SYNTHESIS AND STUDY OF THE STRUCTURES OF NEW PYRIDAZINO[4,5-b]QUINOXALINE AND PYRAZINO-[2,3-d]PYRIDAZINE DERIVATIVES

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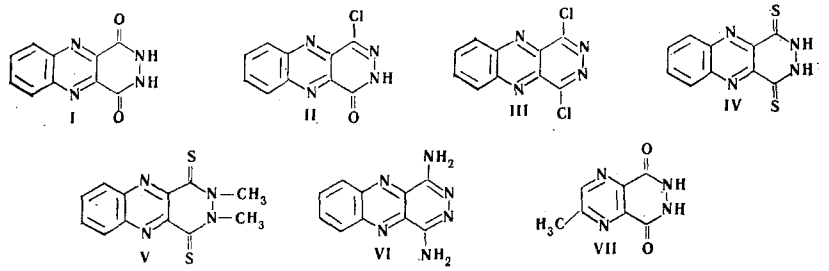
The goal of this study was the synthesis and investigation of the structures of new pyridazino[4,5-b]-quinoxaline and pyrazino[2,3-d]pyridazine derivatives, the first representatives of which were recently obtained in [1, 2]. Both of these systems are of interest as a consequence of their structural similarity to benzopteridine and pteridine systems which are the basis of biologically important compounds.

The reaction of quinoxaline-2,3-dicarboxylic acid anhydride [3] with hydrazine hydrate in glacial acetic acid yielded I, which is capable of existing in three tautomeric forms. The problem of its structure is the subject of a second investigation. Products II or III are obtained by the action of a mixture of $POCl_3$ and PCl_5 on I, depending on the ratio of the reagents. The IR spectrum of II contains a band at 1685 cm^{-1} for the C=O group of the cyclic amide. Treatment of I with P_2S_5 in pyridine yielded IV, the IR spectrum of which contains a strong band at 1490 cm^{-1}, which is characteristic for thioamides, and a band at 1220 cm^{-1}, which corresponds to the valence vibrations of C=S [4]. No bands were observed at 2550-2600 cm^{-1} Thus, IV has the thione form in the solid state. Compound IV is readily converted to V by reaction with CH_3I. The IR spectrum of V contains bands at 1485 cm^{-1} (thioamide) and 1220 cm^{-1} for the valence vibrations of the C=S group. Compound VI was obtained by condensation of the dinitrile of quinoxaline-2,3-dicarboxylic acid [5] with hydrazine hydrate in methanol. Product VII is formed by the reaction of dimethyl 2-methylpyrazine-5,6-dicarboxylate [6] with hydrazine hydrate in methanol.



EXPERIMENTAL

1,4-Dioxopyridazino[4,5-b]quinoxaline (I). This compound melted above 350° (from dimethylformamide). Found %: C 55.8; H 3.1; N 26.3. $C_{10}H_6N_4O_2$. Calculated %: C 56.1; H 2.8; N 26.1.

1-Chloro-4-oxopyridazino[4,5-b]quinoxaline (II). This compound had mp 328-330°. Found %: C 51.8; H 2.2; N 23.8. $C_{10}H_5ClN_4O$. Calculated %: C 51.6; H 2.1; N 24.1.

1,4-Dichloropyridazino[4,5-b]quinoxaline (III). This compound had mp 294-296° (decomp., from butanol). Found %: C 47.7; H 2.0; N 22.5. $C_{10}H_4Cl_2N_4$. Calculated %: C 47.8; H 1.6; N 22.3.

1,4-Dithiopyridazino[4,5-b]quinoxaline (IV). This compound had mp 240-242°. Found %: N 22.4. $C_{10}H_6N_4S_2$. Calculated %: N 22.7.

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1,4-Dithio[2,3-dimethylpyridazino[4,5-b]quinoxaline (V). This compound had mp 295-296° (from butanol). Found %: C 52.4; H 3.8; N 20.4. $C_{12}H_{10}N_4S_2$. Calculated %: C 52.5; H 3.6; N 20.42.

1,4-Diaminopyridazino[4,5-b]quinoxaline (VI). This compound had mp 280-282° (from water). Found %: C 57.1; H 3.6. $C_{10}H_8N_6$. Calculated %: C 56.6; H 3.7.

2-Methyl-5,8(6H,7H)pyrazino[2,3-d]pyridazinone (VII). This compound melted above 350° (from water). Found %: C 46.7; H 3.5; N 31.6. $C_7H_6N_4O_2$. Calculated %: C 47.1; H 3.4; N 31.5.

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