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N-(3-Phenyl-2-propinoyl)benzamide

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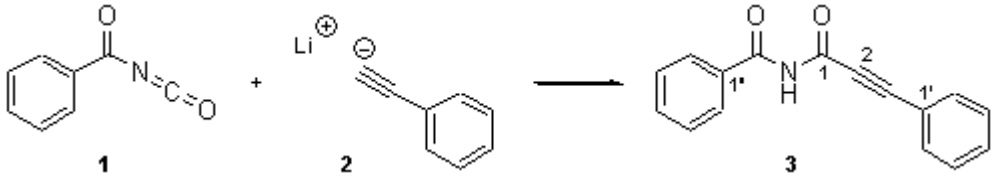

During the synthesis of a series of carboximides using acyl isocyanates [1], the title compound **3** was synthesised as a model compound from benzoyl isocyanate (**1**) and lithium phenylacetylide (**2**).

To benzoyl isocyanate (342 ml, 2.72 mmol, Aldrich) in tetrahydrofuran (8 ml), a solution of lithium phenylacetylide in tetrahydrofuran (2.72 ml, 1.0 M, 2.72 mmol, Aldrich) was added under argon at -15°C, and the mixture stirred for 90 min at -15°C. Dilute hydrochloric acid (20 ml, 2 M) was added and the mixture was extracted three times with dichloromethane (20 ml each). The combined organic layers were dried (Na_2SO_4), filtered, and the solvent removed *in vacuo*. The residue was chromatographed on SiO_2 (60 g, dichloromethane) to give 414 mg (61%) of **3** as yellowish needles.

Yellowish nedles, m.p. 110-112°C

IR (KBr): 3266; 3079; 2235; 2192; 1713; 1648; 1459; 1325; 1238; 761; 694.

^{1}H-NMR (300 MHz, $CDCl_3$): 10.02 (*s br*, 1H, NH); 7.97 (*d*, *J* = 7.1, 2H, H-C(2"), H-C(6")); 7.63 - 7.30 (*m*, 8H, H-C(3"), H-C(4"), H-C(5"), H-C(2'), H-C(3'), H-C(4'), H-C(5'), H-C(6')).

^{13}C-NMR (75 MHz, $CDCl_3$): 165.1 (*s*, C_6H_5-*C*=O); 153.3 (*s*, C(1)); 133.2 (*d*, C(4")); 132.9 (*d*, C(2'), C(6')); 131.9 (*s*, C(1")); 130.7 (*d*, C(4')); 128.6, 128.3, 127.9 (3*d*, C(2"), C(3"), C(5"), C(6"), C(3'), C(5')); 119.5 (*s*, C(1')); 93.0 (*s*, C(3)); 82.9 (*s*, C(2)).

EI-MS (70 eV): 249 (5, M^+); 221 (8); 178 (18); 129 (16, $[C_6H_5C^oCC{=}O]^+$); 118 (100); 105 (40, $[C_6H_5CO]^+$); 90 (39); 77 (21, $[C_6H_5]^+$); 63 (6); 51 (11).

CI-MS (NH_3): 250 (100, $[M{+}H]^+$); 118 (10).

Anal. Calcd for $C_{16}H_{11}NO_2$ (249.27): C 77.10, H 4.45, N 5.62, O 12.84; Found: C 76.92, H 4.60, N 5.59, O 12.74.

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References

1. Hubmann, D.; Liechti, C.; Trinks, U.; Traxler, P.; Séquin, U. Synthesis of *N*-Phenylpyrrole Carboximides. *Molecules* 1999, *4*, 151-158.

Sample availability: available from the authors and from MDPI. MDPI ID 17925.