NOTE

Mechanism Regarding Pyrimidine Ring Formation

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In this note, the authors discussed the mechanism regarding pyrimidine ring formation.

In view of the rare availability and importance of condensed ring compounds of pyrimidine¹⁻³ with other ring system, it is desirable to study in detail the chemistry of pyrimidines.

The compounds '2-methyl mercapto 3-substituted 7,9-diphenyl pyrido {3',2',4,5}-thieno {3,2-d}-pyrimidine⁴, 2-amino-4-(methyl thio) 5-cyano-6(1-H)-pyrimidine thion⁵, thiazolo pyrimidinium salt⁶, steroidal amino pyrimidines⁷ and pyrimidines condensed with other ring⁸ are also reported to exhibit biological activity. To form pyrimidine ring, the carbonyl (>C=O) groups present in other compounds or ring have an important role.

$$C = CH + H_2N - C - NH_2 \longrightarrow C - NH_2$$

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1354 Singh et al. Asian J. Chem.

The alternate possibility

The mechanism of pyrimidine ring formation is not very clearly understood. However, it is considered to proceed as follows. The compounds containing α - β unsaturated carbonyl form compounds with urea and thiourea by way of attack on electrophylic carbonyl carbon, followed by elimination of water. The urea or thiourea undergoes intramolecular rearrangement to yield Δ^2 -pyrimidine.

The other possible alternative arising by 3,4 addition of urea or thiourea results in the formation of Δ^3 -pyrimidines. In literature it is reported that Δ^2 -pyrimidine structure is more stable and is more likely to form Δ^3 -pyrimidine.

If it is taken for granted that Δ^2 -pyrimidines are formed during the reaction, then the adjoining ring is converted into other ring by possible tautomerisation. If this compound is formed then >C—N frequencies should into disappear from the infrared spectrum. But contrary to this expectation, >C—N absorption takes place in all the pyrimidines. Therefore Δ^3 -structure for pyrimidine does not come into picture.

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(Received: 6 May 2000; Accepted: 26 July 2000) AJC-2109