Chemistry of Heterocyclic Compounds, Vol. 36, No. 11, 2000

AN UNUSUAL RECYCLIZATION OF A SUBSTITUTED PYRROLO[1,2-*a*]-QUINOXALINE-1,2,4-TRIONE UNDER THE ACTION OF BENZYLAMINE

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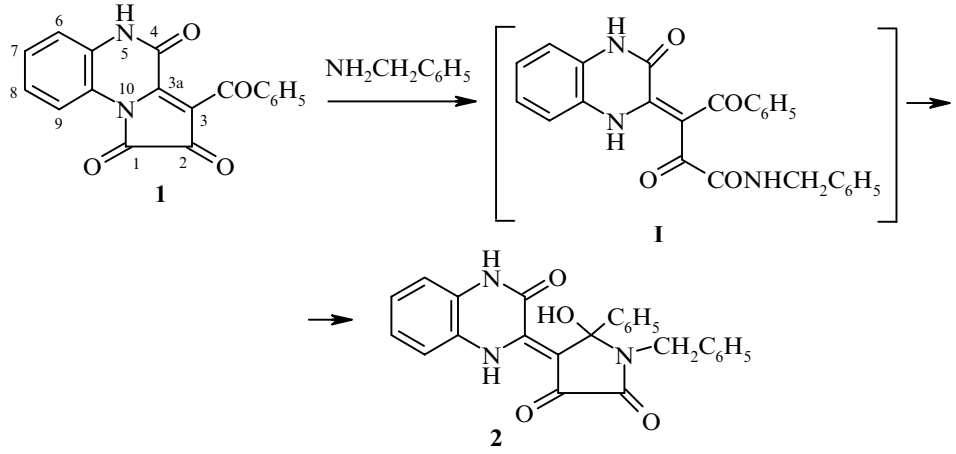
Keywords: benzylamine, pyrrolo[1,2-*a*]quinoxaline-1,2,4-trione, tetrahydropyrrolylidene-1,4-quinoxaline-2-one.

When 3-aroyl-1,2,4,5-tetrahydropyrrolo[1,2-*a*]quinoxaline-1,2,4-triones react with nucleophilic reagents the products usually formed are either products of addition at the $C_{(3a)}$ carbon atom or products of the pyrroledione ring opening at the $C_{(1)}$–$N_{(10)}$ bond to give an open structure, and under more vigorous conditions fission to give 2-quinoxalones [1]. We unexpectedly obtained *Z*-3-(1-benzyl-5-hydroxy-2,3-dioxo-5-phenyl-2,3,4,5-tetrahydro-4-pyrrolylidene)-1,2,3,4-tetrahydroquinoxaline-2-one (**2**) from the reaction of 3-benzoyl-1,2,4,5-tetrahydropyrrolo-[1,2-*a*]quinoxaline-1,2,4-trione (**1**) with benzylamine.



1 **I** **2**

Compound **2** is formed as a result of nucleophilic attack of benzylamine at $C_{(1)}$ atom of compound **1**, opening of the pyrroledione ring at the $C_{(1)}$–$N_{(10)}$ bond with subsequent addition of the benzylamide NH group to the carbonyl of the benzoyl substituent.

Geometric and electronic characteristics of intermediate **I** were calculated by semiempirical methods in order to explain the direction of the reaction. It follows from the calculations that the carbonyl carbon atom of the benzoyl substituent is the most electrophilic and this probably explains the nucleophilic attack by the benzylamide amino group at this atom and the closing of the pyrrolylidene ring.

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Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 11, 1569-1570, November, 2000. Original article submitted August 14, 2000.

This recyclization is the first method for construction of the pyrrolylidenequinoxaline heterocyclic system.

***Z*-3-(1-Benzyl-5-hydroxy-2,3-dioxo-5-phenyl-2,3,4,5-tetrahydro-4-pyrrolylidene)-1,2,3,4-tetrahydroquinoxaline-2-one (2).** Benzylamine (0.95 ml, 10 mmol) was added dropwise to a solution of compound **1** (3.18 g, 10 mmol) in absolute acetonitrile (50 ml), the mixture was boiled for 3-5 min, cooled, and the precipitate filtered off to give compound **2** (3.19 g, 75%); mp 265-267°C (acetonitrile). IR spectrum (nujol mull), ν, cm^{-1}: 3450 sh (OH), 3230 (CONH), 3100 sh ($N_{(4)}H$), 1730 ($C_{(3)}=O)_{pyrrol.}$, 1690 ($C_{(2)}=O)_{quin.}$, 1630 sh ($C_{(2)}=O)_{pyrrol.}$. ^1H NMR spectrum (80 MHz, DMSO-d_6), δ, ppm, *J*, Hz: 4.20, 4.45 (2H, dd, CH_2N, *J* = 3.6); 6.57 (1H, s, OH); 7.12-7.61 (9H, m, C_6H_4 + C_6H_5); 13.01 (1H, s, $N_{(1)}H$); 14.36 (1H, s, $N_{(4)}H$). Found, %: C 70.49; H 4.42; N 9.71. $C_{25}H_{19}N_3O_4$. Calculated, %: C 70.58; H 4.50; N 9.88.

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