H), 7.95 (d, ³J(H,H) = 15.8 Hz, 1H); MS (70 eV): *m/z* 285 [*M*⁺], 240, 156, 128, 112, 101, 83, 70.

2-Ethylhexyl *p*-nitrocinnamate

¹H NMR (400 MHz, CDCl₃, 23 °C): δ = 0.85 (m, 6H), 1.25-1.60 (m, 9H), 4.08 (m, 2H), 6.50 (d, ³J(H,H) = 16.0 Hz, 1H), 7.61 (m, 3H), 8.18 (d, ³J(H,H) = 8.7 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃, 23 °C): δ = 11.4, 14.5, 23.4, 24.2, 29.4, 30.8, 39.2, 67.8, 123.1, 124.6, 129.1, 141.0, 141.9, 148.9, 166.6; MS (70 eV): *m/z* 305 [*M*⁺], 176, 70.

2-Ethylhexyl cinnamate

Data are in accordance with literature (W. A. Herrmann, V. P. W. Böhm, *J. Organomet. Chem.* **1999**, 572, 141).

2-Ethylhexyl *p*-methylcinnamate

Data are in accordance with literature (A. Ehrentraut, A. Zapf, M. Beller, *Synlett* **2000**, 1589).