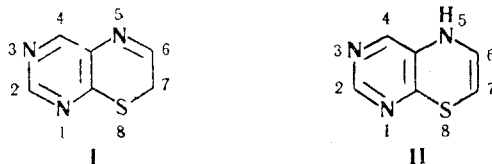


DERIVATIVES OF 5H-PYRIMIDO [4, 5-b] (1, 4) THIAZINE

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The preparation of derivatives of 7H-pyrimido [4, 5-b](1, 4) thiazine (I) is known. Continuing previous research [2, 3], we have now synthesized derivatives of the 5H-pyrimido [4, 5-b](1, 4) thiazine (II) system, hitherto undescribed in the literature. System II differs from system I with respect to the position of the double bond in the thiazine ring (6, 7 instead of 5, 6).



Reaction of 4, 6-dichloro-5-methylaminopyrimidine [4] with KSH gives 4-chloro-5-methylamino-6-mercaptopyrimidine (III). Reaction of the latter with α -bromoacetophenone or its p-nitro derivative gives the S-phenacyl derivatives IV and V, whose structures are confirmed by their IR spectra, which indicate the presence of CO (1600 cm^{-1}) and NH (3400 cm^{-1}) groups. Dehydration of compounds IV and V with POCl_3 gave 4-Cl-5-Me-6-arylpyrimido [4, 5-b](1, 4) thiazine (VI, VII).

4-Chloro-5-methylamino-6-mercaptopyrimidine (III). MP $215^\circ\text{--}217^\circ\text{ C}$ (decomp, EtOH). Found: C 34.43; H 3.69; Cl 20.04; N 23.56; S 18.38%. Calculated for $\text{C}_5\text{H}_6\text{ClN}_3\text{S}$: C 34.21; H 3.44; Cl 20.19; N 23.93; S 18.26%.

4-Chloro-5-methylamino-6-phenacylmercaptopyrimidine (IV). MP $92^\circ\text{--}94^\circ\text{ C}$ (EtOH). Found: C 53.32; H 4.21; Cl 11.97; N 14.31; S 10.94%. $\text{C}_{13}\text{H}_{12}\text{ClN}_3\text{OS}$: C 53.15; H 4.12; Cl 12.07; N 14.305; S 10.91%.

4-Chloro-5-methylamino-6-p-nitrophenacylmercaptopyrimidine (V). MP $151^\circ\text{--}152^\circ\text{ C}$ (benzene). Found: C 45.70; H 3.40; Cl 10.24; N 16.70; S 9.41%. Calculated for $\text{C}_{13}\text{H}_{11}\text{ClN}_4\text{O}_3\text{S}$: C 46.09; H 3.27; Cl 10.47; N 16.54; S 9.46%.

4-Chloro-5-methyl-6-phenylpyrimido [4, 5-b](1, 4) thiazine (VI). MP $73^\circ\text{--}75^\circ\text{ C}$ (petrol ether). Found: C 56.40; H 3.50; Cl 13.20; N 14.97; S 11.47%. Calculated for $\text{C}_{13}\text{H}_{10}\text{ClN}_3\text{S}$: C 56.62; H 3.65; Cl 12.86; N 15.24; S 11.63%.

4-Chloro-5-methyl-6-p-nitrophenylpyrimido [4, 5-b](1, 4) thiazine (VII). MP $156^\circ\text{--}158^\circ\text{ C}$ (MeOH). Found: C 48.67; H 3.05; Cl 10.80; N 17.21; S 10.18%. Calculated for $\text{C}_{13}\text{H}_9\text{ClN}_4\text{O}_2\text{S}$: C 48.67; H 2.83; Cl 11.05; N 17.47; S 10.00%.

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