Chemistry of Heterocyclic Compounds, Vol. 38, No. 3, 2002

sym-TRIAZINE DERIVATIVES.
2*. SYNTHESIS, PROPERTIES, AND STRUCTURE OF 2-OXO-1,2-DIHYDRO-*sym*-TRIAZINES

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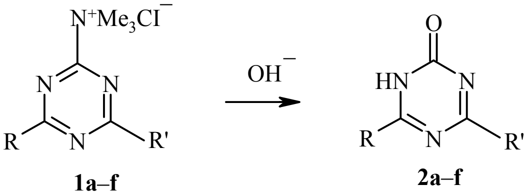
Previously unreported 2-oxo-1,2-dihydro-sym-triazines have been prepared and their alkylation reactions have been studied. It was found that, independently of the structure and nature of the substituent in positions 4 and 6 of the triazine ring or the structure of the alkyl halide used, the reaction occurs regioselectively at the oxygen atom. The stereostructure of the 2-oxo-1,2-dihydro-sym-triazines was investigated by X-ray analysis and it was shown that they exist as dimers in the crystalline state.

Keywords: 2-oxo-1,2-dihydro-*sym*-triazines, alkylation, X-ray analysis.

We have recently described [1] some novel quaternary trimethylammonium salts based on various 2-chloro-4,6-R,R'-*sym*-triazines derivatives and studied certain of their reactions. Attempts to prepare mercaptotriazines from quaternary salts by treatment with an aqueous solution of Na_2S were not successful and 2-oxo-1,2-dihydro-*sym*-triazines were unexpectedly obtained. In this work we have shown that the latter are also formed readily and in good yields (62-84%) by treatment of the quaternary salts **1a-f** with aqueous base solution. It is likely that the oxo compounds are obtained as a result of the isomerization of 2-hydroxy-*sym*-triazines formed through substitution of the trimethylammonium group by hydroxide anion.



1, 2 a R = R' = $N(CH_2CH_2)_2O$; **b** R = R' = $N(CH_2)_5$; **c** R = OMe, R' = $N(CH_2CH_2)_2O$; **d** R = R' = OMe; **e** R = R' = SPh; **f** R = R' = $NHCH_2Ph$

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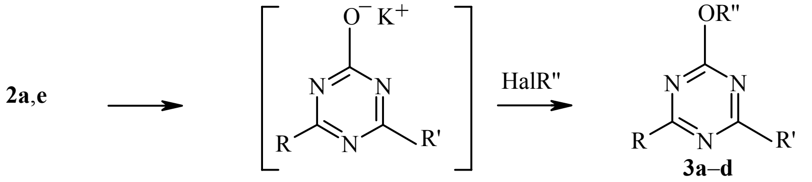
A similar isomerization has been recorded [2] for the Friedel–Crafts reaction of toluene with 6-substituted 2,4-dichloro-1,3,5-triazines and also for the reaction of 4,6-dichloro-2-methoxytriazine with ethyl sodium malonate [3]. It is of interest that, according to [4], cyanuric acid exists principally in the enol form in basic medium but acid hydrolysis of 2-alkoxy-4,6-bisdialkylamino-*sym*-triazines gives the corresponding 2-hydroxy-4,6-bisdialkylamino-*sym*-triazines [5, 6].

The composition and structure of the compounds obtained was confirmed by elemental analysis data, by IR and mass spectrometry, and also by ^{1}H NMR spectroscopy (Table 1). The IR spectra show strong and medium intensity, broad absorption bands which are typical of NH stretching vibrations in the region 3430-3440, the C=O groups at 1670-1690, and also a series of absorption bands in the range 1640-1510 cm^{-1} which are typical of the C=C and conjugated C=N bonds (Table 1).

The ^{1}H NMR spectra of the synthesized compounds show a broad singlet for an NH group at 10.52-13.05 ppm and also signals for the protons of the substituents in the 4 and 6 positions of the triazine ring (Table 1).

Since there is only fragmentary data for the synthesis of 2-oxo-1,2-dihydro-*sym*-triazines in the literature [2, 3] and their properties have been little studied we have examined the alkylation of these compounds in this report.

The reaction of 2-oxo-1,2-dihydro-*sym*-triazines **2a,e** with alkyl halides was carried out in acetonitrile or DMF in the presence of potassium hydroxide with an equimolar ratio of the reagents.



3a-c R = R' = N(CH_2CH_2)$_2$O, **d** R = R' = SPh; **a**, **d** R''= Me; **b** R'' = C_3H_7, **c** R'' = C_4H_9

TABLE 1. Characteristics for the Compounds Synthesized

Compound	Empirical formula	Found, % / Calculated, % C	Found, % / Calculated, % N	Found, % / Calculated, % H	mp, °C	Yield, %
2a	$C_{11}H_{17}N_5O_3$	49.57 / 49.42	26.45 / 26.20	6.63 / 6.41	310-311	62
2b	$C_{13}H_{21}N_5O$	59.52 / 59.29	26.85 / 26.59	8.29 / 8.04	220	84
2c	$C_8H_{12}N_4O_3$	45.41 / 45.28	26.75 / 26.40	5.89 / 5.70	239-241	62
2d	$C_5H_7N_3O_3$	38.37 / 38.22	26.99 / 26.74	4.65 / 4.49	202-203	70
2e	$C_{15}H_{11}N_3OS_2$	57.72 / 57.49	13.54 / 13.41	3.77 / 3.54	231-232	70
2f	$C_{17}H_{17}N_5O$	66.58 / 66.43	22.91 / 22.79	5.82 / 5.58	>400	80
3a	$C_{12}H_{19}N_5O_3$	51.47 / 51.23	25.13 / 24.90	7.02 / 6.81	154-155	65
3b	$C_{14}H_{23}N_5O_3$	54.52 / 54.35	25.05 / 24.90	8.48 / 8.24	146-147	50
3c	$C_{15}H_{25}N_5O_3$	55.87 / 55.71	21.92 / 21.66	7.88 / 7.79	98-99	60
3d	$C_{16}H_{13}N_3OS_2$	58.78 / 58.69	12.99 / 12.83	4.23 / 4.00	55-56	64

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* Compound **2e** found: S 20.57%, calculated: S 20.46%; Compound **3d** found: S 19.75%, calculated: S 19.58%.

TABLE 2. Spectroscopic Characteristics for the Compounds Synthesized*

Com-pound	IR spectrum, ν, cm^{-1}				^1H NMR spectrum, δ, ppm, (spin-spin coupling, *J*, Hz)*[2]				
	N–H	C=O	C=N, C=C	COC	CH_3	NCH_2, OCH_2	OCH_3, s	NH, br. s	Other protons
2a	440		590, 1560	150, 1070	—	3.53-3.73 (16H, m)	—	10.52	—
2b	3430	1670	1630, 1570, 1510	1100, 1140	—	3.55-3.70 (16H, m)	3.9	11.45	—
2c	3440	1690	1630, 1570, 1500	1190, 1120	—	—	3.89	12.30	—
2d	3430	1670	1640, 1570, 1520	1230, 1140	—	—	—	13.05	7.29-7.50 (10H, m, H(Ar)
3a	—	—	1560, 1520	1130, 1090, 1050, 1030	—	3.56-3.78 (16H, m)	3.81	—	—
3b	—	—	1570, 1530	1140, 1100, 1060	0.72 (3H, t, *J* = 9)	3.58-3.73 (16H, m); 4.16 (2H, t, *J* = 6, OCH_2)	—	—	1.64-1.78 (2H, m, $OCH_2\underline{CH_2}CH_3$)
3c	—	—	1570, 1520	1170, 1140, 1100, 1030	0.97 (3H, t, *J* = 9)	3.58-3.73 (16H, m); 4.20 (2H, t, *J* = 8, OCH_2)	—	—	1.37-1.50 (2H; m, $\underline{CH_2}CH_3$); 1.61-1.71 (2H, m, $–\underline{CH_2}CH_2CH_3$)
3d	—	—	1570, 1520	1160, 1140, 1055, 1015	—	—	3.72	—	7.24-7.43 (10H, m, H (Ar)

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* Mass spectroscopic data can be obtained from the authors.

*[2] ^1H NMR spectrum, ppm, *J* (Hz): **3b**: 0.72 (3H, t, *J* = 9, CH_3); **3c**: 0.97 (3H, t, *J* = 9, CH_3).

It was found that, independently of the nature of the halogen derivative, the solvent, and the reaction temperature, the reaction takes place highly regioselectively at the oxygen atom to give the 4,6-disubstituted 2-alkoxy-*sym*-triazines **3a-d** in 60-70% yield. The determining factor in this regioselectivity is evidently the localization of the negative charge on the oxygen atom in the intermediate potassium salt. The structure of the 4,6-disubstituted 2-alkoxy-*sym*-triazines **3a-d** was confirmed by IR, mass spectroscopic, and ^{1}H NMR data (Table 2).

In the IR spectra of compounds **3a-d** the absorption bands typical of C=O and N–H bonds are absent but a series of bands are seen at 1015-1170 cm^{-1}, characteristic of the stretching bands of ethers. The ^{1}H NMR spectra show no broad signal for an NH group proton but show the presence of alkoxy group proton signals (Table 2).

In order to confirm the structure and to study the geometry of the molecule in detail we undertook an X-ray investigation of compounds **2a** and **2c**. Projections of the steric models for the molecules are given in Figure 1 and the atomic coordinates, interatomic distances, and valence and torsional angles are presented in Tables 3-5.

TABLE 3. Atomic Coordinates* (×10^4) for Compounds **2a,c**

Atom	*x*	*y*	*z*	*U (eq)*
Compound **2c**				
O(1)	6966(5)	1229(4)	5770(4)	67(1)
O(2)	-660(5)	8455(5)	1694(4)	71(1)
O(3)	5557(5)	8401(4)	-888(4)	60(1)
N(1)	5005(6)	3646(5)	3192(4)	57(1)
N(2)	2071(6)	5974(5)	2502(4)	54(1)
N(3)	2495(6)	8361(5)	406(4)	56(1)
N(4)	5441(5)	5966(5)	1131(4)	49(1)
C(1)	7221(8)	2698(8)	308(6)	63(2)
C(2)	8015(9)	2275(8)	4560(6)	62(2)
C(3)	4810(8)	2193(8)	5920(6)	59(2)
C(4)	3848(9)	2696(8)	4488(6)	59(2)
C(5)	4108(7)	5244(6)	2252(5)	46(1)
C(6)	1208(8)	7608(6)	1555(5)	53(1)
C(7)	4526(7)	7507(6)	254(5)	49(1)
C(8)	7777(9)	7595(8)	-1123(8)	62(2)
Compound **2a**				
O(1)	102(5)	2524(5)	-156(2)	56(1)
O(2)	9574(5)	4800(4)	3572(2)	58(1)
O(3)	3993(5)	1042(4)	7759(3)	61(1)
N(1)	3199(5)	2475(5)	1775(3)	44(1)
N(2)	6443(5)	3637(5)	2606(3)	42(1)
N(3)	7321(5)	3702(5)	4640(3)	40(1)
N(4)	4034(5)	2488(4)	3751(3)	38(1)
N(5)	4945(5)	2552(5)	5737(3)	39(1)
C(1)	1137(7)	1635(7)	1782(4)	46(1)
C(2)	-35(8)	2477(9)	985(4)	54(1)
C(3)	2086(7)	3446(7)	-124(4)	51(1)
C(4)	3623(7)	2633(8)	607(4)	51(1)
C(5)	4616(6)	2882(5)	2742(3)	36(1)
C(6)	7815(6)	4058(6)	3574(3)	40(1)
C(7)	5421(6)	2917(5)	4698(3)	36(1)
C(8)	6507(8)	2401(9)	6743(4)	52(1)
C(9)	5718(8)	2346(8)	7838(4)	55(1)
C(10)	2439(8)	1401(9)	6884(4)	61(2)
C(11)	3006(8)	1397(8)	5716(4)	53(1)

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* Hydrogen atom coordinates can be obtained from the authors.

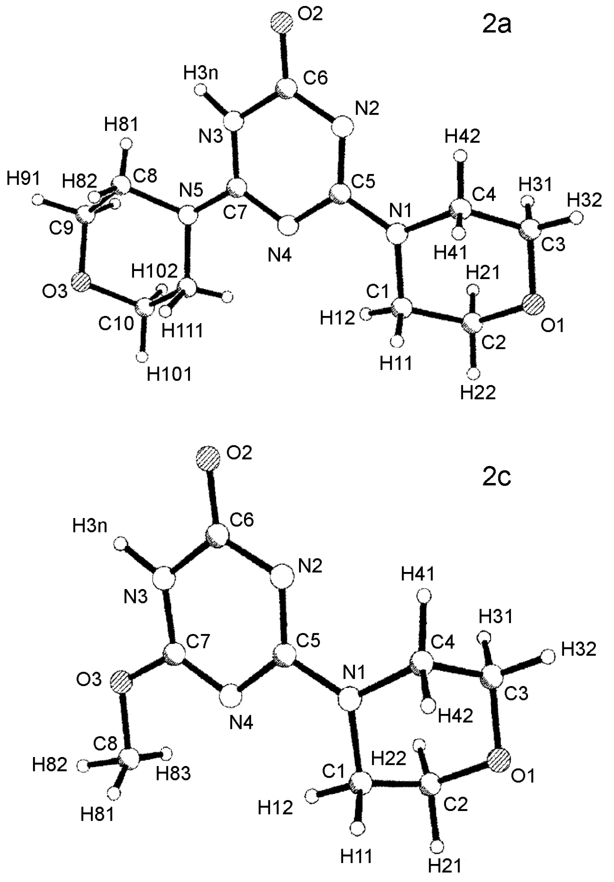

Fig. 1. Projections of the molecules **2a,c**.

TABLE 4. Interatomic Distances in the Molecules **2a,c**

Bond	*d*, Å	Bond	*d*, Å
Compound **2a**		Compound **2c**	
O(1)–C(3)	1.424(5)	O(1)–C(3)	1.420(6)
O(1)–C(2)	1.429(6)	O(1)–C(2)	1.425(6)
O(2)–C(6)	1.250(5)	O(2)–C(6)	1.233(5)
O(3)–C(9)	1.414(6)	O(3)–C(7)	1.320(5)
O(3)–C(10)	1.414(6)	O(3)–C(8)	1.441(6)
N(1)–C(5)	1.343(5)	N(1)–C(5)	1.339(5)
N(1)–C(1)	1.459(6)	N(1)–C(1)	1.451(6)
N(1)–C(4)	1.462(6)	N(1)–C(4)	1.466(6)
N(2)–C(6)	1.328(5)	N(2)–C(5)	1.323(5)
N(2)–C(5)	1.335(5)	N(2)–C(6)	1.355(5)
N(3)–C(7)	1.361(5)	N(3)–C(7)	1.329(6)
N(3)–C(6)	1.385(5)	N(3)–C(6)	1.377(5)
N(4)–C(7)	1.317(5)	N(4)–C(7)	1.288(5)
N(4)–C(5)	1.350(5)	N(4)–C(5)	1.374(5)
N(5)–C(7)	1.351(5)	C(1)–C(2)	1.496(8)
N(5)–C(8)	1.467(6)	C(3)–C(4)	1.504(8)
N(5)–C(11)	1.474(6)		
C(1)–C(2)	1.503(7)		
C(3)–C(4)	1.481(7)		
C(8)–C(9)	1.486(7)		
C(10)–C(11)	1.495(7)		

In crystalline states, compounds **2a,c** exist as dimers which are joined via the oxo and amino group by a hydrogen bond, the length of which is 1.77Å in compound **2a** and 1.836 Å in **2c**. This dimerization is also likely to be the reason for the high melting points, poor solubility, and low reactivity of the compounds **2**. Moreover, incomplete conjugation leads to deformation of the triazine ring. The greatest deformation of this ring occurs with different substituents at positions 4 and 6.

The longest bond in the triazine ring in both compounds is the $N_{(3)}$–$C_{(6)}$ bond which is 1.377 in compound **2c** and 1.385 Å in **2a**. The bond length of the remaining C–N and C=N bonds in compound **2a** varies in the range 1.317 ($C_{(7)}$–$N_{(4)}$) to 1.361 Å ($C_{(7)}$–$N_{(3)}$) while the length of such bonds in the unsubstituted *sym*-triazine is 1.337 Å, according to the authors of [8]. The valence angles of **2a** are also deformed, the greatest distortion of the angles are at atoms $N_{(4)}$ (116.0°), $N_{(2)}$ (115.9°), and $C_{(5)}$ (127.0°).

Compound **2c** contains different substituents at positions 4 and 6 of the triazine ring which leads to a still greater deformation of the valence angles and changes the bond lengths in the triazine ring. The length of the conjugated bonds in this compound varies in the range 1.288 ($C_{(7)}$–$N_{(4)}$) to 1.355 Å ($C_{(6)}$–$N_{(2)}$) and the valence angles from 113.6° ($C_{(7)}$–$N_{(4)}$–$C_{(5)}$) to 126.9° ($N_{(2)}$–$C_{(5)}$–$N_{(4)}$). Such a distortion in the bond lengths and valence angles in the triazine ring of compound **2c** is evidently associated with partial conjugation of the unshared electron pair of the oxygen atom in the methoxy group with the multiple $C_{(7)}$–$N_{(4)}$ bond and with the

TABLE 5. Valence Angles in Compounds **2a,c**

Angle	φ, deg.	Angle	φ, deg.
Compound **2a**		Compound **2c**	
C(3)–O(1)–C(2)	110.5(3)	C(3)–O(1)–C(2)	109.7 (4)
C(9)–O(3)–C(10)	109.4(4)	C(7)–O(3)–C(8)	117.4 (4)
(5)–N(1)–C(1)	123.2(3)	C(5)–N(1)–C(1)	124.1 (4)
C(5)–N(1)–C(4)	123.3(3)	C(5)–N(1)–C(4)	123.2 (4)
C(1)–N(1)–C(4)	113.1(3)	C(1)–N(1)–C(4)	112.6 (4)
C(6)–N(2)–C(5)	115.9(3)	C(5)–N(2)–C(6)	116.6 (4)
C(7)–N(3)–C(6)	119.9(4)	C(7)–N(3)–C(6)	120.4 (4)
C(7)–N(4)–C(5)	116.0(3)	C(7)–N(4)–C(5)	113.6 (4)
C(7)–N(5)–C(8)	121.0(4)	N(1)–C(1)–C(2)	109.8 (4)
C(7)–N(5)–C(11)	116.6(3)	O(1)–C(2)–C(1)	110.0 (5)
C(8)–N(5)–C(11)	114.0(4)	O(1)–C(3)–C(4)	112.1 (5)
N(1)–C(1)–C(2)	110.6(4)	N(1)–C(4)–C(3)	109.4 (5)
O(1)–C(2)–C(1)	111.4(4)	N(2)–C(5)–N(1)	117.8 (4)
O(1)–C(3)–C(4)	111.9(4)	N(2)–C(5)–N(4)	126.9 (4)
N(1)–C(4)–C(3)	110.5(4)	N(1)–C(5)–N(4)	115.3(4)
N(2)–C(5)–N(1)	116.7(3)	O(2)–C(6)–N(2)	123.1(5)
N(2)–C(5)–N(4)	127.0(4)	O(2)–C(6)–N(3)	118.8(4)
N(1)–C(5)–N(4)	116.3(3)	N(2)–C(6)–N(3)	118.1(4)
O(2)–C(6)–N(2)	122.5(4)	N(4)–C(7)–O(3)	122.2(4)
O(2)–C(6)–N(3)	117.2(4)	N(4)–C(7)–N(3)	124.4(4)
N(2)–C(6)–N(3)	120.3(4)	O(3)–C(7)–N(3)	113.4(4)
N(4)–C(7)–N(5)	119.2(3)		
N(4)–C(7)–N(3)	121.0(4)		
N(5)–C(7)–N(3)	119.9(4)		
N(5)–C(8)–C(9)	111.9(4)		
O(3)–C(8)–C(9)	111.9(4)		
O(3)–C(9)–C(8)	111.9(4)		
O(3)–C(10)–C(11)	112.0(5)		
(5)–C(11)–C(10)	111.5(4)		

TABLE 6. Torsional Angles in Compounds **2a,c**

Angle	θ, deg	Angle	θ, deg
Compound **2a**		Compound **2c**	
C(4)–N(1)–C(1)–C(2)	-50.7	C(4)–N(1)–C(1)–C(2)	-54.6
C(5)–N(1)–C(1)–C(2)	136.2	C(5)–N(1)–C(1)–C(2)	123.0
C(3)–O(1)–C(2)–C(1)	-58.5	C(3)–O(1)–C(2)–C(1)	-61.7
N(1)–C(1)–C(2)–O(1)	53.8	N(1)–C(1)–C(2)–O(1)	58.9
C(2)–O(1)–C(3)–C(4)	59.7	C(2)–O(1)–C(3)–C(4)	60.0
C(1)–N(1)–C(4)–C(3)	51.5	C(1)–N(1)–C(4)–C(3)	51.7
C(5)–N(1)–C(4)–C(3)	-135.5	C(5)–N(1)–C(4)–C(3)	-125.9
O(1)–C(3)–C(4)–N(1)	-55.6	O(1)–C(3)–C(4)–N(1)	-54.2
C(7)–N(5)–C(8)–C(9)	168.6		
C(11)–N(5)–C(8)–C(9)	-44.3		
C(10)–O(3)–C(9)–C(8)	-62.0		
N(5)–C(8)–C(9)–O(3)	53.3		
C(9)–O(3)–C(10)–C(11)	61.8		
C(7)–N(5)–C(11)–C(10)	-167.5		
C(8)–N(5)–C(11)–C(10)	44.0		
O(3)–C(10)–C(11)–N(5)	-52.7		

redistribution of electron density in the ring. These effects may also apparently explain somewhat decreased N–H (0.936 Å) and C=O (1.233 Å) bond lengths in compound **2c** when compared with the lengths of the corresponding bonds in compound **2a** (1.004 and 1.25 Å).

It was of interest to note that the morpholine ring in position 6 of compound **2a** has a half chair conformation. Moreover, the lengths of the single C–C bonds in this fragment is somewhat shorter than the mean C–C bond lengths in aliphatic cyclic amines and the valence angles are also somewhat distorted (Table 3). The same substituent in position 4 of the triazine ring has a chair conformation with a smaller distortion of bond lengths and valence angles when compared with the mean values for similar compounds (Tables 4-6).

In compound **2c** the morpholine substituent at position 6 of the triazine ring is also found in a half chair conformation, moreover its torsional angles are virtually identical with those for the substituent in position 6 of compound **2a** (Tables 5, 6). The methyl group carbon atom is situated in the plane of the triazine ring.

Hence these novel 2-oxo-1,2-dihydro-*sym*-triazines have been synthesized and their reactivities towards alkylation studied. The structure determination has identified their tendency towards dimerization in the crystalline state *via* the formation of N–H···O=C hydrogen bonds.

EXPERIMENTAL

IR spectra were recorded for vaseline oil suspension of the samples on a Specord IR-75 instrument. ^{1}H NMR spectra were taken on a Bruker WM-250 spectrometer (250 MHz) for sample solutions in DMSO-d$_6$. Mass spectra were recorded on a Finnigan MAT INCOS50 instrument (70 eV). Monitoring of the reaction course and the purity of the products obtained was performed using TLC on Silufol UV-254 plates in the system acetone-hexane (1: 1).

X-Ray Structural Investigation of Compounds 2a,c. Prismatic crystals grown from ethanol solution.

Compound 2a. $C_{11}H_{17}N_5O_3$. Unit cell parameters: a = 6.877 (1), b = 7.834 (2), c = 11.762 (2) Å; α = 92.08 (3), β = 100.66 (3), γ = 99.80 (3)°; Z = 2; d = 1.450 Mg/m^3; V = 612.1 (2) Å^3. Space group triclinic, *P*-1

Compound 2c. $C_8H_{12}N_4O_3$. Unit cell parameters: a = 7.023 (1), b = 8.573 (2), c = 9.439 (2) Å; α = 69.07 (3), β = 76.33 (3), γ = 67.38 (3)°; Z = 2; d = 1.448 Mg/m^3; V = 486.7 (1) Å^3. Space group triclinic, *P*-1. Experimental data was obtained on an Enraf-Nonius CAD 4 automatic diffractometer using

MoKα-radiation with a β-filter and θ/2θ scanning. In all, 944 reflections were obtained with $I > 2\sigma(I)$. The structure was solved by a direct method using the SHELXTL computer program [8] and refined in the anisotropic (isotropic for hydrogen) approximation to difference factors of $R = 0.0390$, $R_w = 0.0439$ for **2a** and $R = 0.0469$, $R_w = 0.0470$ for **2c**.

2-Oxo-1,2-dihydro-4,6-R,R'-*sym*-triazines (2a-f). A mixture of the 2-trimethylammonium-4,6-R,R'-*sym*-triazine (9 mmol), prepared as in method [1], and NaOH (18 mmol) was stirred at a temperature of 40°C for 3-5 h. The reaction mixture was then acidified with acetic acid to pH 6.5-5.0 and the precipitated product **2** was filtered off, washed with water, and purified by crystallization from alcohol.

2-Alkoxy-4,6-R,R'-*sym*-triazines (3a-d). A 10% aqueous solution of KOH (1.5 ml, 1.9 mmol) was added rapidly to a solution of the compound **2a-f** (1.9 mmol) in DMF (10-15 ml). The solution obtained was then treated with the alkyl halide (1.9 mmol) with stirring and the mixture was held for from 3 h to 2 days at 25-60°C. The contents were diluted with twice the quantity of water and the precipitated product was filtered off, washed with water, and recrystallized from a mixture of hexane and benzene (3:1).

In the case of using acetonitrile as solvent, after completion of the reaction the acetonitrile was evaporated in vacuo and the precipitate was filtered off and worked up as described above.

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