Chemistry of Heterocyclic Compounds, Vol. 36, No. 5, 2000

A SECOND TYPE OF STABILIZATION OF ALKOXYCARBONYL(IMIDOYL)KETENES

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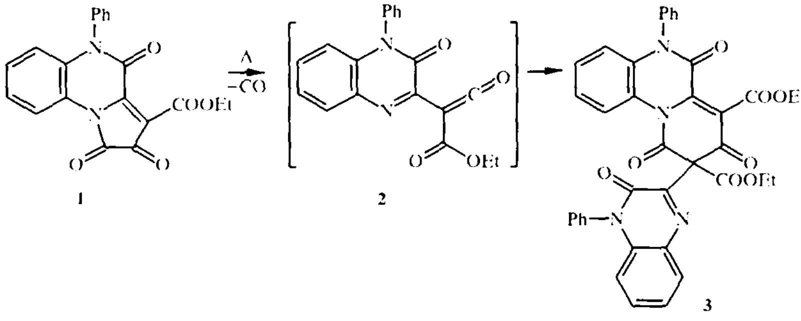
Keywords: alkoxycarbonyl(imidoyl)ketene, 2,3-dihydro-2,3-pyrroledione, pyrrolo[1,2-*a*]quinoxaline, dimerization.

Aroyl(imidoyl)ketenes are stabilized by intramolecular cyclization [1,2] or by participation in a [4+2] cyclodimerization reaction, accompanied by a [1,3] acylotropic shift of the aroyl group [3]. The first studied representative of the class of alkoxycarbonyl(imidoyl)ketenes has a structure suggesting the possibility of intramolecular cyclization, and such a reaction has been realized [4].

We studied thermolysis of 3-ethoxycarbonyl-5-phenyl-1,2,4,5-tetrahydropyrrolo[1,2-*a*]quinoxaline-1,2,4-trione (**1**), in which we might expect formation of 3-oxo-4-phenyl-3,4-dihydroquinoxalin-2-yl(ethoxycarbonyl)ketene (**2**), a representative of the class of alkoxycarbonyl(imidoyl)ketenes which is not capable of intramolecular cyclization of the types described [1, 2, 4].

If compound **1** is held at 185-187°C for 5 min, we obtain 2,4-di(ethoxycarbonyl)-2-(3-oxo-4-phenyl-3,4-dihydroquinoxalin-2-yl)-6-phenyl-2,3,5,6-tetrahydro-1H-pyrido[1,2-*a*]quinoxaline-1,3,5-trione (**3**), identified from X-ray diffraction data.



Probably ketene **2** formed upon thermal decarbonylation of compound **1** is stabilized by participation in a [4+2] cyclodimerization reaction, and one ketene molecule plays the role of the diene with the imidoylketene moiety while the other ketene molecule plays the role of the dienophile with the C=C bond of the ketene moiety. The [1,3] acylotropic shift of the ethoxycarbonyl group described for the aroyl analog does not occur in the cycloadduct **3** formed.

2,4-Di(ethoxycarbonyl)-2-(3-oxo-4-phenyl-3,4-dihydroquinoxalin-2-yl)-6-phenyl-2,3,5,6-tetrahydro-1H-pyrido[1,2-*a*]quinoxaline-1,3,5-trione (3). A solution of compound **1** (0.60 g, 1.66 mmol) in Dowtherm A (4 ml) was held at 185-187°C for 5 min and then cooled down. The precipitate of compound **3** was filtered off. Yield 0.44 g (40%); mp 209-211°C (with decomposition, from benzene). IR spectrum: 1720 (COO), 1645 cm^{-1} (CO). ^{1}H NMR spectrum (DMSO-d_6): 1.24 (3H, t, J = 7.0 Hz, CH_3); 1.42 (3H, t, J = 7.0 Hz, CH_3); 4.17 (2H, q, J = 7.0 Hz, CH_2O); 4.50 (2H, q, J = 7.0 Hz, CH_2O); 6.40-8.03 ppm (18H, m, $2C_6H_5$ + $2C_6H_4$). Mass spectrum, m/z: 668 [M$^+$]. Found, %: C 68.31; H 4.25; N 8.41. $C_{38}H_{28}N_4O_8$. Calculated, %: C 68.26; H 4.22; N 8.38.

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This research was financially supported by the Russian Foundation for Basic Research (grant No. 98-03-32888).

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