

STUDIES ON THE 3-SUBSTITUTED 3H-1,2,3-TRIAZOLO[4,5-d]-
PYRIMIDINES

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Various reactions of 3-methyl- (Im) and 3-phenyl-3H-1,2,3-triazolo[4,5-d]-pyrimidines (Ip) were examined.

In warm alkaline solution or in dilute sulfuric acid I underwent ring fission to give 1-substituted 5-amino-1H-1,2,3-triazole-4-carboxaldehyde (II). However, the reaction on Im with methoxide ion resulted in the formation of 7,7'-dimer of Im (IIIIm) and 3-methyl-7-(5-amino-1-methyl-1H-1,2,3-triazol-4-yl)-3H-1,2,3-triazolo[4,5-d]pyrimidine (IVm). I dimerized in the presence of the cyanide ion to give 7,7'-dimer of I (III). N,N-Dimethylaniline reacted with Im in the presence of dilute sulfuric acid to give 5-amino-4-[bis[4-N,N-dimethylaminophenyl]methyl]-1-methyl-1H-1,2,3-triazole (Vm). Treatment of I with active methylene compounds or ketones in the presence of dilute sulfuric acid gave 3-substituted 3H-1,2,3-triazolo[4,5-b]pyridines (VI).

The substitution reaction of 7-chloro derivative of I (VII) by nucleophiles was carried out.

The reaction with amines and alkoxide ions resulted in the formation of 7-(N-substituted amino) (VIII) and 7-alkoxy derivatives of I (IX). Moreover, VII reacted with carbanions, which were formed by the reaction of active methylene compounds with sodium hydride, to result in the introduction of a carbon chain into the 7-position of I (the formation of the 7-substituted 3-methyl (or phenyl)-3H-1,2,3-triazolo[4,5-d]pyrimidines (X).

Similarly, the p-tolylsulfonyl and the cyano groups at the 7-position of Ip were easily displaced by amines, alkoxide ions and carbanions to give VIII, IX and X, respectively.