LETTERS TO THE EDITOR

BROMOCYCLIZATION OF SOME SUBSTITUTED 3-ALLYL-2-THIOHYDANTOINS

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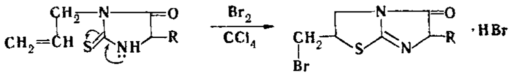
It is known that N-alkenylthioureas with an allylic double bond are cyclized by the action of bromine to 2-thiazoline derivatives [1]. In the present research we have studied the possibility of the preparation of condensed thiazolidine and imidazole systems from 3-allyl-2-thiohydantoin, in which the thiourea fragment enters into the thiohydantoin ring, and an electron-withdrawing group is attached to the same nitrogen atom as the allyl group.

The starting 5-substituted 3-allyl-2-thiohydantoins (I) were obtained by a somewhat modified method [2]. Bromination of I in chloroform or carbon tetrachloride proceeds with simultaneous ring formation to give 2,3,5,6-tetrahydro-6-R-2-bromomethyl-5-oxoimidazo[2,1-b]thiazole (II).



I a-e II a-e

The physical constants and yields of I and II are presented in Table 1.

The ionically and covalently bonded bromine atoms in II were determined. Compounds Ia,d were obtained by two independent methods and were identified from their melting points, UV and IR spectra, and the results of thin-layer chromatography (TLC) (R_f 0.68, 0.65, respectively). The individuality of the re-

TABLE 1. Physical Constants of the Substances Obtained

Compound	5(6) R	mp, °C	R_f[a] A	R_f[a] B	UV spectra, λ_{max}, nm (log ε)	IR spectrum, cm^{-1} $\nu_{C=O}$	ν_{N-H}	$\nu_{C=N}$	$\nu_{C=C}$	Yield, %
Ia	H	88[b]	0,68	0,78	230(3,96), 265(4,11)	1740	3230	—	1640	63
Ib	CH_3	80[b]	0,82	0,88	230(3,85), 270(4,25)	1740	3220	—	1640	66
Ic	C_3H_7	65—66	0,70	0,89	230(4,48), 265(4,85)	1755	3205	—	1650	64
Id	i-C_4H_9	107	0,65	0,91	235(3,83), 265(4,15)	1760	3240	—	1660	60
Ie	CH_2COOH	142—143	0,81	0,82	235(4,24), 270(4,56)	—	—	—	—	72
IIa	H	165—166	—	0,52	260(3,17), 320(2,64)	1715	—	1580	—	57
IIb	CH_3	220—222[c]	—	0,53	250(3,00)	1720	—	1590	—	85
IIc	C_3H_7	167	—	0,48	235(3,69)	1760	—	1585	—	70
IId	i-C_4H_9	188	—	0,47	250(3,05)	1750	—	1580	—	91
IIe	CH_2COOH	119—121	—	0,67	—	—	—	—	—	92

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[a] The following systems were used for chromatography on Silufol: A) chloroform–methanol (9:1); B) butanol–acetic acid–water (5:2:2).

[b] These compounds were previously described in [2].

[c] With decomposition.

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maining substances was also established by TLC, and their structures were confirmed by the analytical results and the UV and IR spectra.

The IR spectra of I contain a high-intensity band at 1740-1760 cm^{-1} (C=O). The formation of two-ring compound II from I is confirmed by the absence in its spectrum of absorption bands of an NH bond at 3205-3230 cm^{-1} and of a C=C bond at 1640-1660 cm^{-1}, which are present in the spectrum of the starting substances, and by the appearance of C–Br stretching vibrations at 570-580 cm^{-1}.

LITERATURE CITED

1. I. V. Smolanka and N. P. Man'o, Ukr. Khim. Zh., 36, 589 (1970).
2. W. Marckwald, M. Neumark, and R. Stelzner, Ber., 24, 3287 (1891).