SYNTHESIS AND PROPERTIES OF N-[ω-(p-TOLUENESULFONOXYL)ALKYL]URACILS

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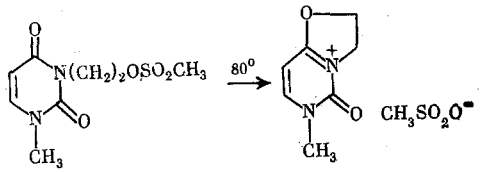
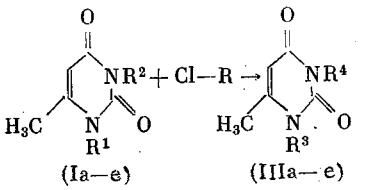
While studying pyrimidones with various functional groups in the N-alkyl radical we synthesized a number of N-[ω-(p-toluenesulfonoxy)alkyl]uracils and studied some of their chemical transformations. The literature data is scanty on the intramolecular cyclization of such compounds to give labile bicyclic quaternary salts [1, 2]; thus, 1-methyl-3-[β-(methylsulfonoxy)ethyl]uracil when heated undergoes cyclization by the following scheme:



A similar cyclization was established for N-(3-bromopropyl)uracils when they are reacted with the Na salt of p-toluenesulfonamide [2].

The present study was undertaken in order to ascertain the ability of the tosylate derivatives of uracil to undergo intramolecular cyclization. Tosylates (IIIa-e) were obtained by the reaction of N-(ω-hydroxyalkyl)uracils (Ia-e) with p-toluenesulfonyl chloride (II) by the following scheme:

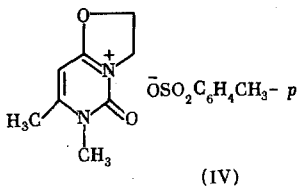


(Ia—e) (IIIa—e)

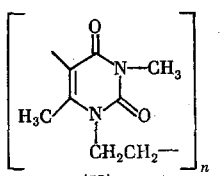
$R^1 = CH_3$, $R^2 = (CH_2)_2OH$ (Ia);
$R^1 = (CH_2)_2OH$, $R^2 = CH_3$ (Ib);
$R^1 = R^2 = (CH_3)_2OH$ (Ic);
$R^1 = CH_3$, $R^2 = (CH_2)_3OH$ (Id);
$R^1 = (CH_2)_3OH$, $R^2 = CH_3$ (Ie)

$R^3 = CH_3$, $R^4 = (CH_2)_2OR$ (IIIa);
$R^3 = (CH_2)_2OR$, $R^4 = CH_3$ (IIIb);
$R^3 = R^4 = (CH_2)_2OR$ (IIIc);
$R^3 = CH_3$, $R^4 = (CH_2)_3OR$ (IIId);
$R^3 = (CH_2)_3OR$, $R^4 = CH_3$ (IIIe);
$R = SO_2C_6H_4CH_3$-*p*.

Tosylates (IIIb, c) are formed in 40-60% yields by running the reaction in triethylamine (TEA) at ∿30°C. A sharp decrease in the yield, especially in the case of (Ic), occurs when the temperature exceeds 30°. Tosylate (IIIe) can be obtained only by running the reaction in abs. CH_3CN in the presence of TEA at −5 to −10°. In general, (IIId) cannot be isolated under these conditions, and instead of (IIIa) the bicyclic salt (IV) is formed in ∿7% yield.



(IV)



(V)

Tosylates (IIIb, c, e) are crystalline compounds that are soluble in $CHCl_3$, moderately soluble in benzene, and insoluble in water. Salt (IV) is a crystalline compound that is soluble in water or alcohol, and insoluble in benzene, ether or $CHCl_3$. The IR spectra of (IIIb, c, e) lack the νOH and νNH bands; those of νC=O appear at 1660-1710 cm^{-1} (two bands); the position of the νSO_2 bands at 1180-1200 and 1360-1365 cm^{-1} is characteristic for sulfonic

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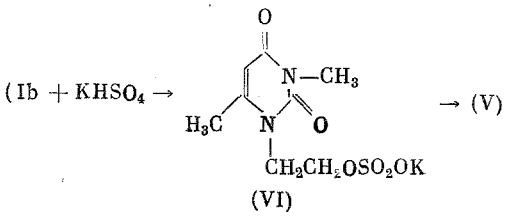
acid esters [3]. The long-wave absorption maxima in the UV spectra of (IIIb, c, e) lie in the 259-263 nm region, which is characteristic for 1,3-bis-substituted uracils [4]. In harmony with the structure, the IR spectrum of (IV) has one νC=O band at 1745 cm^{-1} and an intense band at 1610 cm^{-1}, which belongs to an aromatic pyrimidine ring. The position of the νSO_2 bands at 1020-1035 and 1190-1220 cm^{-1} (doublets) is characteristic for the ν_s and ν_{as} of sulfonic acid salts [3]; νOH and νNH are absent. The long-wave maximum of the UV spectrum lies at 294 nm, which is in agreement with [1].

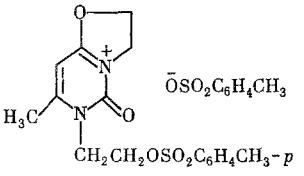
Tosylates (IIIb, c, e) could not be converted to the corresponding bicyclic salts, analogous to (IV). When (IIIb) is heated at 160-165°, it forms an infusible and insoluble oligomer, whose elemental analysis corresponds to the structural unit of (V). The IR spectrum of (V) has bands at 1670 and 1710 cm^{-1} (C=O), while the νNH, OH, and SO_2 bands are absent, and also the vibrations of the C–H bond at the C^5 atom of the pyrimidine ring (usually 3060-3090 cm^{-1}). Similar results are also obtained when tosylate (IIIe) is heated. The structure of (V) is also confirmed by the fact that (V) is also formed when (Ib) is heated in molten $KHSO_4$ at 240-250°, probably via the intermediate formation of (VI):



(VI)

The IR spectra and properties of the (V) compounds, obtained in these reactions, are identical. The formation of (VI) is postulated on the basis that when 6-methyluracil is heated in $KHSO_4$ under analogous conditions it forms the K salt of 6-methyluracil-5-sulfonic acid (VII), which was identified via elemental analysis and the presence of the stretching vibrations of C=O, NH, and SO_2 in the IR spectrum of (VII). In the case of (Ib) the condensation initially takes place at the hydroxyethyl radical.

When tosylate (IIIc) is heated in an ampul at 130°, it forms a glassy mass, which is soluble in CH_2Cl_2, CH_3CN, or water. The NH_4 salt of p-toluenesulfonic acid deposits when it is dissolved in CH_3CN. This testifies to the complete destruction of the pyrimidine ring with the liberation of NH_3, although, by analogy with (IIIa), the formation of the bicyclic salt (VIII) could be expected. However, it is possible that the presence of a second complex substituent at N^1 of the pyrimidine ring substantially destabilizes the (VIII) molecule.

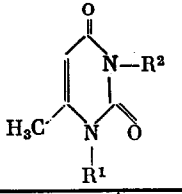


(VIII)

This conclusion is also confirmed by the fact that when (IIIb) is heated with excess NaBr in methyl ethyl ketone (MEK) it quantitatively forms 3,6-dimethyl-1-(β-bromomethyl)uracil (IX), whereas 1,3-bis(β-bromoethyl)uracil is not formed from (IIIc) under analogous conditions.

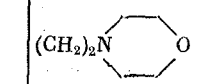
As a result, on the basis of the above said, and also the data given in [1, 2], it may be assumed that the intramolecular cyclization is realized predominantly under the conditions where the alkyl radical, containing a functional group, is found on the N^3 atom of the pyrimidine ring. A greater possibility for delocalization of the electrons in the bicyclic salt exists in this position than in the structures with the substituent on N^1. Nevertheless, it is impossible to completely exclude the possibility of the intramolecular cyclization of tosylates of the (IIIb) type to the corresponding salts, since even for the N^3-derivatives the cyclic and acyclic forms are found in a tautomeric equilibrium that is very sensitive to external effects [1]. For derivatives of the (IIIb) type this equilibrium can be shifted more toward the acyclic form. The intermediate formation of bicyclic salt (X) can be trapped by reacting tosylate (IIIb) with amines. This possibility is determined by salt (X) having two electrophilic centers in the oxazole ring that are capable of undergoing nucleophilic attack (designated by asterisks). The formation of the hypothetical iminopyrimidine (XI) is probably only by attack of the amine on the C^2 atom of the bicyclic salt (X), while amino

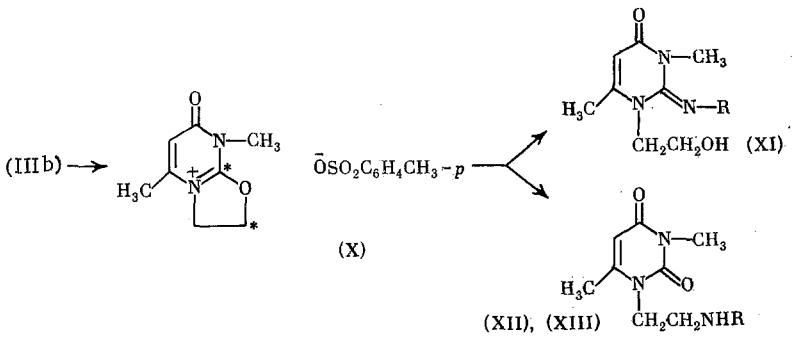
TABLE 1



Compound	R^1	R^2	mp, °C (solvent)	Yield, %	Found/Calculated, %			Empirical formula
					C	H	N	
(Id)	CH_3	$(CH_2)_3OH$	72–73 (n-butanol)	40,0	54,30 / 54,53	7,37 / 7,12	14,11 / 14,13	$C_9H_{14}N_2O_3$
(Ie)	$(CH_2)_3OH$	CH_3	81–82 (benzene)	55,0	54,35 / 54,53	7,29 / 7,12	14,16 / 14,13	$C_9H_{14}N_2O_3$
(IIIb)	$(CH_2)_2OR$ *	CH_3	158–160 (benzene)	80,0	53,10 / 53,24	5,66 / 5,36	8,13 / 8,28	$C_{15}H_{18}N_2O_5S$
(IIIc)	$(CH_2)_2OR$	$(CH_2)_2OR$	126–128 (benzene)	41,0	52,87 / 52,86	4,81 / 5,01	5,15 / 5,36	$C_{23}H_{26}N_2O_8S_2$
(IIIe)	$(CH_2)_3OR$	CH_3	108–109 (benzene)	39,0	53,10 / 53,53	5,66 / 5,72	8,13 / 7,95	$C_{16}H_{20}N_2O_5S$
(IV)	Bicyclic salt		185–187 (decompn.)	7,5	53,20 / 53,24	5,30 / 5,36	8,30 / 8,28	$C_{15}H_{18}N_2O_5S$
(V)	Oligomeric product		Decompn. > 300 (water)	81,0	57,32 / 57,81	6,16 / 6,06	16,77 / 16,85	$C_8H_{10}N_2O_2$
(VII)	K salt of 6-methyl-uracil-5-sulfonic acid		Decompn. > 350 (water)	54,5	21,44 / 21,42	2,93 / 3,23	9,79 / 10,00	$C_5H_9N_2O_7SK$
(IX)	$(CH_2)_2Br$	CH_3	93–95 (ether)	85,0	38,82 / 38,80	4,23 / 4,46	11,13 / 11,30	$C_8H_{11}N_2O_2Br$

TABLE 1 (Continued)

Compound	R^1	R^2	mp, °C (solvent)	Yield, %	Found/Calculated, %			Empirical formula
					C	H	N	
(XII)	$(CH_2)_2NHC_6H_5$	CH_3	176–179 (benzene)	71,0	64,77 / 64,86	6,50 / 6,56	15,82 / 16,21	$C_{14}H_{17}N_3O_2$
(XIII)	$(CH_2)_2NH(CH_2)_2OH$	CH_3	112–114 (benzene)	30,0	52,81 / 52,86	7,36 / 7,48	18,60 / 18,50	$C_{10}H_{17}N_3O_3$
(XVII)		CH_3	83–85 (benzene–hexane)	69,5	56,44 / 56,91	7,65 / 7,50	16,61 / 16,60	$C_{12}H_{19}N_3O_3$
(XVIII)	$(CH_2)_2NHC_6H_5$	$(CH_2)_2NHC_6H_5$	123–125 (benzene–hexane)	38,0	69,68 / 69,23	6,82 / 6,68	15,57 / 15,68	$C_{24}H_{24}N_4O_2$
(XIX)	$(CH_2)_2NH_2$	$(CH_2)_2NH_2$	216–220 (acetone)	36,5	50,88 / 51,20	7,34 / 7,56	26,05 / 26,40	$C_9H_{16}N_4O_2$
(XX)	CH_3	$(CH_2)_2NHC_6H_5$	162–163,5 (benzene–hexane)	76,6	64,56 / 64,86	6,84 / 6,56	15,61 / 16,21	$C_{14}H_{17}N_3O_2$
(XXI)	$(CH_2)_2\overset{+}{N}(C_2H_5)_3 \cdot RO^-$	CH_3	112–116 (methyl ethyl ketone)	64,5	54,68 / 55,10	7,61 / 7,66	9,31 / 9,20	$C_{21}H_{33}N_3O_5S \cdot H_2O$
(XXII)	$(CH_2)_2OC_6H_{13}$-*n*	CH_3	n_D^{20} 1,5003	88,5	62,55 / 62,80	9,36 / 8,95	10,27 / 10,43	$C_{14}H_{24}N_2O_3$
(XXIII)	$(CH_2)_2SC_4H_9$-*n*	CH_3	n_D^{20} 1,5440	85,5	56,39 / 56,30	7,93 / 7,82	11,15 / 10,92	$C_{12}H_{20}N_2O_2S$



derivatives (XII) and (XIII) can be formed both via salt (X) (attack on C^5) and by direct attack of the amine on the β-C atom of the alkyl radical of (IIIb).

The reaction of (IIIb) with aniline (XIV), monoethanolamine (XV), and morpholine (XVI) gives the corresponding 1-(β-anilinoethyl)-(XII), 1-[β-(2-hydroxyethylamino)ethyl]-(XIII), and 1-(β-N-morpholinylethyl)-3,6-dimethyluracils (XVII). In a similar manner, the reaction of tosylate (IIIc) with (XIV) and NH_3 respectively gave 1,3-bis(β-anilinoethyl)-(XVIII) and 1,3-bis(β-aminoethyl)-6-methyluracils (XIX). The formation of imino derivatives in this manner could not be recorded. These results also do not exclude the progress of the indicated reactions via the step of intramolecular cyclization. In addition, the reaction of authentic salt (IV) with (XIV) also leads to 3-(β-anilinoethyl)-1,6-dimethyluracil (XX), i.e., the amine attacks the C^5 atom of the oxazole ring of (IV). The structures of (XII)-(XIII) and (XVII)-(XX) were confirmed via the IR spectra. The spectra of the compounds each have two C=O bands at 1660-1710 cm^{-1} and NH bands at 3320-3400 cm^{-1}; (XVIII) has a doublet at 3360 and 3400 cm^{-1}, while (XIX) has two broad bands with maxima at 3200 (ν_s) and 3370 cm^{-1} (ν_{as}). In addition, (XIX) has two δNH_2 bands at 1550 and 1580 cm^{-1}. In the spectrum of the solid (XIII) the N–H and O–H appear as one band at 3300 cm^{-1}, while in CH_2Cl_2 solution (1 mm) are observed the bands of a free (3630 cm^{-1}) and bound (3490 cm^{-1}) O–H and the bands of N–H (3320 and 3370 cm^{-1}).

When (IIIb) is heated in TEA, n-hexanol or n-butyl mercaptan it respectively forms β-(3,6-dimethyl-2,4-dioxo-1,2,3,4-tetrahydro-1-pyrimidinyl)ethyltriethylammonium tosylate (XXI) and the 1-β-(n-hexoxy)ethyl-(XXII) or 1-β-(n-butylthio)ethyl-3,6-dimethyluracil (XXIII). In harmony with the structures, the IR spectra of these compounds each have two νC=O bands at 1660-1710 cm^{-1}, while the νN–H and νO–H bands are absent. The IR spectrum of (XXI) also has νSO_2 bands in the region characteristic for sulfonic acid salts [3].

EXPERIMENTAL

The IR spectra were taken on a UR-10 spectrophotometer, the solids as Nujol mulls, and the liquids as a film between KBr plates. The UV spectra were taken on a Specord UV-VIS spectrophotometer. The constants of the obtained compounds are given in Table 1.

1,6-Dimethyl-3-(γ-hydroxypropyl)uracil (Id) and 3,6-Dimethyl-1-(γ-hydroxypropyl)uracil (Ie). To the dry Na salt of 1,6-dimethyluracil (from 11 g of 1,6-dimethyluracil and 1.8 g of Na in 400 ml of i-PrOH) in 300 ml of abs. DMF was added 9.6 g of 1,3-pyropylene chlorohydrin and the mixture was stirred at 80-85° to pH 7, filtered, and the filtrate was evaporated in vacuo. The residue was heated in $CHCl_3$, filtered, and the filtrate was evaporated to give 6.2 g of (Id).

In a similar manner, from 11 g of 3,6-dimethyluracil, 1.8 g of Na, and 9.6 g of 1,3-propylene chlorohydrin we obtained 8.5 g of (Ie).

1-[β-(p-Toluenesulfonoxy)propyl]-3,6-dimethyluracil (IIIe). With stirring, to 4.3 g of (Ie) and 2.2 g of abs. triethylamine (TEA) in 100 ml of abs. MeCN was added in drops, at −5 to −10°, a solution of 4.1 g of o-toluenesulfonyl chloride (II) in 30 ml of MeCN, and the mixture was stirred for 1 h and then heated to 20°. The precipitate was filtered and the filtrate was evaporated in vacuo. To the residue was added 100 ml of abs. benzene, the mixture was left standing 1 h, the precipitate was filtered, and the filtrate was treated with active carbon, filtered, and evaporated in vacuo to give 3.1 g of (IIIe).

1-[β-(p-Toluenesulfonoxy)ethyl]-3,6-dimethyluracil (IIIb). With stirring, to a suspension of 20 g of 1-(β-hydroxyethyl)-3,6-dimethyluracil in 200 ml of TEA was gradually added

20.7 g of (II) (temperature kept below 30°), and the precipitate was filtered, treated with water, filtered, and recrystallized from benzene to give 29.3 g of (IIIb).

In a similar manner, from 20 g of 1,3-bis(β-hydroxyethyl)-6-methyluracil and 35.6 g of (II) in 300 ml of TEA we obtained 20 g of 1,3-bis[β-(p-toluenesulfonoxy)ethyl]-6-methyluracil (IIIc).

5-Oxo-6,7-dimethyl-5,6-dihydrooxazolidino[3,2-c]pyrimidinium Tosylate (IV). To a solution of 3.4 g of 3-(β-hydroxyethyl)-1,6-dimethyluracil and 3.5 g of (II) in 50 ml of abs. MeCN at 20° was added 1.9 g of abs. TEA in 0.5 h. The mixture was stirred for 3 h, evaporated in vacuo to 1/3 volume, and 100 ml of abs. ether was added. The obtained precipitate was filtered and the filtrate was evaporated. To the residue was added 50 ml of abs. benzene and the precipitate was filtered, boiled in benzene, and filtered to give 0.45 g of (IV).

Heating of Tosylate (IIIb). Compound (IIIb) (5 g) was heated in an ampul for 6 h at 160-165°. The mass was cooled, treated with water, and the precipitate was filtered, boiled in water, and filtered to give 2 g of (V).

K salt of 6-Methyluracil-5-sulfonic Acid (VII). 6-Methyluracil (50 g) was heated for 3 h in 150 g of molten $KHSO_4$ at 245-250°. The mass was treated with water, and the precipitate was filtered and recrystallized from water using active carbon to give 48 g of (VII).

1-(β-Bromoethyl)-3,6-dimethyluracil (IX). A mixture of 10 g of (IIIb) and 10 g of NaBr in 100 ml of methyl ethyl ketone (MEK) was refluxed for 15 h, filtered, and the filtrate was evaporated in vacuo. The residue was treated with 150 ml of ether, filtered, and the filtrate was evaporated to 1/2 volume to give 6.2 g of (IX).

1-(β-Anilinoethyl)-3,6-dimethyluracil (XII). A mixture of 5 g of (IIIb) and 2.7 g of (XIV) in 50 ml of abs. benzene was refluxed for 3 h, and the precipitate was filtered, washed with hot benzene, the filtrate was evaporated, and the residue was recrystallized from benzene to give 2.8 g of (XII).

1-[β-(2-Hydroxyethylamino)ethyl]-3,6-dimethyluracil (XIII). A mixture of 5 g of (IIIb) and 1.8 g of (XV) in 50 ml of abs. n-butanol was refluxed for 5 h, cooled, 300 ml of ether was added, and the solution was decanted from the separated oil, which crystallized on standing. The residue was treated with boiling benzene, filtered, the filtrate was evaporated, and the residue was recrystallized from benzene to give 1 g of (XIII).

1-(β-N-Morpholinylethyl)-3,6-dimethyluracil (XVII). A mixture of 5 g of (IIIb) and 2.6 g of (XVI) in 50 ml of abs. benzene was refluxed for 6 h, filtered, the precipitate was washed with benzene, the filtrate was evaporated, and the residue was recrystallized from a 1:1 benzene–petroleum ether mixture to give 2.6 g of (XVII).

1,3-Bis(β-anilinoethyl)-6-methyluracil (XVIII). A mixture of 3 g of (IIIc) and 5 ml of (XIV) was heated for 1 h at 70°, after which 50 ml of abs. benzene was added, the separated salt was filtered, and the filtrate was evaporated in vacuo. The residue was treated with ether, and the solution was decanted and evaporated to 2/3 volume to give 0.8 g of (XVIII).

1,3-Bis(β-aminoethyl)-6-methyluracil (XIX). A stream of NH_3 was passed into a solution of 5 g of (IIIc) in 150 ml of n-propanol for 4 h at 20°, the ammonium salt was filtered, and the filtrate was evaporated in vacuo. The residue was treated with acetone, and the solution was decanted from the insoluble residue, evaporated to 2/3 volume, and filtered to give 0.45 g of (XIX).

3-(β-Anilinoethyl)-1,6-dimethyluracil (XX). A mixture of 0.34 g of (IV) and 3 g of (XIV) was heated for 3 h at 40-60°, 150 ml of a 2:1 ether–petroleum ether mixture was added, the obtained precipitate was filtered, treated with boiling benzene, filtered, the filtrate was evaporated, and the residue was recrystallized from a 4:1 benzene–petroleum ether mixture to give 0.2 g of (XX).

β(3,6-Dimethyl-2,4-dioxo-1,2,3,4-tetrahydro-1-pyrimidinyl)ethyltriethylammonium Tosylate (XXI). A solution of 10 g of (IIIb) in 50 ml of abs. TEA and 60 ml of abs. benzene was refluxed for 10 h, the precipitate was filtered, washed with ether, treated with MEK in the cold and the insoluble portion was filtered to give 8.5 g of (XXI) (crystallohydrate·$1H_2O$).

1-(β-n-Hexoxyethyl)-3,6-dimethyluracil (XXII). A solution of 5 g of (IIIb) in 30 ml of n-hexanol was refluxed for 8 h. The mass was dissolved in 200 ml of benzene, and the solution was washed with Na_2CO_3 solution, treated with active carbon, filtered, evaporated in vacuo, and dried at 150° (0.01 mm) to give 3.8 g of (XXII) as an oil.

1-(β-n-Butylthioethyl)-3,6-dimethyluracil (XXIII). A solution of 5 g of (IIIb) in 10 ml of n-butyl mercaptan was refluxed for 8 h then poured into KOH solution. The separated oil was extracted with benzene, and the extract was washed with water, dried over Na_2SO_4, and evaporated in vacuo to give 3.5 g of (XXIII) as an oil.

CONCLUSIONS

The possibility of N-(ω-hydroxyalkyl)uracil tosylates undergoing intramolecular cyclization to give bicyclic pyrimidinium salts was studied.

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SYNTHESIS AND PROPERTIES OF PYRIMIDINYLALKYLSULFONAMIDES

5. REACTION OF Na SALT OF p-TOLUENESULFONAMIDE WITH SOME N-(ω-BROMOALKYL)URACILS, DEVOID OF GROUPINGS CAPABLE OF TAUTOMERISM IN THE PYRIMIDINE RING

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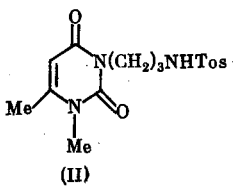
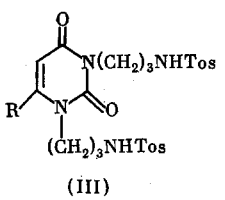
The reaction of N-(ω-bromoalkyl)uracils, devoid of NH—CO groupings capable of tautomerism in the pyrimidine ring, with the Na salt of p-toluenesulfonamide (I) gives N-[ω-(p-toluenesulfonamido)alkyl]uracils [1, 2]. The IR and UV spectra of the products, which were assigned the structures of (II) and (IIIa, b), differed from the spectra of the other compounds of this series.



(II)



(III)

R=H (IIIa); Me (IIIb).

A possible reason for this difference could be the interaction of the unshared electron pairs of the N and O atoms of the sulfonamido group with the π system of the pyrimidine ring, which also postulated a different geometry of the compounds [2]. In order to explain the spectral data and establish the specific structural traits of compound (II) we undertook an x-ray structure study of it. From the obtained x-ray structure data it followed that the molecule of the studied compound is composed of pyrimidine and benzene rings, connected by a sulfonimido group, constituting in combination a practically planar (excluding the O^1 and O^2 atoms) system, and has the structure shown in Fig. 1 (the bond lengths are given in Table 1).

The S atom has a somewhat distorted tetrahedral coordination. The lengths of the bonds S—O^1 1.441(3) and S—O^2 1.440(3) Å correspond to the sums of the double-bonded covalent radii of S and O [3], while the bond S—C^{10} 1.766(4) Å is ordinary; the interatomic distance S—N^1 1.601(4) is shortened substantially and exceeds by only 0.04 Å the sum of the double-bonded radii of the S and N atoms (1.56 Å [3]).

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