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TAUTOMERISM OF 3,5-DISUBSTITUTED 1,2,4-TRIAZOLES

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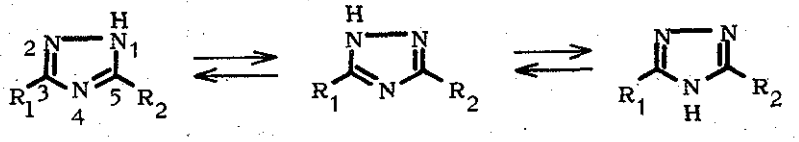
Tautomerism of 3,5-disubstituted 1,2,4-triazoles, which may exist in three forms, has been studied.

Comparison of the nuclear magnetic resonance and ultraviolet spectra of these 1,2,4-triazoles with those of the N-methylated derivatives showed that the location of the ring hydrogen is influenced by the electronic effects of the substituents at positions 3 and 5, and that the hydrogen of the predominant tautomer is located at the position (N-1 or N-2) close to the more electron releasing substituent. For example, 3-p-nitrophenyl, 3-p-chlorophenyl, and 3-γ-pyridyl derivatives of 5-methylthio-1,2,4-triazole exist in the N_1-H form, and 3-p-aminophenyl and 3-p-methoxyphenyl derivatives of 5-methylthio-1,2,4-triazole exist in the N_2-H form predominantly. However, 5-methylthio-3-γ-pyridyl-1,2,4-triazole exists solely in the N_2-H form, since it is different from the other derivatives in the type of hydrogen bond formation.



N_1-H form N_2-H form N_4-H form