2,3,4,5-TETRAHYDRO-7H,12bH-1,3-THIAZEPINO[3,2-*c*]-1,3-BENZOXAZINE. A NEW HETEROCYCLIC SYSTEM

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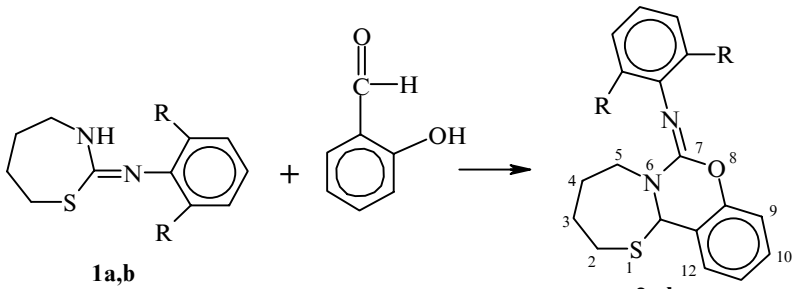
Keywords: 2-aryliminohexahydro-1,3-thiazepines, salicylaldehyde, 2,3,4,5-tetrahydro-7H,12bH-1,3-thiazepino[3,2-*c*]-1,3-benzoxazine.

2-Aminothiazepine derivatives and their hydrogenated analogs have not yet been studied extensively although they are convenient synthones for the preparation of potential biologically active compounds. In a continuation of our study of the chemical behavior and spectral properties of 2-aminotetrahydro- and 2-iminohexahydro-1,3-thiazepines [1, 2], we investigated the reaction of **1a** and **1b** with salicylaldehyde. Derivatives of a new heterocyclic system, 2,3,4,5-tetrahydro-7H,12bH-1,3-thiazepino[3,2-*c*]-1,3-benzoxazines (**2a** and **2b**) were obtained instead of the expected bis(N-aryl-N-hexahydrothiazepinylamino)-2-hydroxyphenylmethanes.



1a,b **2a,b**

1a R = H, **b** R = Me

These transformations proceed with an equimolar reagent ratio and prolonged heating in isoamyl alcohol. The structures of these products were confirmed in the case of **2a** by X-ray diffraction structural analysis.

The X-ray diffraction study of the structure of **2a** showed that the $C_{(7)}$–$N_{(13)}$ exocyclic bond (1.266 Å) is much shorter than the $C_{(12b)}$–$N_{(6)}$ endocyclic bond (1.363 Å) and closer to a formal C=N double bond (1.265 Å). The mean values of C_{sp3}–C_{sp3} (1.519 Å) and C_{arom}–C_{arom} bond lengths (1.383 Å) are somewhat shorter than the generally accepted values.

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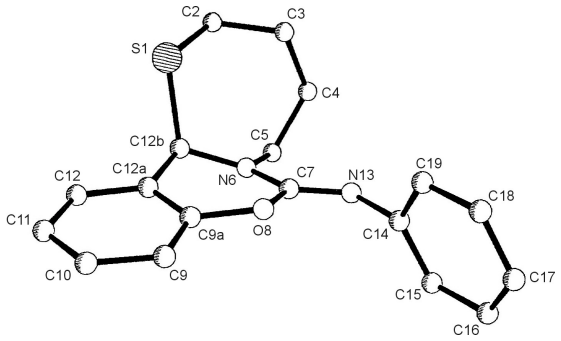

Fig. 1. Molecular structure of compound **2a**.

7-Phenylimino-2,3,4,5-tetrahydro-7H,12bH-1,3-thiazepino[3,2-*c*]-1,3-benzoxazine (2a) was obtained in 41.3% yield; mp 133-134°C (ethanol). IR spectrum, ν, cm^{-1}: 1590 (C=C), 1657 (C=N), 2952, 3015 (Ph). Mass spectrum, *m/z* (I_{rel}, %): M^+ 310 (38). Found, %: C 69.42; H 5.80; N 9.17. $C_{18}H_{18}N_2OS$. Calculated, %: C 69.65; H 5.84; N 9.02.

7-(2^1,6^1-Dimethylphenylimino)-2,3,4,5-tetrahydro-7H,12bH-1,3-thiazepino[3,2-*c*]-1,3-benzoxazine (2b) was obtained in 59.2% yield; mp 136.5-137.5°C (aqueous ethanol). IR spectrum, ν, cm^{-1}: 1589 (C=C), 1669 (C=N), 2955, 3046 (Ar). Mass spectrum, *m/z* (I_{rel}, %): 338 (37). Found, %: C 70.68; H 6.51; N 8.34. $C_{20}H_{22}N_2OS$. Calculated, %: C 70.97; H 6.55; N 8.28.

X-ray Diffraction Structural Analysis of 2a. The unit cell parameters and space group were determined and refined on a Siemens diffractometer: a = 13.514(4), b = 10.142(2), c = 12.010(3) Å, β = 110.26(2)°; V = 1544.1(7) $Å^3$; d_{calc} = 1.335 g/cm^3; space group $P2_1/c$; Z = 4. The final R_1 = 0.0348, wR_2 = 0.1090 for reflections with $I > 2\theta(I)$ and R_1 = 0.0348 and wR_2 = 0.1090 for all reflections.

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