Molecules **2000**, *5*, M171

1-(4-Nitrophenyl)-1-octyne

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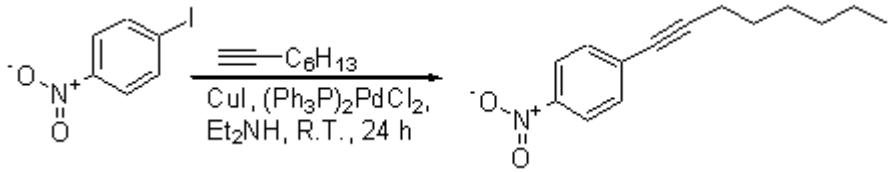
Received: 27 June 2000 / Accepted: 17 July 2000 / Published: 30 July 2000



Following the procedure of Takahashi, et al (1), to a mixture of 1-iodo-4-nitrobenzene (7.76 mmol, 1.90g) and 1-octyne (9.3 mmol, 1.023g) in diethylamine (40 mL) are added bis[triphenylphosphine]palladium dichloride (0.2mmol, 0.14g) and copper(I) iodide (0.1mmol, 0.01g). The reaction is stirred at room temperature under a nitrogen atmosphere for 24 hours. The solvent is then removed by rotary evaporation. The remaining solution is suspended in petroleum ether. The resulting suspension is filtered, and the solvent removed. The crude oily product is purified by means of column chromatography using a 19:1 petroleum ether: diethyl ether as the eluent. Yield: 1.17g (65.6%)

IR (NaCl plates, cm^{-1}): 3080, 2931, 2858, 2227, 1594, 1518, 1342, 1108, 854, 750, 734, 688.

^{1}H-NMR (300 MHz, $CDCl_3$): 0.83 (3H, t, J=6.87 Hz), 1.25 (4H, m), 1.38 (2H, m), 1.53 (2H, q, J=7.38 Hz), 7.43 (2H, d, J=8.94), 8.07 (2H, d, J=8.94).

^{13}C-NMR (75.5 MHz, $CDCl_3$): 146.88, 132.52, 131.56, 123.73, 97.08, 79.62, 31.69, 28.99, 28.76, 22.91, 19.88, 14.34.

GC-MS (ion trap, m/e, in order of decreasing peak size): 128, 142, 232 (M + 1), 202, 115, 116, 156, 215, 102, 188.

Reference

1. Takahashi, S.; Kuroyama, Y.; Sonogashira, K.; Hagihara, N. *Synthesis* **1980**, 627-630.

Sample Availability: available from MDPI. MDPI 18996.