Letters to the Editor

N-(2-Nitroxyethyl)nicotinamide (Nicorandil) as a monomer in quaternization polymerization

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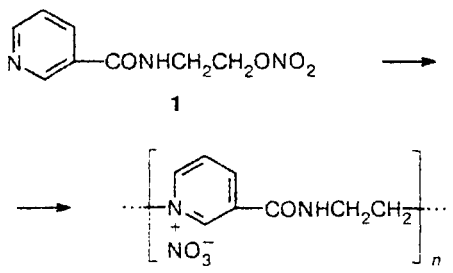
The chemical properties of *N*-(2-nitroxyethyl)-nicotinamide (**1**), known as a cardioactive medicine (Nicorandil),[1] have been studied in aqueous solutions.[2] We showed that compound **1** (m.p. 92—93 °C) undergoes solid-state polymerization at 40—70 °C. The polymer obtained is well soluble in water and virtually insoluble in organic solvents. Based on the data from elemental analysis, IR and ^{1}H NMR spectroscopy, and thermomechanical analysis,[3,4] one can conclude that the major reaction product is polymer (**2**) (95 wt %) with relatively high molecular mass ($3 \cdot 10^4$—$5 \cdot 10^4$) and low glass-transition temperature (−48 °C), which results from quaternization polymerization of **1**.



1

2

The rest of the reaction products is a low-molecular-mass (10^3) polymer with higher glass-transition temperature (76 °C). Supposedly, it is a product of quaternization polymerization of 2-(3-pyridyl)-4,5-dihydrooxazole, which seems to be formed from compound **1**[2] and composed of the corresponding *N*-acylethylenimine units.[5]

The possibility of these solid-state reactions was confirmed by X-ray diffraction analysis[6,7] of compound **1**. In its molecule, the side chain exists in a twisted, cisoid conformation so that there are short distances between the corresponding reaction centers.

Polymerization of compound 1. Compound **1**[7] (1 g, 4.7 mmol) was heated in an evacuated sealed tube at 70 °C for 3 days. The weight and appearance of the sample remained unchanged. It was dissolved in hot 50% MeOH to give a colorless powder in almost quantitative yield on cooling. Found (%): C, 45.55; H, 4.48; N, 19.95. $(C_8H_9N_3O_4)_x$. Calculated (%): C, 45.50; H, 4.30; N, 19.90. IR (KBr), ν/cm^{-1}: 3250 (NH); 1675 (C=O, CONH); 1590 (pyridinium ring); 1555 (NH); 1495 (pyridinium ring); 1385 (NO_3^-); 1365 (CH_2); 1310 (C—N, CONH); 1195, 1145, 1090, 1045, 1030, 830 (pyridinium ring); 745, 680 (pyridinium ring). ^{1}H NMR (DMSO-d_6), δ: 3.95 (br.m, 2 H, NHC$\underline{H_2}$CH$_2$); 4.85 (br.m, 2 H, NHCH$_2$C$\underline{H_2}$); 8.22 (dd, 1 H, H-5, $^3J_{H\text{-}5,H\text{-}6} \approx 5.6$ Hz, $^3J_{H\text{-}5,H\text{-}4} \approx 8.0$ Hz); 8.80 (d, 1 H, H-4, $^3J_{H\text{-}4,H\text{-}5} \approx 8.0$ Hz); 9.18 (d, 1 H, H-6, $^3J_{H\text{-}6,H\text{-}5} \approx 5.6$ Hz); 9.38 (br.m, 1 H, CONH); 9.44 (br.s, 1 H, H-2).

Published in *Izvestiya Akademii Nauk. Seriya Khimicheskaya*, No. 8, pp. 1493—1494, August, 2000.

1066-5285/00/4908-1487 $25.00

This work was financially supported by the International Scientific and Technical Center (Project No. 123-94).

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Received December 15, 1999;
in revised form May 25, 2000