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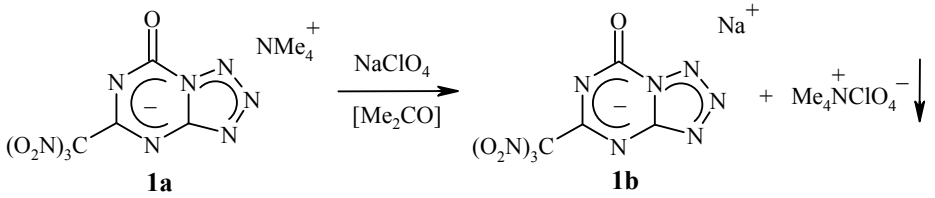
CONDENSED TETRAZOLO-1,3,5-TRIAZINES. 2*. ALKYLATION AND NUCLEOPHILIC SUBSTITUTION OF 5-TRINITROMETHYL-TETRAZOLO[1,5-*a*]-1,3,5-TRIAZIN-7-ONES

B. S. Fedorov[1], A. N. Utienyshev[1], A. A. Ghidaspov[2], E. V. Kachanovskaya[2], V. V. Bakharev[2], and M. A. Fadeev[1]

A new heterocyclic compound, 3-methyl-5-trinitromethyltetrazolo[1,5-a]-1,3,5-triazin-7-one, was synthesized by the reaction of methyl iodide and the silver salt of 5-trinitromethyltetrazolo[1,5-a]-1,3,5-triazin-7-one. An X-ray diffraction structural analysis of this product was carried out and feasibility was demonstrated for the nucleophilic substitution of the trinitromethyl group in this compound by the action of phenol, phenol derivatives, and thiophenol.

Keywords: condensed tetrazolo-1,3,5-triazines, 5-aryloxy-3-methyl- and 5-arylthio-3-methyl-tetrazolo[1,5-*a*]-1,3,5-triazin-7-ones, 3-methyl-5-trinitromethyltetrazolo[1,5-*a*]-1,3,5-triazin-7-one, alkylation, nucleophilic substitution of the trinitromethyl group.

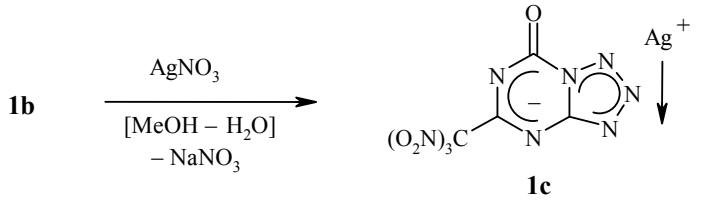
In a continuation of a study of condensed tetrazolo-1,3,5-triazines [1], we synthesized covalent derivatives of substituted tetrazolo[1,5-*a*]-1,3,5-triazin-7-one by the alkylation of various salts of 5-trinitromethyltetrazolo[1,5-*a*]-1,3,5-triazin-7-one using methyl iodide in DMF and acetonitrile. Alkylation could not be obtained using the tetramethylammonium salt of 5-trinitromethyltetrazolo[1,5-*a*]-1,3,5-triazin-7-one (**1a**) [1] despite broad variation of the reaction conditions such as the solvent, reaction temperature, and reaction time. The desired product could be obtained by alkylation only through use of the silver salt of 5-trinitromethyltetrazolo[1,5-*a*]-1,3,5-triazin-7-one [2].



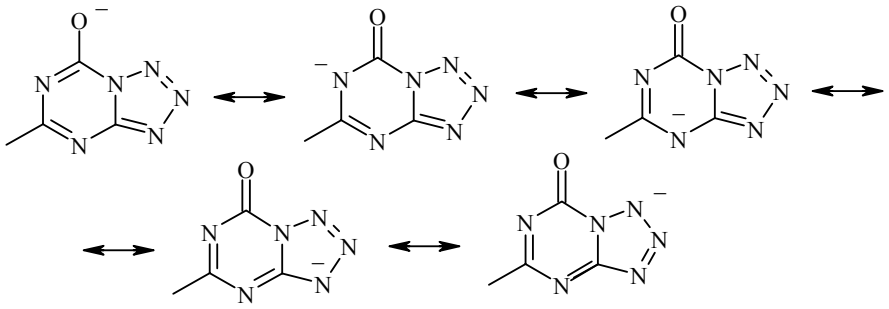
1a **1b**

* Communication 1, see ref. [1].

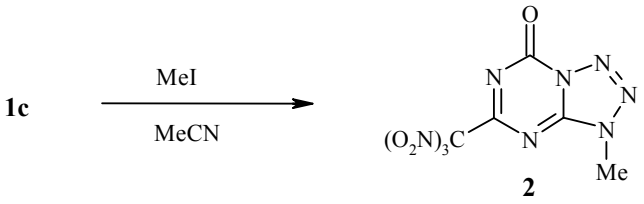
[1] Institute of Problems of Chemical Physics, Russian Academy of Sciences, 142432 Chernogolovka, Moscow Region, Russia; e-mail: boris@icp.ac.ru. [2] Samara State Technical University, 443010 Samara, Russia; e-mail: knil@sstu.smr.ru. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 4, pp. 582-588, April, 2005. Original article submitted December 19, 2002.



The structure of the polydentate anion in **1c** may be represented by resonance forms having a single conjugated electronic system. The alkylation might occur at five sites: the exocyclic oxygen atom, $N_{(1)}$ and $N_{(3)}$ of the tetrazole fragment, and $N_{(4)}$ and $N_{(6)}$ of the triazine ring.



The alkylation of silver salt **1c** by methyl iodide proceeds both in an excess of the alkylating agent and in acetonitrile solution. The only reaction product is 3-methyl-5-trinitromethyltetrazolo[1,5-*a*]-1,3,5-triazin-7-one (**2**), i.e., alkylation under the conditions studied proceeds at $N_{(3)}$ of the tetrazole fragment.



The yield of the methylation product was found to be greater when the reaction is carried out in acetonitrile.

The X-ray diffraction structural analysis data for **2** given in Fig. 1 and Tables 1-3 clearly support this structural assignment.

The covalent tetrazolo[1,5-*a*]-1,3,5-triazin-7-one heterocyclic system and exocyclic $O_{(1a)}$–$C_{(1a)}$ and $C_{(2a)}$–$C_{(5a)}$ bonds lie virtually in a single plane. The exocyclic $C_{(4a)}$–$N_{(2a)}$ bond is extruded from the plane of the heterocyclic system by about 4°. The length of the exocyclic $O_{(1a)}$–$C_{(1a)}$ bond corresponds to a double bond [3]. The length of three bonds, namely, $N_{(9a)}$–$C_{(1a)}$, $C_{(1a)}$–$N_{(5a)}$, and $N_{(5a)}$–$N_{(4a)}$, of the ten bonds of the heterocyclic system is close to single bond length (1.40-1.44 Å) [3]. The length of five bonds, namely, $C_{(2a)}$–$N_{(1a)}$, $N_{(1a)}$–$C_{(3a)}$, $C_{(3a)}$–$N_{(5a)}$, $C_{(3a)}$–$N_{(2a)}$, and $N_{(2a)}$–$N_{(3a)}$, corresponds to a bond intermediate between single and double (1.345-1.365 Å). The length of the $N_{(9a)}$–$C_{(2a)}$ and $N_{(3a)}$–$N_{(4a)}$ bonds is close to double bond length (1.28-1.30 Å) [3]. These findings indicate rather unique conjugation of the π-bonds in the heterocyclic system, which probably results from the electronic effect of the trinitromethyl group, which is a strong electron-withdrawing substituent, and the exocyclic $O_{(1a)}$–$C_{(1a)}$ double bond. The nitro group planes form a propeller conformation in the trinitromethyl group in **2**, similar to other covalent trinitromethyl compounds [4, 5]. As a consequence of the

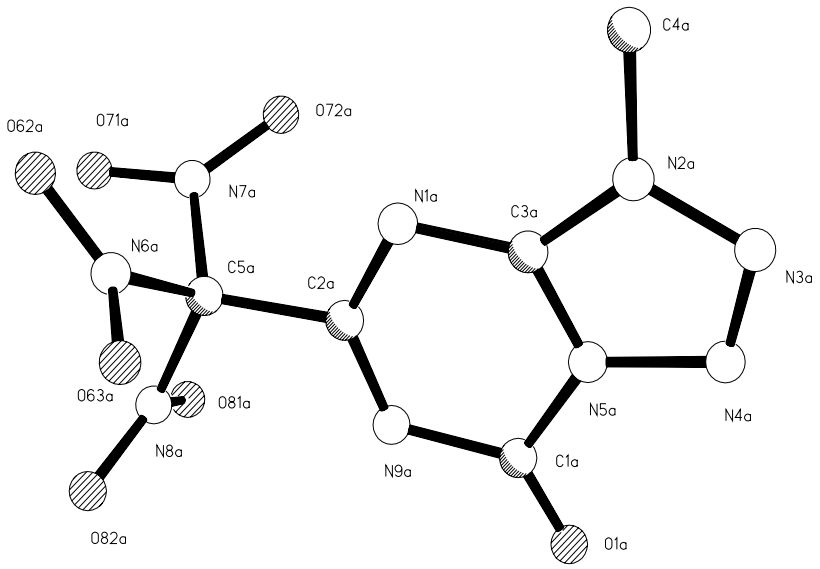


Fig. 1. Structure of 3-methyl-5-trinitromethyltetrazolo[1,5-*a*]-1,3,5-triazin-7-one (**2**).

slight differences in the lengths of the O–N and C–N bonds (up to 0.3 Å) and in the O–N–O and O–N–C bond angles (up to 4°), the twist angles of the planes of nitro groups A = $C_{(5a)}$–$N_{(6a)}$–$O_{(62a)}$–$O_{(63a)}$, B = $C_{(5a)}$–$N_{(7a)}$–$O_{(71a)}$–$O_{(72a)}$, and C = $C_{(5a)}$–$N_{(8a)}$–$O_{(81a)}$–$O_{(82a)}$ differ slightly from each other. The twist angle between A and B is 64.9°, the twist angle between B and C is 68.7°, and the twist angle between A and C is 67.8°.

The crystal of triazinone **2** features two independent molecules, **2A** and **2B**, which differ in bond lengths by 0.01-0.05 Å and in bond angles by 1-3°. However, the nitro groups in molecule **2B** are disordered, which may be a consequence of instability either of the crystal structure or of triazinone **2** itself during the exposure. This phenomenon probably accounts for the rather high R factor. Hence, the data on the structure of **2B** will not be given or discussed in this article.

TABLE 1. Bond Lengths (*d*) in the Structure of **2**

Bond	*d*, Å	Bond	*d*, Å
$N_{(1A)}$–$C_{(2A)}$	1.345(3)	$N_{(6A)}$–$C_{(5A)}$	1.548(3)
$N_{(1A)}$–$C_{(3A)}$	1.347(3)	$N_{(7A)}$–$O_{(72A)}$	1.223(4)
$N_{(2A)}$–$C_{(3A)}$	1.362(3)	$N_{(7A)}$–$O_{(71A)}$	1.234(4)
$N_{(2A)}$–$N_{(3A)}$	1.367(3)	$N_{(7A)}$–$C_{(5A)}$	1.548(3)
$N_{(2A)}$–$C_{(4A)}$	1.461(3)	$N_{(8A)}$–$O_{(81A)}$	1.218(4)
$N_{(3A)}$–$N_{(4A)}$	1.281(3)	$N_{(8A)}$–$O_{(82A)}$	1.227(4)
$N_{(4A)}$–$N_{(5A)}$	1.401(3)	$N_{(8A)}$–$C_{(5A)}$	1.523(3)
$N_{(5A)}$–$C_{(3A)}$	1.343(3)	$N_{(9A)}$–$C_{(2A)}$	1.301(3)
$N_{(5A)}$–$C_{(1A)}$	1.446(3)	$N_{(9A)}$–$C_{(1A)}$	1.411(3)
$N_{(6A)}$–$O_{(63A)}$	1.198(4)	$O_{(1A)}$–$C_{(1A)}$	1.171(3)
$N_{(6A)}$–$O_{(62A)}$	1.202(4)	$C_{(2A)}$–$C_{(5A)}$	1.553(3)

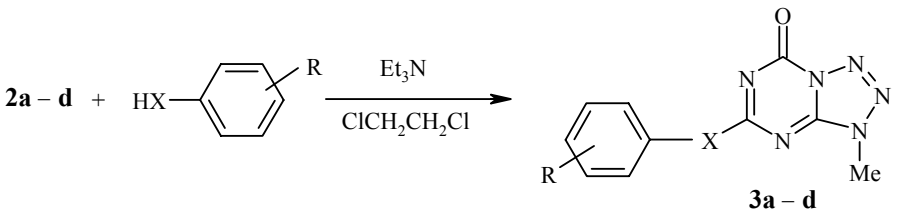
TABLE 2. Bond Angles (ω) in the Structure of **2**

Angle	ω, deg.	Angle	ω, deg.
$C_{(2A)}–N_{(1A)}–C_{(3A)}$	109.76(19)	$O_{(82A)}–N_{(8A)}–C_{(5A)}$	119.0(3)
$C_{(3A)}–N_{(2A)}–N_{(3A)}$	110.75(19)	$C_{(2A)}–N_{(9A)}–C_{(1A)}$	119.7(2)
$C_{(3A)}–N_{(2A)}–C_{(4A)}$	127.1(2)	$O_{(1A)}–C_{(1A)}–N_{(9A)}$	127.9(2)
$N_{(3A)}–N_{(2A)}–C_{(4A)}$	122.0(2)	$O_{(1A)}–C_{(1A)}–N_{(5A)}$	120.8(3)
$N_{(4A)}–N_{(3A)}–N_{(2A)}$	108.8(2)	$N_{(9A)}–C_{(1A)}–N_{(5A)}$	111.3(2)
$N_{(3A)}–N_{(4A)}–N_{(5A)}$	106.4(2)	$N_{(9A)}–C_{(2A)}–N_{(1A)}$	131.4(2)
$C_{(3A)}–N_{(5A)}–N_{(4A)}$	111.11(19)	$N_{(9A)}–C_{(2A)}–C_{(5A)}$	115.21(19)
$C_{(3A)}–N_{(5A)}–C_{(1A)}$	122.0(2)	$N_{(1A)}–C_{(2A)}–C_{(5A)}$	113.39(19)
$N_{(4A)}–N_{(5A)}–C_{(1A)}$	126.8(2)	$N_{(5A)}–C_{(3A)}–N_{(1A)}$	125.71(19)
$O_{(63A)}–N_{(6A)}–O_{(62A)}$	125.2(3)	$N_{(5A)}–C_{(3A)}–N_{(2A)}$	103.0(2)
$O_{(63A)}–N_{(6A)}–C_{(5A)}$	114.3(3)	$N_{(1A)}–C_{(3A)}–N_{(2A)}$	131.3(2)
$O_{(62A)}–N_{(6A)}–C_{(5A)}$	120.5(3)	$N_{(8A)}–C_{(5A)}–N_{(7A)}$	104.4(2)
$O_{(72A)}–N_{(7A)}–O_{(71A)}$	129.6(3)	$N_{(8A)}–C_{(5A)}–N_{(6A)}$	108.16(19)
$O_{(72A)}–N_{(7A)}–C_{(5A)}$	116.3(3)	$N_{(7A)}–C_{(5A)}–N_{(6A)}$	107.8(2)
$O_{(71A)}–N_{(7A)}–C_{(5A)}$	114.1(2)	$N_{(8A)}–C_{(5A)}–C_{(2A)}$	112.2(2)
$O_{(81A)}–N_{(8A)}–O_{(82A)}$	126.5(3)	$N_{(7A)}–C_{(5A)}–C_{(2A)}$	111.86(19)
$O_{(81A)}–N_{(8A)}–C_{(5A)}$	114.4(2)	$N_{(6A)}–C_{(5A)}–C_{(2A)}$	112.0(2)

In the presence of triethylamine as base, the trinitromethyl group in **2** is readily replaced by the action of various nucleophiles such as phenol, substituted phenols, and thiophenol to give the corresponding covalent 5-aryloxy-3-methyl- and 5-arylthio-3-methyltetrazolo[1,5-*a*]-1,3,5-triazin-7-ones **3a-d**:

TALE 3. Torsion Angles (φ) in the Structure of **2**

Angle	φ, deg.	Angle	φ, deg.
$C_{(3A)}–N_{(2A)}–N_{(3A)}–N_{(4A)}$	-1.9	$O_{(62A)}–N_{(6A)}–C_{(5A)}–N_{(7A)}$	6.1
$C_{(4A)}–N_{(2A)}–N_{(3A)}–N_{(4A)}$	-177.7	$O_{(62A)}–N_{(6A)}–C_{(5A)}–N_{(8A)}$	-106.2
$N_{(2A)}–N_{(3A)}–N_{(4A)}–N_{(5A)}$	1.2	$O_{(62A)}–N_{(6A)}–C_{(5A)}–C_{(2A)}$	129.6
$N_{(3A)}–N_{(4A)}–N_{(5A)}–C_{(1A)}$	-179.8	$O_{(63A)}–N_{(6A)}–C_{(5A)}–N_{(7A)}$	-171.8
$N_{(3A)}–N_{(4A)}–N_{(5A)}–C_{(3A)}$	-0.2	$O_{(63A)}–N_{(6A)}–C_{(5A)}–N_{(8A)}$	75.9
$N_{(4A)}–N_{(5A)}–C_{(1A)}–N_{(9A)}$	-178.9	$O_{(63A)}–N_{(6A)}–C_{(5A)}–C_{(2A)}$	-48.3
$N_{(4A)}–N_{(5A)}–C_{(1A)}–O_{(1A)}$	0.5	$O_{(71A)}–N_{(7A)}–C_{(5A)}–N_{(6A)}$	-66.8
$C_{(3A)}–N_{(5A)}–C_{(1A)}–N_{(9A)}$	1.6	$O_{(71A)}–N_{(7A)}–C_{(5A)}–N_{(8A)}$	48.1
$C_{(3A)}–N_{(5A)}–C_{(1A)}–O_{(1A)}$	-179.0	$O_{(71A)}–N_{(7A)}–C_{(5A)}–C_{(2A)}$	169.6
$C_{(2A)}–N_{(9A)}–C_{(1A)}–N_{(5A)}$	-1.0	$O_{(72A)}–N_{(7A)}–C_{(5A)}–N_{(6A)}$	113.8
$C_{(2A)}–N_{(9A)}–C_{(1A)}–O_{(1A)}$	179.7	$O_{(72A)}–N_{(7A)}–C_{(5A)}–N_{(8A)}$	-131.4
$C_{(3A)}–N_{(1A)}–C_{(2A)}–N_{(9A)}$	2.6	$O_{(72A)}–N_{(7A)}–C_{(5A)}–C_{(2A)}$	-9.8
$C_{(3A)}–N_{(1A)}–C_{(2A)}–C_{(5A)}$	-179.3	$O_{(81A)}–N_{(8A)}–C_{(5A)}–N_{(6A)}$	158.1
$C_{(1A)}–N_{(9A)}–C_{(2A)}–N_{(1A)}$	-1.2	$O_{(81A)}–N_{(8A)}–C_{(5A)}–N_{(7A)}$	43.4
$C_{(1A)}–N_{(9A)}–C_{(2A)}–C_{(5A)}$	-179.3	$O_{(81A)}–N_{(8A)}–C_{(5A)}–C_{(2A)}$	77.9
$C_{(2A)}–N_{(1A)}–C_{(3A)}–N_{(2A)}$	179.7	$O_{(82A)}–N_{(8A)}–C_{(5A)}–N_{(6A)}$	-25.7
$C_{(2A)}–N_{(1A)}–C_{(3A)}–N_{(5A)}$	-1.8	$O_{(82A)}–N_{(8A)}–C_{(5A)}–N_{(7A)}$	-140.3
$N_{(3A)}–N_{(2A)}–C_{(3A)}–N_{(1A)}$	-179.6	$O_{(82A)}–N_{(8A)}–C_{(5A)}–C_{(2A)}$	98.4
$N_{(3A)}–N_{(2A)}–C_{(3A)}–N_{(5A)}$	1.7	$N_{(1A)}–C_{(2A)}–C_{(5A)}–N_{(6A)}$	-52.2
$C_{(4A)}–N_{(2A)}–C_{(3A)}–N_{(1A)}$	-4.0	$N_{(1A)}–C_{(2A)}–C_{(5A)}–N_{(7A)}$	69.0
$C_{(4A)}–N_{(2A)}–C_{(3A)}–N_{(5A)}$	77.3	$N_{(1A)}–C_{(2A)}–C_{(5A)}–N_{(8A)}$	-174.1
$N_{(4A)}–N_{(5A)}–C_{(3A)}–N_{(1A)}$	-179.8	$N_{(9A)}–C_{(2A)}–C_{(5A)}–N_{(6A)}$	126.2
$N_{(4A)}–N_{(5A)}–C_{(3A)}–N_{(2A)}$	-0.9	$N_{(9A)}–C_{(2A)}–C_{(5A)}–N_{(7A)}$	-112.6
$C_{(1A)}–N_{(5A)}–C_{(3A)}–N_{(1A)}$	-0.1	$N_{(9A)}–C_{(2A)}–C_{(5A)}–N_{(8A)}$	4.3
$C_{(1A)}–N_{(5A)}–C_{(3A)}–N_{(2A)}$	78.7		



3a – d

3 a X = O, R = H, **b** X = S, R = H, **c** X = O, R = *p*-NHAc, **d** X = O, R = *p*-*t*-Bu

The capacity of the trinitromethyl group to undergo replacement by the action of various nucleophilic agents such as amines, alcohols, and azides has been demonstrated for trinitromethyl derivatives of 1,3,5-triazine [1, 6, 7].

Thus, we are the first to report covalent derivatives of 3,5-disubstituted tetrazolo[1,5-*a*]-1,3,5-triazin-7-ones.

EXPERIMENTAL

The ^{1}H and ^{13}C NMR spectra were taken on a Bruker AM-300 spectrometer at 300 and 75 MHz, respectively, and in DMSO-d_6 using HMDS as the internal standard (δ = 0.055 ppm) and TMS (δ = 2.00 ppm), respectively. The IR spectra were taken on a Specord M-80 spectrometer for KBr pellets. The starting compound **1a** was prepared according to our previous procedure [1].

Silver Salt of 5-Trinitromethyltetrazolo[1,5-*a*]-1,3,5-triazin-7-one (1c). A sample of $NaClO_4$ (1.29 g, 0.0105 mol) was added with stirring to a solution of salt **1a** (3.60 g, 0.01 mol) in acetone (25 ml) at 20-25°C and maintained for 2 h. The tetramethylammonium perchlorate precipitate was filtered off and the acetone containing salt **1b** was evaporated. Then, $AgNO_3$ (1.79 g, 0.0105 mol) was added to a solution of the resultant crystalline precipitate in water (25 ml) and maintained for 30 min. The precipitate of salt **1c** was filtered off and dried in the air under black paper. The yield of **1c** was 3.35 g (85%); mp 158°C (dec). IR spectrum, ν, cm^{-1}: 1734, 1626, 1612, 1592, 1572, 1518, 1476, 1368, 1332, 1300, 1168, 1144, 932, 844, 802, 776. Found, %: C 12.26; N 31.92%. $C_4AgN_9O_7$. Calculated, %: C 12.19; N 32.00.

3-Methyl-5-trinitromethyltetrazolo[1,5-*a*]-1,3,5-triazin-7-one (2). A sample of methyl iodide (1.52 ml, 0.03 mol) was added to a suspension of salt **1c** (3.94 g, 0.01 mol) in acetonitrile (40 ml). The reaction mixture was heated for 6 h at 55-65°C. The precipitate of AgI was filtered off and washed on the filter with two 10-ml acetonitrile portions. The combined filtrate was evaporated. The residue was stirred in water. The crystals were filtered off, washed on the filter with water, and dried in the air to give 2.11 g (70%) **2**; mp 159-161°C (dichloroethane). IR spectrum, ν, cm^{-1}: 2880, 1770, 1628, 1596, 1534, 1476, 1420, 1380, 1342, 1296, 1238, 1148, 1056, 1018, 926, 848, 806, 772. ^{1}H NMR spectrum, δ, ppm: 4.15 (3H, s, NCH_3). ^{13}C NMR spectrum, δ, ppm: 158.74 (C–$C(NO_2)_3$), 151.85 (N–C=N), 144.88 (C=O), 34.07 (NCH_3). Found: C 19.97; H 1.06; N 41.79. $C_5H_3N_9O_7$. Calculated, %: C 19.94; H 1.00; N 41.86.

5-Aryloxy- and 5-Arylthio-3-methyltetrazolo[1,5-*a*]-1,3,5-triazin-7-ones 3a-d (General Procedure). A sample of corresponding phenol or thiophenol (0.011 mol) was added with stirring to a solution of **2** (3.01 g, 0.01 mol) in dichloroethane (30 ml) at 20-25°C. Then, maintaining the temperature below 25°C, triethylamine (1.68 ml, 0.012 mol) was added. The reaction mixture was stirred at 20-25°C until all starting **2** had been consumed as indicated by thin-layer chromatography (from about 1 to 3 h). The reaction mixture was evaporated without filtration and the residue was stirred with water. The crystalline precipitate was filtered off, washed on the filter with water, and dried in the air.

3-Methyl-5-phenoxytetrazolo[1,5-*a*]-1,3,5-triazin-7-one (3a) was obtained in 76% yield (1.85 g), mp 250-252°C. IR spectrum, ν, cm^{-1}: 3064, 2964, 1748, 1664, 1654, 1598, 1482, 1456, 1396, 1318, 1252, 1222, 1040, 1016, 816, 774. ^{1}H NMR spectrum, δ, ppm: 3.92 (3H, s, NCH_3), 7.09-7.45 (5H, m, C_6H_5). ^{13}C NMR spectrum, δ, ppm: 168.90 (N=C–O), 151.86 (N–C=N), 146.37 (C=O), 152.36, 129.54, 125.85, 121.41 (C_6H_5O), 32.97 (NCH_3). Found, %: C 49.24; H 3.35; N 34.35. $C_{10}H_8N_6O_2$. Calculated, %: C 49.18; H 3.30; N 34.41.

3-Methyl-5-phenylthiotetrazolo[1,5-*a*]-1,3,5-triazin-7-one (3b) was obtained in 68% yield (1.56 g); mp 238-240°C. IR spectrum, ν, cm^{-1}: 3068, 1734, 1620, 1596, 1498, 1466, 1448, 1434, 1408, 1380, 1348, 1340, 1330, 1280, 1232, 1192, 1138, 1090, 1032, 1012, 948, 768. ^{1}H NMR spectrum, δ, ppm: 3.86 (3H, s, NCH_3), 7.50 (5H, br. s, C_6H_5). ^{13}C NMR spectrum, δ, ppm: 180.32 (N=C–S), 150.24 (N–C=N), 144.25 (C=O), 134.95, 129.78, 129.19, 127.64 (C_6H_5S), 32.97 (NCH_3). Found, %: C 46.10; H 3.18; N 32.36. $C_{10}H_8N_6OS$. Calculated, %: C 46.15; H 3.10; N 32.29.

5-(*p*-Acetylaminophenoxy)-3-methyltetrazolo[1,5-*a*]-1,3,5-triazin-7-one (3c) was obtained in 65% yield (1.96 g); mp 236-258°C. IR spectrum, ν, cm^{-1}: 3304, 3280, 3152, 3080, 2964, 1756, 1666, 1622, 1570, 1520, 1486, 1392, 1330, 1318, 1276, 1254, 1220, 1036, 1016, 980, 968, 852, 774. ^{1}H NMR spectrum, δ, ppm: 1.98 (3H, s, CH_3CO), 3.90 (3H, s, NCH_3), 7.00-7.10 and 7.53-7.63 (4H, both d, *p*-C_6H_4), 9.97 (1H, s, NH). ^{13}C NMR spectrum, δ, ppm: 169.12 ($CH_3\underline{C}ONH$), 168.17 (N=C–O), 152.38 (N–C=N), 146.40 (C=O), 147.02, 137.06, 121.56, 119.87 (*p*-C_6H_4), 32.98 (NCH_3), 23.82 ($NHCO\underline{C}H_3$). Found, %: C 47.78; H 3.65; N 33.63. $C_{12}H_{11}N_7O_3$. Calculated, %: C 47.84; H 3.68; N 32.55.

5-(*p*-*tert*-Butylphenoxy)-3-methyltetrazolo[1,5-*a*]-1,3,5-triazin-7-one (3d) was obtained in 73% yield (2.19 g); mp 248-251°C. IR spectrum, ν, cm^{-1}: 3060, 2960, 2872, 1758, 1518, 1466, 1390, 1312, 1274, 1224, 1184, 1120, 1032, 1016, 944, 850, 812, 776. ^{1}H NMR spectrum, δ, ppm: 1.26 (9H, s, CH_3), 3.93 (3H, s, NCH_3), 6.99-7.10 and 7.37-7.48 (4H, both d, *p*-C_6H_4). ^{13}C NMR spectrum, δ, ppm: 168.98 (N=C–O), 152.37 (N–C=N), 146.39 (C=O), 149.59; 148.20, 126.22, 120.86 (*p*-C_6H_4), 34.16 ($\underline{C}(CH_3)_3$), 32.69 (NCH_3), 31.08 ($C(\underline{C}H_3)_3$). Found, %: C 59.90; H 5.42; N 28.01. $C_{14}H_{16}N_6O_2$. Calculated, %: C 55.99; H 5.37; N 27.98.

X-ray Diffraction Structural Analysis of Compound 2. The unit cell parameters of monoclinic crystals of **2** (from dichloroethane): space group *P*; a = 24.466(5), b = 14.637(3); c = 6.730(1) Å; β = 90.70(3)°; V = 2415.8 $Å^3$; D_c = 1.651 g/cm^3; Z = 8. The intensities of 4019 independent reflections with $I > 2\sigma(I)$ were obtained on a KM-4 automatic four-circle diffractometer (λ = 0.71069 Å, MoKα, graphite monochromator, θ/2θ-scanning, θ_{max} = 27°). The structure was solved by the direct method using the SHELX-86 programs and refined anisotropically by the method of least squares. The hydrogen atoms were located geometrically and only the positional parameters of these atoms were refined. The final *R*-factor was 0.072.

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