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TAUTOMERIC FORMS OF 5-(2-HYDROXYPHENYL)-7-PHENYLDIHYDRO-1,2,4-TRIAZOLO[1,5-a]PYRIMIDINE

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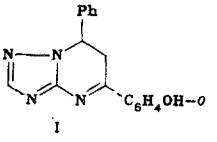
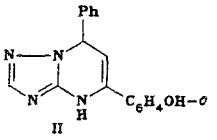
It was previously found [1] that certain aromatic substituted dihydro-1,2,4-triazolo [1,5-a]pyrimidines can form mixtures of imine and enamine tautomeric forms in solution. By exploiting the considerable influence of solvents on the tautomeric composition of 5-(2-hydroxyphenyl)-7-phenyldihydro-1,2,4-triazolo [1,5,-a]-pyrimidine, we isolated the individual 6,7- and 4,7-dihydro forms of this compound by crystallization. Thus, the crystals of tautomer I, obtained by boiling a solution of 2'-hydroxychalcone and 3-amino-1,2,4-triazole in DMFA, after dissolution in DMSO, and slow evaporation of the solution completely convert into the 4,7-dihydro form II. A reversed transition is attained by the crystallization of the latter form from methanol, ethanol, chloroform, DMFA, or mixtures of DMFA and benzene.



I



II

Tautomers I and II differ substantially in their spectral characteristics in the solid phase and also in the electronic absorption spectra of freshly prepared methanolic solutions. The UV spectrum of a solution of compound II is similar to the spectra of 5,7-diaryl-4,7-dihydro-1,2,4-triazolo[1,5-a]pyrimidines [1], the enamine structure of which has been unequivocally established. The results of their calculation by the MO LCAO SCF QI method in a PPP variant, carried out for the π-electronic fragments of these molecules [λ_{max}^{calc} (oscillator force): I 301 (0.32), 358 (0.60); II 243 (0.61), 280 (0.11), 290 (0.12)] also conform well with the spectra of the two tautomers. After 20 to 25 min from the dissolution of the crystals of compounds I and II in methanol, the UV spectra of the solutions obtained become completely identical, characterizing an equilibrium mixture of the two tautomers I:II 65:35.

Tautomer I, mp 222...224°C; $\nu_{C=N}$ (in KBr) 1615 cm^{-1}; λ_{max} nm ($\varepsilon \cdot 10^{-3}$): 305 (13.0) 365 (11.5) (in methanol).

Tautomer II, mp 214...216°C; $\nu_{C=C}$ 1665 cm^{-1}; λ_{max} nm ($\varepsilon \cdot 10^{-3}$): 238 (17.5), 282 (5.6).

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