Chemistry of Heterocyclic Compounds, Vol. 41, No. 5, 2005

LETTERS TO THE EDITOR

β,β-DINITROSTYRENES REACTED WITH PYRROLE

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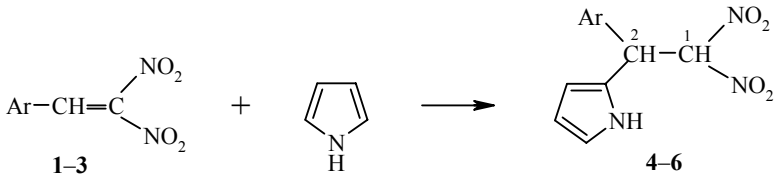
Keywords: heterocycles, β,β-dinitrostyrenes, nitro group, pyrrole.

Pyrrole derivatives occupy a special place among biologically important compounds. It is sufficient to note that the basis for "the pigments of life" (hemoglobin, chlorophyll, cytochrome, and also vitamin B_{12}) are porphyrin tetrapyrrole macrocycles [1, 2]. β,β-Dinitrostyrenes, as highly reactive electron-deficient systems, are valuable intermediates in organic synthesis [3-7]. We might assume that introducing active pharmacophores of the pyrrole and indole type into their molecules may lead to novel heteryl-containing structures with useful properties.

For the first time, we have shown that reactions of β,β-dinitrostyrenes **1-3** with pyrrole occur under very mild conditions (at room temperature, with constant stirring of the reagents in carbon tetrachloride with no catalyst) and end in formation of substituent addition products: 2-aryl-1,1-dinitro-2-(pyrrol-2-yl)ethanes **4-6** in 66-97% yields.



1, **4** Ar = Ph, **2**, **5** Ar = *p*-MeC_6H_4, **3**, **6** Ar = *p*-ClC_6H_4

The structure of products **4-6** was confirmed by IR and 1H NMR spectroscopy.

We synthesized the starting β,β-dinitrostyrenes by the procedures we developed in [8, 9].

1,1-Dinitro-2-(pyrrol-2-yl)-2-phenylethane (4). Pyrrole (0.1 ml, 1.5 mmol) was added dropwise with constant stirring to a suspension of compound **1** (0.29 g, 1.5 mmol) in carbon tetrachloride (6 ml) at room temperature. After 2 h, the reaction solution was poured into a petri dish, the solvent was evaporated, and the residue was recrystallized from carbon tetrachloride. Yield 0.52 g (66%), yellow-green crystals; mp 86-87°C. ^{1}H NMR spectrum ($CDCl_3$, 200 MHz), δ, ppm (*J*, Hz): 5.28 (1H, d, *J* = 11.6, C(2)H); 6.12 (2H, s, CH_{pyr}); 6.69 (1H, s, CH_{pyr}); 7.08 (1H, d, *J* = 11.6, C(1)H); 7.31 (5H, m, Ar); 9.36 (1H, s, NH). IR spectrum ($CHCl_3$), ν, cm^{-1}: 1586, 1327 (NO_2); 3474 (NH). Found, %: C 54.95, 54.98; H 4.30, 4.27; N 15.91, 15.92. $C_{12}H_{11}N_3O_4$. Calculated, %: C 55.17; H 4.21; N 16.09.

Compounds **5** and **6** were obtained similarly.

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1,1-Dinitro-2-(pyrrol-2-yl)-2-(*p*-tolyl)ethane (5). Yield 89%, yellow-green crystals; mp 70-71°C (hexane). ^{1}H NMR spectrum ($CDCl_3$, 200 MHz), δ, ppm (*J*, Hz): 2.31 (3H, s, CH_3); 5.25 (1H, d, *J* = 11.0, C(2)H); 6.11 (2H, s, CH_{pyr}); 6.69 (1H, s, CH_{pyr}); 6.98 (1H, d, *J* = 11.0, C(1)H); 7.21 (4H, m, Ar); 9.08 (1H, s, NH). IR spectrum ($CHCl_3$), ν, cm^{-1}: 1585, 1326 (NO_2); 3470 (NH). Found, %: C 56.46, 56.45; H 5.16, 5.19; N 15.12, 15.17. $C_{13}H_{13}N_3O_4$. Calculated, %: C 56.73; H 4.73; N 15.27.

2-(*p*-Chlorophenyl)-1,1-dinitro-2-(pyrrol-2-yl)ethane (6). Yield 97%, yellow-green crystals; mp 84-85°C (carbon tetrachloride). ^{1}H NMR spectrum ($CDCl_3$, 200 MHz), δ, ppm (*J*, Hz): 5.29 (1H, d, *J* = 11.6, C(2)H); 6.12 (2H, s, CH_{pyr}); 6.70 (1H, s, CH_{pyr}); 7.11 (1H, d, *J* = 11.6, C(1)H); 7.23 (4H, m, Ar); 9.45 (1H, s, NH). IR spectrum ($CHCl_3$), ν, cm^{-1}: 1590, 1322 (NO_2); 3464 (NH). Found, %: C 48.58, 48.63; H 4.17, 4.20; N 14.01, 14.02. $C_{12}H_{10}ClN_3O_4$. Calculated, %: C 48.73; H 3.38; N 14.21.

This research was performed with the financial support of the Ministry of Education of the Russian Federation (grant No. A03-2.11-517).

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