064

ADDUCT FORMATION OF FLUORO-CONTAINING β-DIKETONES, β-KETOESTERS AND THEIR 2-HALOGENO DERIVATIVES WITH OHT AND SHT NUCLEOPHILES

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Interaction of fluoro-containing β -diketones (I), β -ketoesters (II), 2-chloro- β -ketoesters (III) and 2,2-dibromo- β -ketoesters (IV) with OH (water, alcohols) and SH (ethylthiol) nucleophiles has been studied by IR and NMR (¹H, ¹⁹F, ¹³C) spectra without solvent as in deuteriochloroform or deuterioacetone.

The results indicate that the rate of keto-enol equilibrium of compounds (I) and (III) is considerably less than that of adduct formation, therefore one can judge the reactivity of their keto and enol forms correctly.

Addition of OH and SH nucleophiles is found to occur on the enol form (I) and (II) on the carbon atom adjacent to the fluoroalkyl substituent. Keto form is more reactive for compounds (III) and (IV).

The degree of adduct formation is decreased when going from the trifluoromethyl substituent to the nonafluorobutyl substituent.