NITRO AZINES.
21.* REACTIVITIES AND ELECTRON STRUCTURES OF 6-NITROAZOLO[1,5-*a*]PYRIMIDINES

A. V. Myasnikov, P. A. Torgashev, T. L. Pilicheva, V. L. Rusinov, S. A. Gromova, M. G. Trofimova, A. V. Velik, and O. N. Chupakhin

6-Nitroazolopyrimidines react with the acetonyl anion to give 6-nitro-7-acetonyl-4,7-dihydroazolo[1,5-a]pyrimidines. The reactivity of this class of compounds with respect to charged and uncharged nucleophiles is determined by their aromatic character and the deficit of electron density in the pyrimidine ring, while the direction of attack is determined by the overall charge on fragments of the valence-bonded atoms.

6-Nitroazolo[1,5-*a*]pyrimidines I react with a whole host of C-nucleophiles such as indoles [2], pyrroles [3], and polyphenols [4] or O-nucleophiles such as alcohols and water [5] to give stable adducts that have a 4,7-dihydro structure. All of these transformations take place without additional activation of the reagent and substrate.

In this paper we present new data on the reaction of azolo-annelated nitropyrimidines with a charge-activated C-nucleophile, viz., the acetonyl anion, and we also discuss the results of quantum-chemical calculations of a series of 6-nitroazolo[1,5-*a*]pyrimidines that make it possible to predict the reactivity and direction of addition of the nucleophile.

We found that acetone, in contrast to aromatic C-nucleophiles, does not, without additional activation, react with 6-nitroazolo[1,5-*a*]pyrimidines. The utilization of the acetonyl anion, like the reaction of the latter with nitrobenzenes, nitropyridines, and nitropyrimidines [6-8], leads initially to the formation of σ adducts IIa-k. Thus when triethylamine is added to an acetone solution of 6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidine (Ia), one observes a bathochromic shift of the absorption maximum to 410 nm ($\Delta\lambda$ = 70 nm), and signals of 7-H and 5-H protons (5.83 and 8.34 ppm, respectively) and equivalent-to-them (with respect to integral intensity) signals of the acetonyl anion and the triethylammonium cation appear in the PMR spectrum of a mixture of azolopyrimidine Ia, deuteroacetone, and triethylamine in d_6-DMSO.

Stable protonated forms IIIa-k can be isolated from the reaction mixtures when the resulting σ adducts IIa-k are acidified. Acetone reacts similarly with 6-nitro-1,2,4-triazolo[1,5-*a*]pyrimidine, as well as with a number of other azolo[1,5-*a*]pyrimidines Ib-k in the presence of sodium carbonate and alkali.

The proton spectra of III (Table 1) contain characteristic signals of an acetone fragment at 2.00-2.05 ppm (CH_3) and 3.08-3.25 ppm (CH_2), as well as signals of the 7-H and 5-H protons of the pyrimidine ring at 5.80-5.95 ppm and 8.10-8.42 ppm, respectively. The location of the signals of the protons of the azolopyrimidine fragment of III does not undergo appreciable changes with respect to the anionic σ adducts II; this apparently attests to dissociation of the N−H bond in III in solution in DMSO. The IR spectra contain characteristic absorption bands corresponding to symmetrical (1330-1335 cm^{-1}) and asymmetrical (1590-1615 cm^{-1}) vibrations of a nitro group, as well as bands corresponding to a carbonyl group at 1720-1730 cm^{-1} and to an NH group at 3100-3300 cm^{-1}. Mass-spectral studies made it possible to record peaks of a molecular ion (M^+) and an [M^+ — 46] ion, which corresponds to detachment of a nitro group.

As with uncharged C-nucleophiles, the nature of the substituents in the azole fragment of the molecule affects the reactivities of 6-nitroazolopyrimidines in their reaction with the acetonyl ion. The donor substituents CH_3 and SCH_3 do not

*For Communication 20 see [1].

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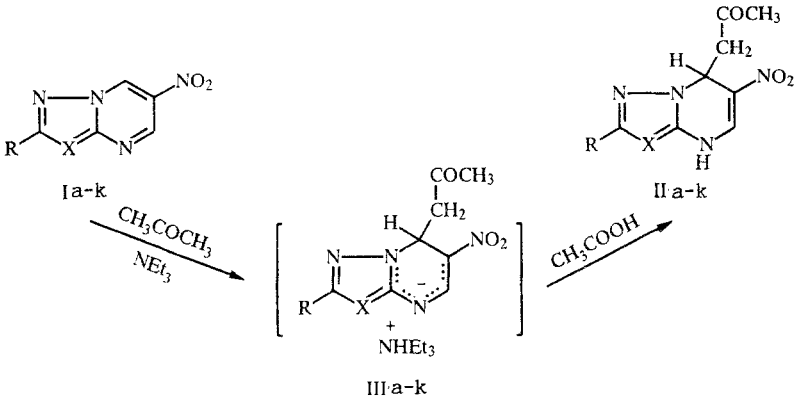
TABLE 1. Characteristics of the Synthesized 6-Nitro-7-acetonyl-4,7-dihydroazolo[1,5-*a*]pyrimidines

Compound	Empirical formula	mp, °C	PMR spectrum, δ, ppm	IR spectrum, ν, cm^{-1}			UV spectrum, λ_{max}, nm (log ε)	Yield, %	
				NO_2	C=O	NH		spectral	preparative
IIIa	$C_8H_9N_5O_3$	228	2,02 (3H, s, CH_3); 3,07 (2H, d, CH_2); 5,83 (1H, t, 7-H); 7,68 (1H, s, 2-H); 8,34 (1H, s, 5-H)	1330, 1605	1730	3130	213 (3,85); 374 (4,06)	100	84
IIIb	$C_9H_{11}N_5O_3$	226	2,00 (3H, c, CH_3); 2,18 (3H, s, CH_3); 3,14 (2H, d, CH_2); 5,80 (1H, t, 7-H); 8,28 (1H, s, 5-H)	1335, 1610	1720	3100	213 (3,80); 376 (4,01)	100	82
IIIc	$C_{10}H_{12}N_5O_3$	201	1,14 (3H, t, CH_3); 2,00 (3H, s, CH_3); 2,53 (2H, q, CH_2); 3,13 (2H, d, CH_2); 5,81 (1H, t, 7-H); 8,33 (1H, s, 5-H)	1310, 1585	1705	3080	227 (3,63); 380 (3,92)	100	82
IIId	$C_{14}H_{13}N_5O_3$	204	2,10 (3H, s, CH_3); 3,20 (2H, d, CH_2); 5,94 (1H, t, 7-H); 7,65 (5H, сл. C_6H_5); 8,40 (1H, s, 5-H); 11,96 (1H, br.s, NH)	1325, 1580	1690	3120	232 (2,91); 259 (3,02); 381 (3,04)	100	73
IIIe	$C_9H_{11}N_5O_3S$	168	2,00 (3H, s, CH_3); 2,45 (3H, s, SCH_3); 3,15 (2H, d, CH_2); 5,82 (1H, t, 7-H); 8,32 (1H, s, 5-H)	1330, 1590	1720	3300	212 (4,06); 287 (3,57); 384 (3,98)	100	80
IIIf	$C_{11}H_{13}N_5O_5$		1,30 (3H, t, CH_3); 2,03 (3H, s, CH_3); 3,25 (2H, d, CH_2); 4,30 (2H, q, CH_2); 5,95 (1H, t, 7-H); 8,42 (1H, s, 5-H)	1330, 1610	1730			100	76
IIIg	$C_9H_8N_5O_3F_3$	178	2,05 (3H, s, CH_3); 3,10 (2H, d, CH_2); 5,94 (1H, t, 7-H); 8,38 (1H, s, 5-H)	1325, 1610	1720	3170	221 (3,81); 367 (3,95)	100	71
IIIh	$C_8H_8N_5O_3Cl$	204	2,04 (3H, s, CH_3); 3,12 (2H, d, CH_2); 5,74 (1H, t, 7-H); 8,29 (1H, s, 5-H)	1320, 1575	1700	3070	208 (3,99); 266 (3,95); 369 (3,86)	100	74
IIIi	$C_8H_{10}N_6O_3$	212	2,07 (3H, s, CH_3); 3,09 (2H, d, CH_2); 5,59 (1H, t, 7-H); 7,02 (2H, br.s, NH_2); 8,21 (1H, s, 5-H)				210 (3,93); 294 (3,70); 392 (3,90)	32	26
IIIj	$C_{10}H_{13}N_6O_3$	195	2,02 (3H, s, CH_3); 2,81 (6H, s, $N(CH_3)_2$); 3,06 (2H, д, CH_2); 5,66 (1H, t, 7-H); 8,27 (1H, s, 5-H)				213 (2,80); 317 (2,84); 396 (3,06)	33	28
IIIk	$C_{12}H_{13}N_4O_5$	162	1,39 (3H, t, CH_3); 2,10 (3H, s, CH_3); 3,25 (2H, d, CH2); 4,35 (2H, q, CH_2); 5,92 (1H, t, 7-H); 7,83 (1H, s, 2-H); 8,16 (1H, s, 5-H)	1330, 1615	1720	3200		100	83

hinder the reaction (the yields of the σ adducts are quantitative). However, groups that have a significant +M effect [NH_2, $N(CH_3)_2$] deactivate the system. The σ adducts in this case are formed in only 32-33% yields (Table 1).



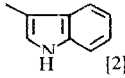
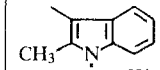
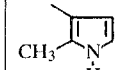
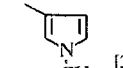
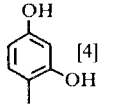
I—IIIa R = H, X = N; b R = CH_3, X = N; c R = C_2H_5, X = N; d R = C_6H_5, X = N; e R = SCH_3, X = N; f R = $COOC_2H_5$, X = N; g R = CF_3, X = N; h R = Cl, X = N; i R = NH_2, X = N; j R = $N(CH_3)_2$, X = N; k R = H, X = $CCOOC_2H_5$

To analyze the reactivities of 6-nitroazolo[1,5-*a*]pyrimidines with respect to the acetonyl ion, as well as other nucleophilic agents, we examined their electron structures. In our research we carried out a quantum-chemical study of 16 nitro azines (Table 2). The calculations were performed by the CNDO/2 method [9] by means of the modified CNINDO program [10]. It has been previously shown [11, 12] that for calculations of nitro compounds within the framework of the CNDO/2 method it is sufficient to use the "averaged" geometrical parameters. In this connection, in selecting the geometries of the compounds under consideration we took into account the results of x-ray diffraction analysis for molecules with similar structures [2, 13].

One of the factors that determine the direction of nucleophilic attack is the distribution of the electron density in the molecule. In the compounds under consideration here, the positive charges are located on the $C_{(2)}$, $C_{(5)}$, $C_{(7)}$, and $C_{(9)}$ atoms (Table 3). All of them are theoretically possible centers of nucleophilic attack. In previous studies [14, 15] it was shown that the direction of nucleophilic attack is determined not so much by the charge on an individual atom as it is by the overall charge of the fragment of valence-bonded atoms. In our case one can single out four fragments, viz., F_1, F_2, F_3, and F_4, with central carbon atoms $C_{(2)}$, $C_{(9)}$, $C_{(5)}$, and $C_{(7)}$, respectively, and their immediate environment, i.e., the F_1 fragment includes central atom $C_{(2)}$ and the $R_{(2)}$, $N_{(1)}$, and $X_{(3)}$ atoms that are valence-bonded to it; the F_2 fragment includes central atom $C_{(9)}$ and the $C_{(9)}$, $X_{(3)}$, $N_{(4)}$, and $N_{(8)}$ atoms valence-bonded to it; the F_3 fragment includes central atom $C_{(5)}$ and the $H_{(5)}$, $N_{(4)}$, and $C_{(6)}$ atoms valence-bonded to it; the F_4 fragment includes central atom $C_{(7)}$ and the $H_{(7)}$, $R_{(7)}$, $N_{(8)}$, and $N_{(6)}$ atoms valence-bonded to it. An analysis of the charge distribution (Table 4) shows that the F_4 fragment is the most positive. The charges on the other fragments are either substantially smaller in magnitude or have negative values. An exception to this is 2-trifluoromethyl-6-nitrotriazolo[1,5-*a*]pyrimidine (Ig), in which, due to the high charge on the carbon atom of the trifluoromethyl group, the maximum positive charge is located on the F_1 fragment. However, in this case steric hindrance must be overcome for addition of the nucleophile to the $C_{(2)}$ atom, since the 2 position is already occupied by a trifluoromethyl group. In addition, the high negative charge ($Q = -0.2037$) on the fluorine atoms shields the positive charge on the F_1 fragment. Thus, proceeding from the results of the calculation, the most likely center of nucleophilic addition in the investigated compounds is the F_4 fragment with central atom $C_{(7)}$; this is in good agreement with the experimental results and, consequently, may serve as a diagnostic indication of the direction of nucleophilic attack in each individual compound of this series. However, these results are not adequate for predicting their reactivities with respect to charged and uncharged nucleophiles.

To solve this problem we undertook a search for characteristics that reflect the reactivities of the compounds. We examined the topological, structural, and electronic indexes (descriptors). We ultimately arrived at two descriptors (Table 4): $\Delta\bar{N}_S$ — the average value of the fluctuations of the orders of the ring bonds taking into account the effect of the substituents [16] (the bond orders were calculated within the framework of the Wiberg CNDO/2 method [17]) and ΣQ — the overall charge of the pyrimidine fragment calculated on the basis of the charges on the atoms of the pyrimidine ring and valence-bonded to it. The reactivity of this class of compounds also depends on the aromatic character of the system, which is reflected by the

TABLE 2. Reactivities of 6-Nitroazolo[1,5-*a*]pyrimidines Ia-c*

Compound	R	X	D_2O [5]	CD_3O_2 [5]	 [2]	 [2]	 [3]	 [3]	 [4]	$\bar{C}H_2COCH_3$
Ia	H	N	+	+	+	+	+	+	+	+
Ib	CH_3	N	+	+	+	+	+	+	+	+
Ic	C_2H_5	N	+	+	+	+	+	+	+	+
Ie	SCH_3	N	+	+	+	+	+	+	+	+
If	$COOC_2H_5$	N	+	+	+		+			+
Ig	CF_3	N	+	+	+	+			+	+
Ih	Cl	N	-	+	-		-		+	+
Ii	NH_2	N	-	-	-	-				+
Ij	$N(CH_3)_2$	N	-	-	-	-	-	-		+
Ik	H	C-$COOC_2H_5$	+	+	+	+	+	+	+	+
Il	CH_3	CH	-	+	-	-	-	-	-	+
Im	H	CH	-	-	-	-	-	-	-	
In	C_6H_5	CH	-	+			+		-	+
Io	H	C-NO_2		+	+		+		+	
Ip	CH_3	C-NO_2		+	+		+		+	
Iq	H	C-CN	+	+	+		+		+	

*A "+" indicates that the compound did react, while a "−" indicates that the compound did not.

TABLE 3. Charges on the Ring Atoms of Condensed Nitro Azines

Compound	$N_{(1)}$	$C_{(2)}$	$X_{(N,C)}$	$N_{(4)}$	$C_{(5)}$	$C_{(6)}$	$C_{(7)}$	$N_{(8)}$	$C_{(9)}$
Ia	-0,2247	0,2105	-0,2430	-0,1787	0,1405	-0,0391	0,1049	0,0013	0,3040
Ib	-0,2279	0,2372	-0,2892	-0,2159	0,1422	-0,0451	0,1218	0,0378	0,3041
Ic	-0,2203	0,2304	-0,3074	-0,2310	0,1409	-0,0479	0,1292	0,0607	0,3051
Ie	-0,2094	0,2407	-0,3181	-0,2404	0,1412	-0,0484	0,1360	0,0772	0,3068
If	-0,1496	0,1428	-0,2979	-0,2322	0,1403	-0,0416	0,1385	0,0756	0,2944
Ig	-0,2103	0,1673	-0,2015	-0,1493	0,1410	-0,0337	0,0962	-0,0143	0,3071
Ih	-0,2136	0,3145	-0,2706	-0,2049	0,1437	-0,0373	0,1256	0,0411	0,3095
Ii	-0,2476	0,3060	-0,3012	-0,2218	0,1449	-0,0484	0,1261	0,0407	0,3103
Ij	-0,2493	0,3054	-0,3027	-0,2219	0,1446	-0,0484	0,1256	0,0395	0,3019
Ik	-0,1973	0,1454	-0,1893	-0,1944	0,1170	-0,0255	0,1173	0,0764	0,2233
Il	-0,2117	0,1595	-0,1874	-0,2464	0,1244	-0,0265	0,1334	0,1102	0,2057
Im	-0,2224	0,1363	-0,1482	-0,1498	0,1224	-0,0313	0,8889	0,0388	0,2185
In	-0,2105	0,1421	-0,1821	-0,2286	0,1234	-0,0312	0,1257	0,1010	0,2080
Io	-0,1898	0,1434	-0,1169	-0,1661	0,1347	-0,0242	0,1181	0,0738	0,2283
Ip	0,2144	0,1844	-0,1361	-0,1716	0,1355	-0,0270	0,1172	0,0736	0,2306
Iq	-0,2037	0,1334	-0,1081	-0,1795	0,1285	-0,0277	0,1177	0,0661	0,2163

$\Delta\bar{N}_S$ index, and on the deficit of the electron density in the pyrimidine ring determined by the overall positive charge ΣQ. These indexes, taken separately, are not linked linearly with the reactivities. Thus the smaller the $\Delta\bar{N}_S$ index, the greater the aromatic character of the compound and, consequently, the lower the reactivity.

At the same time, a reverse dependence is observed for Im and Ip. The same exceptions can also be found for the separately taken ΣQ index. In addition, the values of the selected criteria depend on the type of system, i.e., they change on passing from triazolopyrimidines to pyrazolopyrimidines. For agreement of these indexes with one another we used methods involving the recognition of samples [18, 19], for which we used the SNARM program and Aidarkhanov's method [20].

All of the subjects used (16 compounds) can be divided into three types. Type 1 consists of Ia, b, c, f, g, k, n, p, q, which react with all of the nucleophiles presented in Table 2. Compounds Ii, j, *l*, m, which do not react with any of the nucleophiles comprise the third type, and, finally, type 2 consisted of Ie, h, which have intermediate activity. Of the 16 compounds, six were standard objects (SO), which determine the concept regarding each group, and 10 were control objects (CO), by means of which the quality of recognition was determined. Thus the concept regarding each type was determined by only two SO. In solving the problem we varied the possible SO in order to obtain the maximum amount of recognition, which was determined for the CO. Finally, we obtained the following values: if Ib, e, h, l, o, q are taken as the SO (Table 2), for the CO we obtain a 90% quality of recognition, i.e., of the 10 CO, nine are correctly classified. This means that, by using the above-indicated SO one can, with a probability of 90%, predict the behavior of nitro azines in nucleophilic addition reactions.

Thus the reactivities of nitro azines depend on the aromatic character and the deficit of electron density of the pyrimidine ring, while the center of nucleophilic attack is determined by the overall charge of the fragment of valence-bonded atoms and is located on the $C_{(7)}$ atom; this is in agreement with the experimental data on the reaction of the investigated series of compounds with charged and uncharged nucleophiles.

EXPERIMENTAL

The PMR spectra of solutions in d_6-DMSO were obtained with a Bruker WH-90 spectrometer at 80 MHz with tetramethylsilane (TMS) as the internal standard. The UV spectra of solutions in ethanol (10^{-4} mole/liter) and acetone (10^{-4} mole/liter) were recorded with a Specord UV-vis spectrophotometer. The IR spectra of suspensions in mineral oil and KBr pellets were recorded with a UR-20 spectrometer. The mass spectra were recorded with a Varian MAT-311A spectrometer. The following standard recording conditions were used: the accelerating voltage was 3 kV, the cathode emission current was 1 mA, the ionizing-electron energy was 70 eV, and the samples were introduced directly into the ion source. The calculated data were obtained with an EC-1033 computer with a maximum base of 140 AO and a memory capacity of no more than 250 kilobytes.

TABLE 4. Total Charges on the Fragments and Descriptors for the Recognition Problem

Compound	QF_1	QF_2	QF_3	QF_4	$\Delta\bar{N}_s$	ΣQ
Ia	-0,2542	-0,1734	-0,0469	0,1364	0,1991	0,4570
Ib	-0,3340	-0,1632	-0,0898	0,1790	0,1918	0,4146
Ic	-0,3115	-0,1726	-0,1089	0,2047	0,1915	0,4131
Ie	-0,3465	-0,1755	-0,1171	0,2278	0,1927	0,4301
If	0,0380	-0,1602	-0,1007	0,2383	0,1904	0,5187
Ig	0,3190	-0,0580	-0,0063	0,1246	0,1924	0,5377
Ih	-0,3110	-0,1249	-0,0620	0,2015	0,1935	0,4968
Ii	-0,4657	-0,1720	-0,0956	0,1834	0,1896	0,3910
Ij	-0,3960	-0,1832	-0,0963	0,1813	0,1896	0,3767
Ik	-0,2190	-0,0840	-0,0697	0,2366	0,1688	0,5200
Il	-0,2820	-0,1179	-0,1198	0,2766	0,1544	0,4863
Im	-0,2274	-0,0407	-0,0307	0,1642	0,1662	0,5000
In	-0,2444	-0,1017	-0,1081	0,2561	0,1528	0,4880
Io	-0,1267	0,0191	-0,0136	0,2424	0,1670	0,6668
Ip	-0,2124	-0,0035	-0,0228	0,2368	0,1592	0,6132
Iq	-0,1618	-0,0052	-0,0450	0,2189	0,1657	0,5978

2-R-6-Nitroazolo[1,5-*a*]pyrimidines. These compounds were obtained by the methods previously described in [5, 21].

2-R-6-Nitro-7-acetonyl-4,7-dihydroazolo[1,5-*a*]pyrimidines IIIa-k. An equimolar amount of triethylamine (Na_2CO_3, NaOH) was added to a solution of 0.01 mole of azolopyrimidine I in 15 ml of acetone, and the mixture was refluxed for 15 min. It was then cooled and acidified to pH 5 with acetic acid. The resulting precipitate was removed by filtration, dried, and recrystallized from ethanol.

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