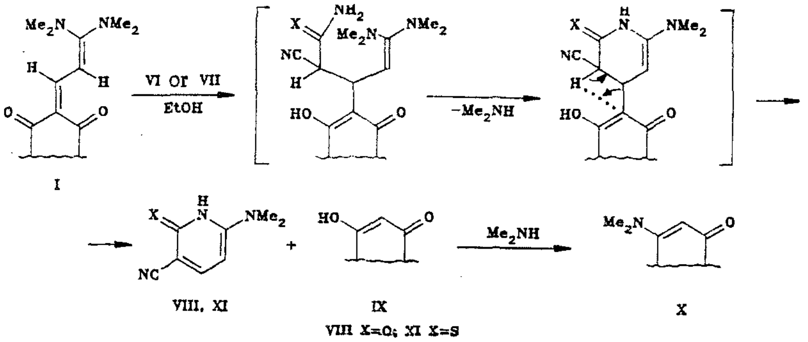

I

VIII, XI

IX

X

VIII X=O; XI X=S

Elemental analyses of compounds VIII and XI were consistent with calculated values.

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2-IMINO-cis-PERHYDROTHIENO[3,4-d]THIAZOLE-5,5-DIOXIDES

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UDC 547.732'789.6

It has previously been demonstrated that 4-amino-2-thiolene-1,1-dioxides react with aryl(alkyl)isothiocyanates at 70-110°C, or with thiophosgene and amines at 20-30°C, to give thioureas, which undergo cyclization in the presence of amines to give cis-perhydrothieno-[3,4-d]imidazole-2-thione-5,5-dioxides [1].

We have now found that reaction with benzoylisothiocyanate occurs in a different manner. In the case of sulfone Ia, which is substituted on the nitrogen atom, the reaction stops at the thiourea stage II. Subsequent basic hydrolysis (refluxing with potash in a 2:1 water–dioxane mixture) leads to the formation of a bicycle with an imidazolidine fragment, III. Acidic hydrolysis of thiourea II (refluxing in concentrated HCl) results in an isomeric compound belonging to a new series of compounds, namely, 1-phenyl-2-imino-cis-perhydrothieno[3,4-d]thiazole-5,5-dioxide, which was isolated in the form of its hydrochloride IVa. Compounds belonging to this series are interesting as potential antihypertensive agents [2].

In contrast to the N-substituted sulfone Ia, amine Ib reacts with benzoylisothiocyanate to give the bicyclic thiazolidine IVb immediately; the latter reacts with hydrochloric acid to form the unsubstituted (with respect to nitrogen) hydrochloride IVc.

Products: III [yield 62%; mp 277°C (from dioxane); IR spectrum (KBr): 3160, 1505, 1310, 1110 cm^{-1}; ^{13}C-NMR spectrum (CF$_3$COOD): 52.6 t, 56.6 t, 59.0 d, 67.1 d, 129.6 d, 133.7 d, 134.7 s, 173.1 ppm]; IVa [yield 61%, mp 208°C (from aqueous alcohol); IR spectrum (KBr): 3310, 1640, 1320, 1120 cm^{-1}; ^{13}C-NMR spectrum (CF$_3$COOD): 43.9 d, 54.2 t, 58.6 t, 72.3 d, 130.5 d, 135.6 d, 135.8 s, 136.0 d, 175.8 ppm]; IVb [yield 90%; mp 226°C (from alcohol);

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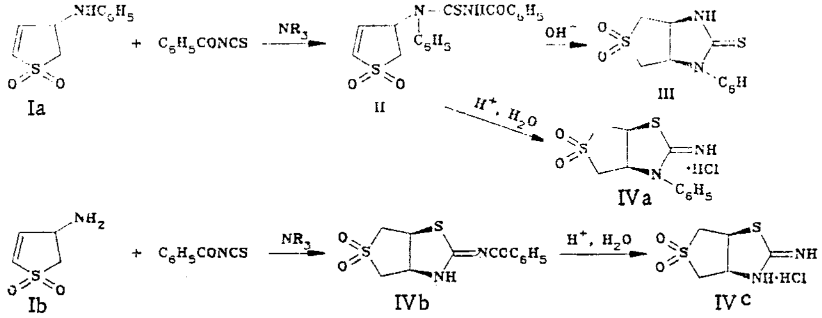

IR spectrum (KBr): 3230, 1620, 1340, 1130 cm^{-1}; ^{13}C-NMR spectrum (CF_3COOD): 46.0 d, 55.8 t, 57.5 t, 64.3 d, 131.8 d, 132.0 d, 133.0 d, 139.6 s, 171.2 s, 177.6 ppm]; IVc [yield 80%; mp 240°C (from aqueous alcohol); IR spectrum (KBr): 3300, 1640, 1300, 1100 cm^{-1}; ^{13}C-NMR spectrum (CF_3COOD): 45.6 d, 55.2 t, 56.4 t, 63.3 d, 175.7 ppm].

Elemental analyses of these synthesized compounds were consistent with calculated values.

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