

SHORT
COMMUNICATIONS

Dedicated to Full Member of the Russian Academy of Sciences
N.S. Zefirov on His 70th Anniversary

N-(4,6-Diphenylpyrimidin-2-yl)thiourea from 1-Benzoyl-2-phenylacetylene and *N*-Carbamimidoylthiourea

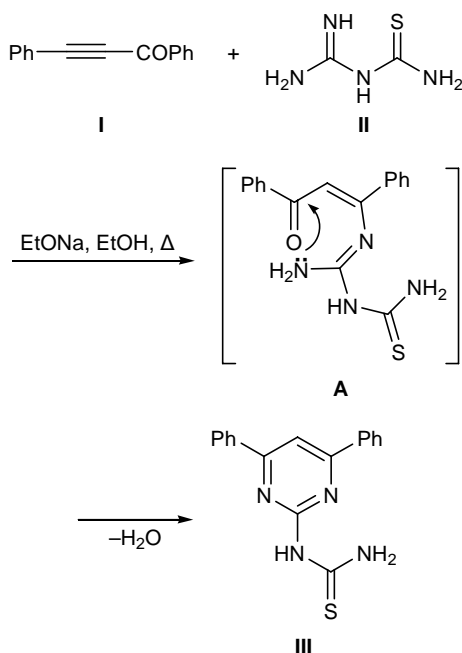
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In continuation of our previous studies on reactions of activated acetylenic compounds with sulfur- and nitrogen-containing polyfunctional nucleophiles [1–4] as a convenient route to various N,S-heterocycles, we examined the reaction of 1-benzoyl-2-phenylacetylene with *N*-carbamimidoylthiourea.

Heteroaromatic α -halo ketones are known to react with *N*-carbamimidoylthiourea to give 4-aryl-2-guandinothiazoles which exhibit strong antiulcer and spasmolytic activity [5, 6]. Reactions of 2-acylcycloalkanones with *N*-carbamimidoylthiourea lead to formation of substituted pyrimidines which attract interest as potential analgetics and chemical means for plant protection [7].



We have found that 1-benzoyl-2-phenylacetylene (**I**) reacts with *N*-carbamimidoylthiourea (**II**) in anhydrous ethanol in the presence of an equimolar amount of sodium ethoxide in an inert atmosphere to afford *N*-(4,6-diphenylpyrimidin-2-yl)thiourea (**III**) in 55% yield. Presumably, the reaction involves intermediate formation of *N*-adduct **A** which undergoes dehydration leading to pyrimidine ring closure.

***N*-(4,6-Diphenylpyrimidin-2-yl)thiourea (III).** A mixture of 1.03 g (5 mmol) of 1-benzoyl-2-phenylacetylene (**I**) and 0.34 g (5 mmol) of sodium ethoxide in 20 ml of anhydrous ethanol was added under stirring in a stream of argon to a suspension of 0.59 g (5 mmol) of *N*-carbamimidoylthiourea in 5 ml of anhydrous ethanol. The mixture was heated to the boiling point, stirred for 10 h at that temperature under argon, and kept for 12 h at 5–8°C. The precipitate was filtered off, washed with 5 ml of cold ethanol, and dried under reduced pressure. Yield 0.84 g (55%), colorless crystals, mp 222–224°C (from EtOH). IR spectrum, ν , cm^{-1} : 3150, 3300, 3390 (NH, NH₂); 1490–1585 (C=C, C=N). ¹H NMR spectrum, δ , ppm: 8.22 s (1H, CH=); 7.56–8.25 m (10H, Ph); 9.24 br.s, 10.38 br.s, and 10.54 br.s (1H each, NH, NH₂). ¹³C NMR spectrum, δ_{C} , ppm: 107.32 (C⁵); 127.45, 129.00, 131.55, 135.87 (C_{arom}); 157.97 (C²); 165.09 (C⁴, C⁶); 181.10 (C=S). Found, %: C 66.45; H 4.48; N 18.35; S 10.24. C₁₇H₁₄N₄S. Calculated, %: C 66.64; H 4.60; N 18.28; S 10.46.

The IR spectrum was recorded in KBr on a Specord 75IR spectrometer. The ¹H and ¹³C NMR spectra were obtained on a Bruker-DPX 400 spectrometer at 400.13 MHz for ¹H and 100.61 MHz for ¹³C using DMSO-*d*₆ as solvent.

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