Synthesis of 1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 4,6-dioxide and its methyl derivatives*

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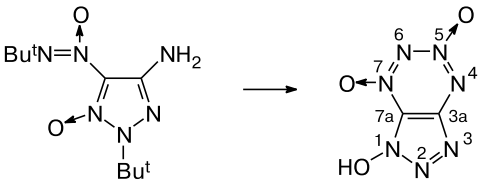
1*H*-[1,2,3]Triazolo[4,5-*e*][1,2,3,4]tetrazine 4,6-dioxide (**3**) was synthesized by reduction of 1-hydroxy-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 5,7-dioxide (**1**) with PCl_3, reduction of 1-methoxy-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 5,7-dioxide (**4**) with $Na_2S_2O_4$, and by the reaction of compound **4** with Et_3N. Both methylation of compound **3** with diazomethane and reaction of Ag-salt of compound **3** with MeI occur at the triazole cycle to give all three possible isomers. The structures of the synthesized compounds were confirmed by ^1H, ^{13}C, ^{14}N, and ^{15}N NMR spectroscopy.

Key words: 1,2,3-triazole 1-oxides, 1,2,3-triazoles, 1,2,3,4-tetrazine 1,3-dioxides, methylation, deoxigenation, ^{14}N and ^{15}N NMR spectroscopy.

Fused 1,2,3,4-tetrazine 1,3-dioxides first synthesized in our research group[1] are potential energetic compounds and attract great attention as the objects for quantum chemistry calculations and properties predicting.[2—6] Therefore, synthesis of these type of compounds and study of their properties are important.

We have recently developed procedure towards triazolotetrazine (TT) **1** (see Ref. 7) *via* reaction of triazole oxide **2** (see Ref. 8) with the $HNO_3/H_2SO_4/Ac_2O$ mixture. Upon the reaction, *tert*-butyl group of the starting compound **2** is cleaved to give target compound **1** (Scheme 1).

Scheme 1

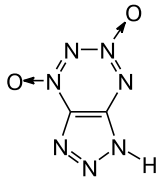


2 **1**

Reagents: HNO_3, H_2SO_4, Ac_2O.

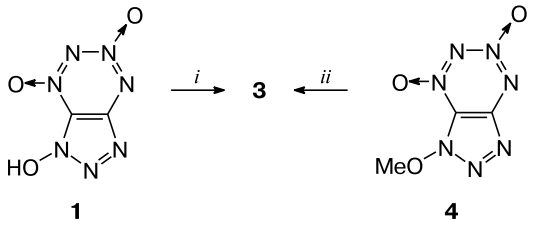
Triazolotetrazine **3** and its derivatives are also of interest as high energy density compounds. In the present work, we describe synthesis of TT **3** and study of its methylation.

Synthesis of TT 3. We developed two synthetic approaches to access TT **3** (Scheme 2).



3

Scheme 2



1 **4**

Reagents: *i*. PCl_3, MeCN; *ii*. $Na_2S_2O_4$, MeOH.

The first approach is the reduction of hydroxy-substituted TT **1** with PCl_3 in anhydrous MeCN at room temperature. The reaction is completed within 18 h to give target TT **3** in 94% yield (see Scheme 2).

The second approach involves the reduction of methoxy-substituted TT **4**** with $Na_2S_2O_4$ in MeOH at room temperature. The reaction is very fast and affords TT **3** in the yield of 89% (see Scheme 2).

To our surprise, treatment of methoxy-substituted TT **4** with strong base also results in TT **3**. We were interested in this unexpected result and studied this reaction in more

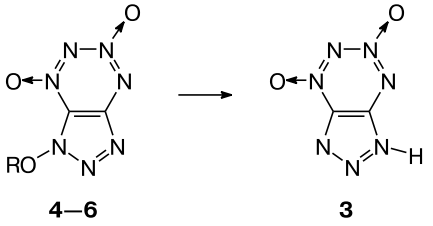
* Dedicated to Academician of the Russian Academy of Sciences V. I. Minkin on the occasion of his 80th birthday.

Published in Russian in *Izvestiya Akademii Nauk. Seriya Khimicheskaya,* No. 3, pp. 0699—0703, March, 2015.

1066-5285/15/6403-0699

detail including in consideration compounds **5** and **6**[9,*] bearing more acidic protons then the methyl group protons (Scheme 3).

Scheme 3



4—6 **3**

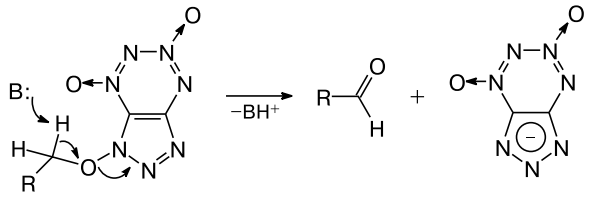
R = Me (**4**), $CH_2C(O)Me$ (**5**), $CH_2C(O)Ph$ (**6**)

Reagents: 1) Et_3N, MeOH; 2) silica gel.

Triethylamine was found to be very convenient as a base. For transformation to occur, 1 equiv. Et_3N is enough for TTs **5** and **6**, and 2 equiv. Et_3N for TT **4**. Triazolotetrazine **3** was obtained in the yields of 77—80%. Thus, this reaction can be regarded as another approach to TT **3**.

The reaction mechanism involves, apparently, the proton abstraction and the O—N bond breaking to give the triazolotetrazine anion and aldehyde (Scheme 4). The reaction proceeds more easily in the case of compounds **5** and **6** bearing acidic methylene protons. At the same time, the triazolotetrazine anion is a very good leaving group and the reaction readily proceeds even in the case of TT **4** bearing the *O*-methyl group.

Scheme 4



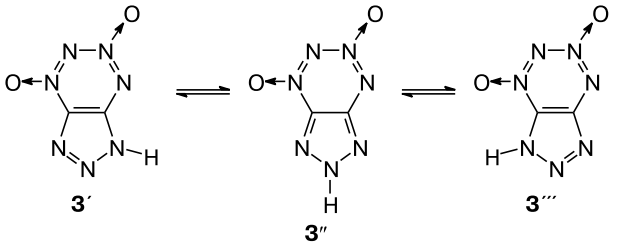
The formation of 2-oxo-2-phenylacetaldehyde (phenylglyoxal) in the reaction of TT **6** with Et_3N (see Scheme 4) was confirmed by its transformation into the corresponding bis-hydrazone upon the reaction with 2,4-dinitrophenylhydrazine. The structure of bis-hydrazone was confirmed by a comparison with a product of counter synthesis.

Earlier,[10,11] similar reactions were described for a series of tetrazole derivatives. Thus, treatment of 1-(2-oxopropoxy)-1*H*-tetrazole derivatives with a K_2CO_3 excess in refluxing EtOH resulted in tetrazole and methylglyoxal.

* Compounds **4—6** were synthesized by alkylation of TT **1** (see Ref. 9).

Prototropic tautomerism of TT 3. Acidic proton of TT **3** can formally be attached to any nitrogen or oxygen of the triazolotetrazine framework. Preliminary quantum chemical calculations (Gaussian 09[12], B3LYP 6-311+G(d,2p) level of theory, gas phase) reveal that tautomers **3′**, **3″**, and **3‴** (Scheme 5) are most thermodynamically favorable. It was found that TT **3′** is more stable than tautomers **3″** and **3‴** by 1.1 and 4.9 kcal mol^{-1}, respectively. Accounting for the solvation effect (H_2O, self-consistent reaction field (SCRF) PCM) does not virtually impact on the relative stability of tautomers. Triazolotetrazine **3′** is more thermodynamically favorable then tautomers **3″** and **3‴** by 1.2 and 4.1 kcal mol^{-1}, respectively.

Scheme 5



3′ **3″** **3‴**

Similar calculations were performed for methylated derivatives **7a—c** (Scheme 6). The results of calculations are close to those obtained for H-form of TT **3**. Triazolotetrazine **7b** is more thermodynamically stable then **7a** and **7c** by 0.3 and 5.3 kcal mol^{-1}, respectively.

Thus, thermodynamic stabilities of tautomers **3′** and **3″** are close. The same conclusion can be drawn for isomers **7a** and **7b**. At the same time, TTs **3‴** and **7c** are relatively less stable.

Methylation of TT 3. Diazomethane methylation of TT **3** leads to a mixture of all three isomers with a ratio of **7a** : **7b** : **7c** = 41 : 33 : 26 (^{1}H NMR data) in 34% total yield (see Scheme 6).

Methylation of Ag-salt **8** with iodomethane in anhydrous MeCN also affords a mixture of three isomers (83% total yield); however, in this case the reaction proceeds more selectively and produces isomers in the ratio of **7a** : **7b** : **7c** = 30 : 56 : 14 (^{1}H NMR data).

In both cases, the lowest content was found for less thermodynamically stable isomer **7c**.

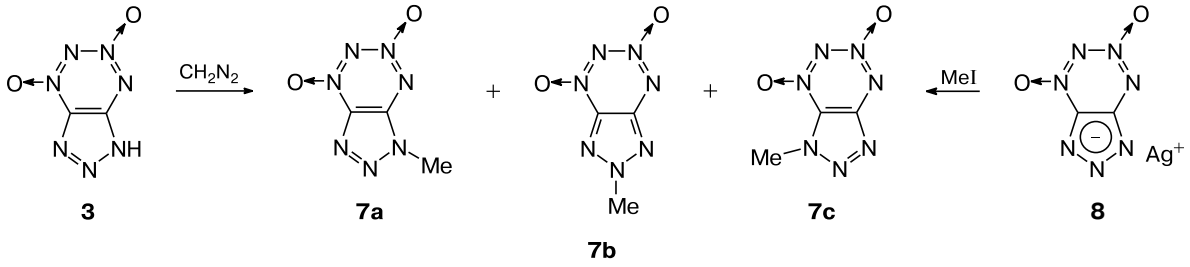
NMR spectroscopy. We succeeded to assign all ^{1}H and ^{13}C NMR signals and observed ^{14}N and ^{15}N NMR signals of TTs **3**, **7a—c**, and **8** (Table 1, Fig. 1). In ^{13}C NMR spectra, the signal of the C(7a) carbon atom bonded to *N*-oxide fragment of tetrazine-dioxide (TDO) cycle is broadened due to spin-spin coupling to ^{14}N. We failed to observe the acidic proton signal for compound **3** by ^{1}H NMR spectroscopy (acetone-d_6 and DMSO-d_6) owing to fast proton exchange. Special NMR techniques (INEPT,

Table 1. ^{1}H, ^{13}C, ^{14}N, and ^{15}N NMR spectra of compounds **3**, **7a**—**c**, and **8**[a]

Compound	NMR								
	^{13}C, δ[b]			^{1}H, δ (J/Hz)[b]	^{14}N, δ ($\Delta\nu_{1/2}$/Hz) [^{15}N, δ][b]				
	C(3a)	C(7a)[c]	R		N(1)	N(2)	N(3)	N(5)	N(7)
3	156.8	137.0	—	—	—[d]	—[d]	—[d]	−43 (60)	−57 (30)
8	156.9	137.6	—	—	—[d]	—[d]	—[d]	−43 (280)	−57 (200)
7a	147.9	137.1	35.1 (CH_3)	4.39 (s, 3 H, CH_3)	—[d]	—[d]	[−161][e]	−39 (40)	−53 (25)
7b[f]	153.3	136.4	46.0 (CH_3)	4.64 (s, 3 H, CH_3)	[−65][e]	[−112][e]	[−65][e]	−42 (50)	−50 (20)
7c	155.5	125.9	37.4 (CH_3)	4.51 (s, 3 H, CH_3)	[−158.8][g]	—[d]	—[d]	−42(55)	−60(20)

[a] Numbering scheme for atoms in compounds **3**, **7a**—**c**, and **8** is given in Fig. 1.
[b] ^{1}H, ^{13}C, ^{14}N, and ^{15}N NMR spectra of TTs **3** and **7a**,**c** were recorded in acetone-d_6, and spectra of TT **8** were run in DMSO-d_6.
[c] Signal of the C(7a) atom bonded to the N→O group of TDO cycle is broadened.
[d] No signals were observed.
[e] ^{1}H—^{15}N HSQC data.
[f] See Ref. 7
[g] INEPT data: δ −158.8, $^{2}J_{N(1),Me}$ = 3.65 Hz.

Scheme 6



^{1}H—^{15}N HSQC, ^{1}H—^{13}C HMBC, ^{1}H—^{13}C HSQC) were applied to evaluate the positions of the substituent at the N atom of 1,2,3-triazole moiety. ^{14}N NMR spectra of compounds **3**, **7a**—**c**, and **8** contain signals of the N(5) and N(7) atoms of TDO cycle at δ −(40—60) ($\Delta\nu_{1/2}$ = = 25—60 Hz). In ^{15}N NMR (^{1}H—^{15}N HSQC) spectra of TTs **7a**,**c**, the signals of the N(1) (compound **7a**) and N(3) (compound **7c**) of 1,2,3-triazole cycle, which are directly bonded to the methyl group, were found about δ −160. In the case of TT **7b**, the N(2) atom directly bonded to the methyl groups resonates at δ −112. This large difference in the chemical shifts can be used to distinguish isomers.

Thermal stability of TTs were examined by monitoring the behavior of compounds upon heating with a Kofler apparatus. Although this method is not accurate, it serves for drawing a number of preliminary conclusions.

H-Form of TT **3** melts with decomposition at 150—152 °C and has inferior stability then hydroxytriazolotetrazine **1** (m.p. 180—185 °C (decomp.)[7]). Stability of Ag-salt **8** is higher as compared to H-form of compound **3** being comparable to the stability of Ag-salt of hydroxytriazolotetrazine **1** (m.p. >197 °C (decomp.)[7]).

Triazolotetrazines **7a**—**c** melt with decomposition over a temperature range of ~200—220 °C (Table 2). These compounds are noticeably more stable then structurally related furazano-1,2,3,4-tetrazine 1,3-dioxide melting with decomposition at 112—114 °C.[13,14]

In summary, we developed versatile procedures to access TT **3** by reduction of TT **1** and by treatment of

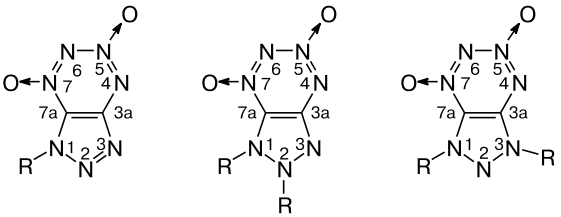


Fig. 1. Numbering scheme for compounds **3**, **7a**—**c**, and **8** used for the description of the NMR spectra.

Table 2. Melting points for TT **3**, **7a—c**, and **8**

Compound	M.p. (decomp.)/°C
3	150—152
8	182—192
7a	213—214
7b	198—199*
7c	200—201

* See Ref. 7.

O-substituted TTs **4—6** with bases. It is found that both TT **3** and Ag-salt **8** react non-selectively with diazomethane to afford a mixture of three isomers.

Experimental

^1H, ^{13}C, ^{14}N, and ^{15}N NMR spectra were run with a Bruker DRX-500 spectrometer (working frequencies of 500.1, 125.8, 36.1, and 50.7 MHz, respectively). The chemical shifts are given in the δ scale relative to Me_4Si (^1H, ^{13}C) and $MeNO_2$ (^{14}N, ^{15}N, internal standard), strong field shifts are negative. Electron impact mass spectra (70 eV) were recorded with a Kratos MS-300 instrument. High resolution mass spectra were obtained on a Bruker micrOTOF II instrument. The course of the reactions was monitored by TLC on precoated Merck 60 F_{254} plates. Silica gel Merck 40—63 was used for column chromatography. Melting points are given uncorrected. A solution of diazomethane in Et_2O,[15] the Brady reagent (a solution of 2,4-dinitrophenyl hydrazine in H_2SO_4),[16] and 1-hydroxy-1*H*-[1,2,3]triazolo[4,5-*e*]-[1,2,3,4]tetrazine 5,7-dioxide **1**)[7,*] were obtained by the known procedures.

Caution! All compounds synthesized in the present work are sensitive to impact and friction and have to be handled as explosives.

Synthesis of 1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 4,6-dioxide (3) by the reaction of 1-hydroxy-1*H*-[1,2,3]triazolo[4,5-*e*]-[1,2,3,4]tetrazine 5,7-dioxide (1) with PCl_3. To a stirred solution of hydroxytriazolotetrazine monohydrate **1** (61 mg, 0.32 mmol) in anhydrous MeCN (2.5 mL), PCl_3 (132 mg, 0.96 mmol) was added dropwise at 25 °C under argon. The reaction mixture was stirred at this temperature for 18 h until complete consumption of the starting TT **1** (TLC monitoring) and the solvent was removed *in vacuo*. Purification of the residue by column chromatography (elution with EtOAc) afforded triazolotetrazine **3** in the yield of 47 mg (94%); yellow crystals well soluble in polar solvents (MeCN, H_2O, MeOH). MS (ESI), *m/z*: 154.0114 $[M - H]^-$. $C_2N_7O_2$. Calculated: 154.0108 $[M - H]^-$. IR (KBr), ν/cm^{-1}: 1636 s, 1612 s, 1601 s, 1484 w, 1436 s, 1388 s, 1340 s, 1312 s. Found (%): C, 15.79; H, 0.91; N, 58.51. $C_2HN_7O_2$. Calculated (%): C, 15.49; H, 0.65; N, 63.23. Note that content of nitrogen is often underestimated upon microanalysis of polynitrogen compounds (see, for instance, Refs 17 and 18).

Synthesis of 1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 4,6-dioxide (3) by the reaction of 1-methoxy-1*H*-[1,2,3]triazolo-[4,5-*e*][1,2,3,4]tetrazine 5,7-dioxide (4) with $Na_2S_2O_4$. To a vigorously stirred solution of TT **4** (198 mg, 1.07 mmol) in 95% MeOH (15 mL), $Na_2S_2O_4$ (186 mg, 1.07 mmol) was added at 25 °C. The reaction mixture was stirred at this temperature for 15 min and precipitate was filtered off. Small amount of silica gel (Merk 40—63) was added to the filtrate, and the volatiles were removed *in vacuo*. Triazolotetrazine **3** was isolated by silica gel column chromatography (elution with AcOEt—MeOH, 4 : 1) in the yield of 140 mg (85%), yellow crystals.

Synthesis of TT 3 by the reaction of 1-R-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 4,6-dioxides 4—6 with Et_3N (general procedure). To a stirred solution of *O*-alkyl derivative **4**, **5** or **6** (1 mmol) in MeOH, Et_3N (2 mmol for TT **4** or 1 mmol for TTs **5** and **6**) was added dropwise at 25 °C. The reaction mixture was stirred at this temperature until complete consumption of the starting TTs **4—6** (TLC monitoring), the solvent was removed *in vacuo*. Triazolotetrazine **3** was purified by silica gel column chromatography (elution with EtOAc—MeOH, 5 : 1). The yields of TT **3** were as follows: 77% from TT **4** (R = Me), 80% from TT **5** (R = $CH_2C(O)Me$), and 80% from TT **6** (R = $CH_2C(O)Ph$).

Synthesis of phenylglyoxal bis(dinitrophenyl)hydrazone. To a vigorously stirred solution of TT **6** (30 mg, 0.104 mmol) in MeCN (2 mL), a solution of triethylamine (14.5 μL, 10.5 mg, 0.104 mmol) in MeCN (0.2 mL) was added at 25 °C. The reaction mixture was stirred at this temperature until complete consumption of the starting TT **6** (TLC monitoring). Then freshly prepared Bradly reagent (1 mL) was added and the mixture was kept for 20 min. Precipitated bishydrazone was collected by filtration, washed with chilled MeCN (2×0.5 mL), and dried. 2-[2-(2,4-Dinitrophenyl)hydrazono-1-phenylpropan-1-one was obtained in the yield of 34 mg (58%), red brown crystals. From mother liquor, TT **3** was isolated by silica gel column chromatography (elution with petroleum ether—EtOAc, 3 : 1 (removal of non-polar impurities), then EtOAc—MeOH, 4 : 1) in the yield of 8 mg (50%), yellow crystals.

1*H*-[1,2,3]Triazolo[4,5-*e*][1,2,3,4]tetrazine 4,6-dioxide Ag-salt (8). *Caution! Ag-Salt is very sensitive to impact and friction and has to be handled as a primary explosive.* To a vigorously stirred solution of TT **3** (166 mg, 1.07 mmol) in H_2O (3 mL), $AgNO_3$ (272 mg, 1.6 mmol) was added at 25 °C. The reaction mixture was stirred at 25 °C for 5 min and the precipitate was collected using porous metal funnel, washed with H_2O (3×5 mL) and dried *in vacuo* over P_4O_{10}. Ag-Salt **8** was obtained in the yield of 206 mg (72%); olive-colored crystals.

Diazomethane methylation of TT 3. To a suspension of TT **3** (130 mg, 0.84 mmol) in EtOAc (5 mL), a solution of CH_2N_2 in Et_2O was added portionwise until complete consumption of the starting compound (TLC monitoring). Purification by silica gel column chromatography (elution with petroleum ether—AcOEt, 1 : 1) afforded a mixture of three isomers **7a**, **7b**, and **7c** in the ratio of 41: 33 : 26 (^1H NMR data), yield of 48 mg (34%), yellow crystals. The mixture of isomers were resolved as follows: first, chromatography using $CHCl_3$ as an eluent afforded TT **7c** (5 mg, lemon-colored crystals) and a mixture of TTs **7a** and **7b** (27 mg, light yellow crystals), subsequent resolution of the mixture of TTs **7a** and **7b** with benzene as a solvent afforded TT **7b** (6 mg, yellow crystals) and TT **7a** (7 mg, light yellow crystals).

* Compound **1** synthesized by the described procedure is a monohydrate, which dehydrates at prolonged drying over P_4O_{10} *in vacuo*. Microanalysis data for 1-hydroxy-1*H*-[1,2,3]triazolo-[4,5-*e*][1,2,3,4]tetrazine 5,7-dioxide monohydrate: found (%): C, 13.03; H, 1.68; N, 45.54. $C_2H_3N_7O_4$. Calculated (%): C, 12.70; H, 1.60; N, 51.85.

Physicochemical and spectral data for triazolotetrazine **7b** are in agreement with those published previously.[7]

1-Methyl-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 4,6-dioxide (7a). MS (EI), *m/z*: 169 $[M]^+$. MS (ESI), *m/z*: 192.0247 $[M + Na]^+$. $C_3H_3N_7O_2$. Calculated: 192.0240 $[M + Na]^+$.

1-Methyl-1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 5,7-dioxide (7c). MS (EI), *m/z*: 169 $[M]^+$, 125 $[M - N_2O]^+$, 81 $[M - 2\,N_2O]^+$. MS (ESI), *m/z*: 192.0243 $[M + Na]^+$. $C_3H_3N_7O_2$. Calculated: 192.0240 $[M + Na]^+$.

Methylation of 1*H*-[1,2,3]triazolo[4,5-*e*][1,2,3,4]tetrazine 4,6-dioxide Ag-salt (8) with iodomethane. To a vigorously stirred suspension of Ag-salt **8** (45 mg, 0.172 mmol) in MeCN (1 mL), MeI (122 mg, 0.860 mmol) was added at 25 °C. The reaction mixture was stirred at this temperature for 12 h, the precipitate was collected by filtration, and washed with MeCN (3×2 ml). Removal of the solvent *in vacuo* afforded a mixture of three isomers **7a**, **7b**, and **7c** in the ratio of 30 : 56 : 14 (^{1}H NMR data), yield of 24 mg (83%), yellow crystals. The isomers were resolved as above described.

This work was financially supported by the Russian Science Foundation (Project No. 14-50-00126).

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Received January 15, 2015