

SUPPORTING INFORMATION

Title: Triethanolamine as an Efficient and Reusable Base, Ligand and Reaction Medium for Phosphane-Free Palladium-Catalyzed Heck Reactions

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Selected characterization data for Heck reaction products.

(E)-Stilbene: Yield: 176 mg (98 %). Mp 120–122 °C (lit.^[1] mp 120 °C). ¹H NMR (400 MHz, DMSO): δ = 7.62–7.60 (m, 4H, ArH), 7.40–7.27 (m, 4H, ArH), 7.24–7.13 (m, 4H, ArH and Vinyl-H); IR (KBr): 3020, 1631, 1495, 1451, 1364, 962, 764, 692 cm⁻¹.

(E)-4-Methylstilbene: Yield: 173 mg (89 %). Mp 121–122 °C (lit.^[1] mp 120 °C). ¹H NMR (400 MHz, DMSO): δ = 7.59 (d, J = 7.6 Hz, 2H, ArH), 7.50 (d, J = 8.0 Hz, 2H, ArH), 7.41–7.24 (m, 3H, ArH), 7.21–7.16 (m, 4H, ArH and Vinyl-H), 2.31 (s, 3H, CH₃); IR (KBr): 3018, 2831, 1632, 1574, 1448, 1365, 969, 809, 749, 690 cm⁻¹.

(E)-4-Acetylstilbene: Yield: 220 mg (99 %). Mp 149–151 °C. (lit.^[1] mp 148–150 °C). ¹H NMR (400 MHz, DMSO): δ = 7.97 (d, J = 8.4 Hz, 2H, ArH), 7.75 (d, J = 8.4 Hz, 2H), 7.66 (d, J = 7.6 Hz, 2H, ArH), 7.43–7.32 (m, 5H, ArH and Vinyl-H), 2.51 (s, 3H, COCH₃); IR (KBr): 2897, 1708, 1600, 1517, 1368, 1357, 1265, 1178, 1074, 966, 867, 821, 756, 725, 692 cm⁻¹.

(E)-4-Cyanostilbene: Yield: 195 mg (95 %). Mp 117–119 °C. (lit.^[1] mp 117.4–117.7 °C). ¹H NMR (400 MHz, DMSO): δ = 7.83 (d, J = 8.4 Hz, 2H, ArH), 7.80 (d, J = 8.4 Hz, 2H, ArH), 7.66 (d, J = 7.6 Hz, 2H, ArH), 7.56 (t, J = 7.4 Hz, 2H, ArH), 7.44 (t, J = 8.4 Hz, 1H, ArH), 7.31 (d, J = 16.5 Hz, 1H, Vinyl-H), 7.19 (d, J = 16.5 Hz, 1H, Vinyl-H); IR (KBr): 2834, 2362, 1602, 1504, 1364, 973 cm⁻¹.

(E)-Ethyl 3-(4-methoxyphenyl)-2-propenoate: Yield: 198 mg (96 %). Mp 48–50 °C. (lit.^[1] mp 47–48.8 °C). ¹H NMR (400 MHz, DMSO): δ = 7.62 (m, 3H, ArH and Vinyl-H), 6.92 (d, J = 8.8 Hz, 2H, ArH), 6.43 (d, J = 16.0 Hz, 1H, Vinyl-H), 4.17 (q, J = 7.2 Hz, 2H, CH₂), 3.77 (s, 3H, OCH₃), 1.32 (t, J = 7.2 Hz, 3H, CH₃); IR (KBr): 2981, 1718, 1635, 1517, 1368, 1178, 984, 814 cm⁻¹.

(E)-4-Methoxystilbene: Yield: 208 mg (99 %). Mp 136–138 °C. (lit.^[2] mp 135–137 °C). ¹H NMR (400 MHz, DMSO): δ = 7.60 (d, J = 6.4 Hz, 2H, ArH), 7.50 (d, J = 8.4 Hz, 2H, ArH), 7.36 (t, J = 7.8 Hz, 2H, ArH), 7.24 (t, J = 6.4 Hz, 1H, ArH), 7.16 (d, J

= 16.4 Hz, 1H, Vinyl-H), 7.10 (d, $J = 16.4$ Hz, 1H, Vinyl-H), 6.95 (d, $J = 8.8$ Hz, 2H, ArH), 3.80 (s, 3H, OCH₃); IR (KBr): 2836, 1605, 1512, 1447, 1365, 1297, 1179, 1030, 967, 828, 689 cm⁻¹.

(E)-*n*-Butyl cinnamate: Yield: 198 mg (97 %). Oil.^[2] ¹H NMR (300 MHz, CDCl₃): $\delta = 7.66$ (d, $J = 15.9$ Hz, 1H, Vinyl-H), 7.48–7.45 (m, 2 H, ArH), 7.33–7.31 (m, 3 H, ArH), 6.42 (d, $J = 16.2$ Hz, 1H, Vinyl-H), 4.18 (t, $J = 6.6$ Hz, 2H, CH₂), 1.70–1.61 (m, 2H, CH₂), 1.47–1.37 (m, 2H, CH₂), 0.94 (t, $J = 7.3$ Hz, 3H, CH₃); IR (film): 3068, 2953, 1710, 1628, 1498, 1320, 770, 690 cm⁻¹.

(E)-*n*-Butyl 3-(4-nitrophenyl)-2-propenoate: Yield: 154 mg (62 %). Mp 63–65 °C. (lit.^[2] mp 64–65 °C). ¹H NMR (300 MHz, CDCl₃): $\delta = 8.25$ (d, $J = 9.0$ Hz, 2H, ArH), 7.71 (d, $J = 16.5$ Hz, 1H, Vinyl-H), 7.68 (d, $J = 9.0$ Hz, 2H, ArH), 6.57 (d, $J = 16.2$ Hz, 1H, Vinyl-H), 4.24 (t, $J = 6.8$ Hz, 2H), 1.76–1.66 (m, 2H), 1.49–1.41 (m, 2H), 0.97 (t, $J = 7.4$ Hz, 3H); IR (KBr): 3058, 2943, 1702, 1615, 1498, 1308, 778, 695 cm⁻¹.

(E)-2-Methylstilbene: Yield: 147 mg (76 %). Oil.^[3] ¹H NMR (300 MHz, CDCl₃): $\delta = 7.55$ (d, $J = 8.1$ Hz, 1H, ArH), 7.58 (d, $J = 8.4$ Hz, 2H, ArH), 7.34–7.28 (m, 3H, ArH and Vinyl-H), 7.24–7.12 (m, 4H, ArH), 6.96 (d, $J = 16.2$ Hz, 1H, Vinyl-H), 2.38 (s, 3H, CH₃); IR (film): 2903, 1700, 1608, 1527, 1378, 1260, 1075, 966, 867, 821, 759, 728, 691 cm⁻¹.

(E)-3-Methylstilbene: Yield: 157 mg (81 %). Mp 48–49 °C. (lit.^[4] mp 47–48 °C). ¹H NMR (300 MHz, CDCl₃): $\delta = 7.50$ –7.47 (m, 2H, ArH), 7.35–7.30 (m, 4H, ArH), 7.20–7.15 (m, 2H, ArH), 7.07–7.04 (m, 3H, ArH and Vinyl-H), 2.35 (s, 3H, CH₃); IR (KBr): 2932, 1703, 1605, 1514, 1388, 1263, 1174, 1075, 966, 867, 821, 757, 724, 690 cm⁻¹.

(E)-Ethyl cinnamate: Yield: 165 mg (94 %). Oil.^[5] ¹H NMR (400 MHz, DMSO): $\delta = 7.67$ (d, $J = 16.4$ Hz, 1H, Vinyl-H), 7.62–7.50 (m, 2 H, ArH), 7.41–7.36 (m, 3H, ArH), 6.60 (d, $J = 16.0$ Hz, 1H, Vinyl-H), 4.18 (q, $J = 7.2$ Hz, 2H, CH₂), 1.25 (t, $J = 7.0$ Hz, 3H, CH₃); IR (film): 3074, 2954, 1709, 1621, 1497, 1312, 772, 687 cm⁻¹.

(E)-Ethyl 3-(4-nitrophenyl)-2-propenoate: Yield: 199 mg (90 %). Mp 138–140 °C (lit.^[6] mp 139–139.8 °C). ¹H NMR (400 MHz, DMSO): δ = 8.25 (d, J = 8.8 Hz, 2H, ArH), 8.20 (d, J = 8.8 Hz, 2H, ArH), 7.69 (d, J = 16.0 Hz, 1H, Vinyl-H), 6.57 (d, J = 16.0 Hz, 1H, Vinyl-H), 4.22 (q, J = 7.0 Hz, 2H, CH₂), 1.26 (t, J = 7.0 Hz, 3H, CH₃); IR (KBr): 3075, 2982, 1717, 1644, 1525, 1446, 1354, 1188, 1034, 873, 767, 664 cm⁻¹.

(E)-Ethyl 4-styrylbenzoate: Yield: 232 mg (92 %). Mp 106.0–107.5 °C (lit.^[7] mp 106.0–106.5 °C). ¹H NMR (400 MHz, DMSO): δ = 7.96 (d, J = 8.4 Hz, 2H, ArH), 7.66 (d, J = 7.6 Hz, 2H, ArH), 7.46–7.30 (m, 5H, ArH), 7.22 (d, J = 16.4 Hz, 1H, Vinyl-H), 7.13 (d, J = 16.4 Hz, 1H, Vinyl-H), 4.32 (q, J = 7.1 Hz, 2H, CH₂), 1.34 (t, J = 7.2 Hz, 3H, CH₃); IR (KBr): 3035, 2928, 1711, 1632, 1365, 1277, 1176, 851, 776 cm⁻¹.

(E)-Cinnamonitrile: Yield: 117 mg (91 %). Oil.^[8] ¹H NMR (300 MHz, CDCl₃): δ = 7.65–7.35 (m, 5H, ArH), 7.38 (d, J = 16.8 Hz, 1H, Vinyl-H), 5.87 (d, J = 16.8 Hz, 1H, Vinyl-H); IR (film): 3060, 2952, 2206, 1643, 1614, 1600, 1181, 1110, 978, 801 cm⁻¹.

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