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CONDENSED TETRAZOLO-1,3,5-TRIAZINES. 3*. SYNTHESIS OF 3-R-5-TRINITROMETHYL-TETRAZOLO[1,5-*a*]-1,3,5-TRIAZIN-7-ONES

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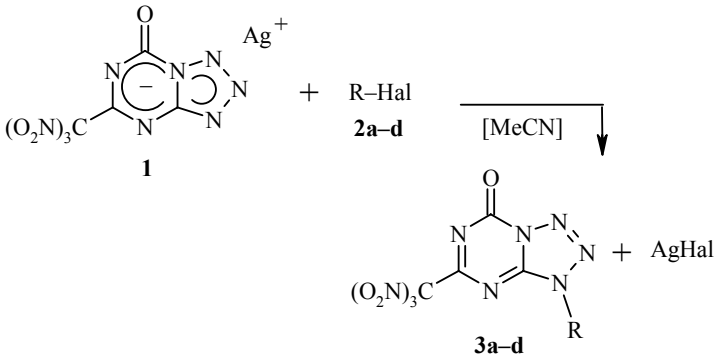
In continuing studies of the properties of the novel heterocyclic system tetrazolo[1,5-*a*]-1,3,5-triazin-7-one [1, 2], we have studied alkylation of 5-trinitromethyltetrazolo[1,5-*a*]-1,3,5-triazin-7-one silver salt (**1**) using structurally different alkylating agents. We have established that in all the studied cases, reaction of the silver salt **1** with halo derivatives **2a-d** leads to formation of the corresponding 3-R-5-trinitromethyltetrazolo[1,5-*a*]-1,3,5-triazin-7-ones **3a-d**.



2 a R = *i*-Pr, Hal = I; **b** R = $(CH_2)_4Me$, Hal = I; **c** R = Bn, Hal = Cl; **d** R = CH_2COAd, Hal = Br;
3a R = *i*-Pr; **b** R = $(CH_2)_4Me$; **c** R = Bn; **d** R = CH_2COAd

Thus despite the structural difference between the alkyl radical and the leaving group (Cl, Br, I), we isolated the products of alkylation at the $N_{(3)}$ atom of the tetrazole ring, as in the case of alkylation of silver salt **1** by methyl iodide in [2].

The IR spectra were recorded on an Avatar 360 ESP spectrophotometer in KBr disks. The ^1H NMR spectra were recorded on a Bruker AM-300 spectrometer (300 MHz) in $CDCl_3$, internal standard TMS.

* For Communication 2, see [1].

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3-R-5-Trinitromethyltetrazolo[1,5-*a*]-1,3,5-triazin-7-ones 3a-d. The corresponding halo derivative **2a-d** (3.0-3.6 mmol) was added to a suspension of silver salt **1** (1.18 g, 3 mmol) in acetonitrile (30 ml). The reaction mass was stirred at a temperature of 20-25°C until compound **1** disappears according to TLC (24-72 h). The corresponding precipitating silver halide was filtered out; the solvent was driven off from the filtrate under reduced pressure using a rotary evaporator. The residue was treated with 10 ml of cold hexane and the crystalline product was filtered out.

Compound 3a. Yield 76%; mp 88-89°C. IR spectrum, ν, cm^{-1}: 3104, 3004, 2960, 2892, 1776, 1612, 1534, 1464, 1404, 1340, 1298, 1214, 1194, 1170, 1138, 1122, 1040, 996, 924, 884, 844, 802, 774. ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 1.62 (6H, d, *J* = 4.8, CH_3); 4.97 (1H, m, CH). Found, %: C 25.62; H 2.27; N 38.18. $C_7H_7N_9O_7$. Calculated, %: C 25.54; H 2.14; N 38.29.

Compound 3b. Yield 84%; mp 61-62°C. IR spectrum, ν, cm^{-1}: 2968, 2936, 2872, 1760, 1620, 1600, 1528, 1474, 1392, 1296, 1156, 1070, 924, 844, 802, 776. ^{1}H NMR spectrum (CDCl3), δ, ppm (*J*, Hz): 0.86 (3H, t, *J* = 7.2, CH_3); 1.30 (4H, m, CH_2); 1.98 (2H, t, *J* = 6.0, CH_2); 4.48 (2H, t, *J* = 6.4, CH_2). Found, %: C 30.19; H 3.17; N 35.36. $C_9H_{11}N_9O_7$. Calculated, %: C 30.26; H 3.10; N 35.29.

Compound 3c. Yield 72%; mp 79-81°C. IR spectrum, ν, cm^{-1}: 3032, 2936, 2898, 1772, 1626, 1604, 1562, 1544, 1532, 1462, 1422, 1360, 1344, 1284, 1252, 1212, 1116, 1072, 1042, 1018, 980, 928, 850, 842, 798, 776. ^{1}H NMR spectrum, δ, ppm: 5.60 (2H, s, CH_2); 7.34 (5H, s, C_6H_5). Found, %: C 34.95; H 1.95; N 33.40. $C_{11}H_7N_9O_7$. Calculated, %: C 35.02; H 1.87; N 33.42.

Compound 3d. Yield 69%; mp 141-143°C. IR spectrum, ν, cm^{-1}: 2924, 2860, 1776, 1728, 1638, 1598, 1564, 1532, 1478, 1464, 1418, 1340, 1294, 1210, 1176, 1150, 1126, 1084, 1022, 984, 968, 948, 924, 848, 802, 772. ^{1}H NMR spectrum ($CDCl_3$), δ, ppm: 1.74, 1.86, and 2.08 (15H, m, Ad); 5.43 (2H, s, CH_2). Found, %: C 41.39; H 3.78; N 27.29. $C_{16}H_{17}N_9O_8$. Calculated, %: C 41.47; H 3.70; N 27.21.

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