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3,5-Bis[5-(4-tert-butylphenyl)-1,3,4-oxadiazol-2-yl]nitrobenzene

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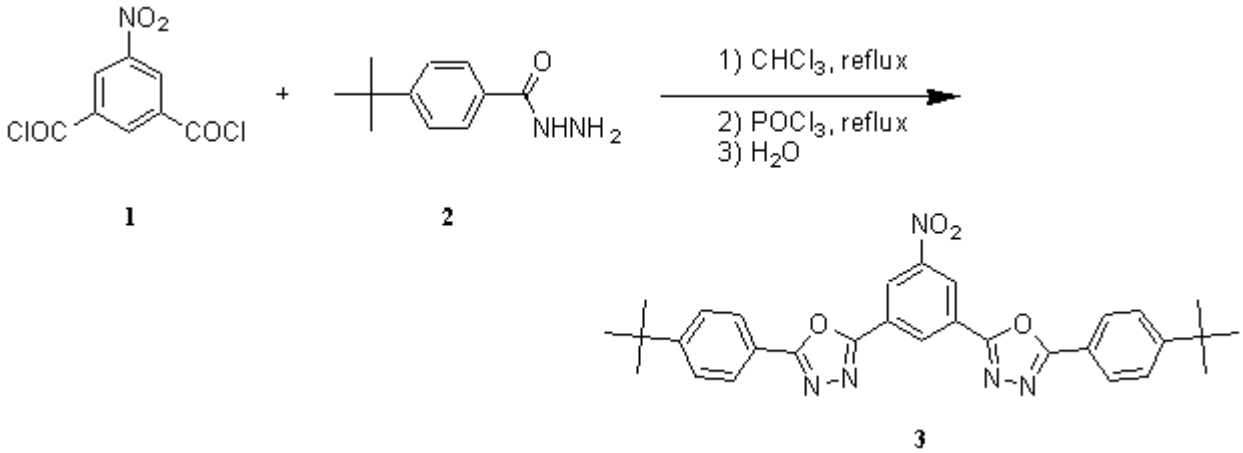

A solution of 5-nitroisophthaloyl dichloride (**1**) [1] (3.92 g, 15.8 mmol) and 4-*tert*-butylbenzhydrazide (**2**) [2] (6.08 g, 31.6 mmol) in $CHCl_3$ (70 mL) was heated to reflux for 12 h. The solvent was then removed in vacuum, the residue was dried and combined with freshly distilled $POCl_3$ (20 mL). The solution was heated to reflux for 3 h until evolution of HCl ceased. The resulting yellow solution was added dropwise to water (300 mL) under vigorous stirring. The precipitate was collected by suction filtration, air-dried, extracted with hot ethanol (200 mL), and dried to afford **3** as a colourless solid (3.11 g, 38%). The yield was not optimised. The extraction with ethanol was responsible for considerable losses in product and should better be replaced by a different method of purification.

Mp. : 288-290°C.

IR (KBr): 2964m; 1615m; 1535s; 1494s; 1349m; 1112m; 884m; 783m; 748m; 717m.

^{1}H NMR ($CDCl_3$, 500 MHz): 9.22 (t, J = 1.5 Hz, 1 H, C_6H_3); 9.12 (t, J = 1.5 Hz, 2 H, C_6H_3); 8.14 (AA'XX', 4 H, C_6H_4); 7.61 (AA'XX', 4 H, C_6H_4); 1.4 (s, 18 H, CH_3).

^{13}C NMR ($CDCl_3$, 125 MHz): 165.9; 161.7; 156.3; 149.2; 129.7; 127.1; 127; 126.3; 123.7; 120.2; 35.2; 31.1.

EI-MS (70 eV): 524 (59, M^+); 161 (92); 136 (57); 77 (100).

Anal. calc. for $C_{30}H_{29}N_5O_4$ (523.59): C 68.68, H 5.76, N 13.34; found: C 68.59, H 5.65, N 13.26.

References

1. Jennings, K. F. *J. Chem. Soc*. **1957**, 1172.

2. Yale, H. L.; Losee, K.; Martins, J.; Holsing, M.; Perry, F. M.; Bernstein, J. *J. Am. Chem. Soc*. **1953**, *75*, 1933.

Sample availability: available from the authors and from MDPI.