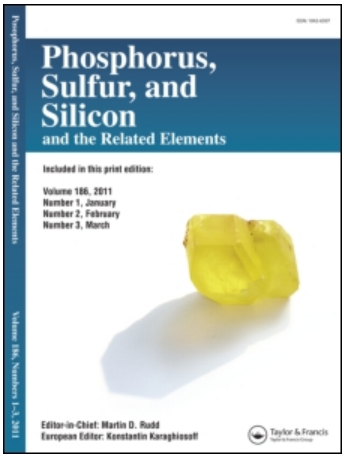

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NMR, PE AND MASS SPECTROSCOPY OF 2-ALKYL- AND 2-ARYL-CARBAMYL- AND THIOCARBAMYL-CYCLOHEXANONES

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NMR, PE AND MASS SPECTROSCOPY OF 2-ALKYL- AND 2-ARYL-CARBAMYL- AND THIOCARBAMYL-CYCLOHEXANONES

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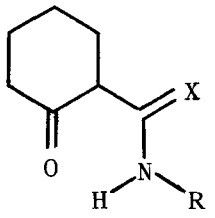
The following β-ketoamides and β-ketothioamides were prepared through Stork reaction.[3-6]



R = Me, Ph

X = O, S

Their behaviour in various solvents has been studied through ^{1}H NMR spectra, which have shown the existence of tautomeric equilibria. As usual, the interconversion between the β-ketoamido (or β-ketothioamido) form and the enolic forms is slow on NMR time scale, therefore giving different peaks. The hydrogen bonded proton resonates at almost the same frequency both in the β-ketoamides and in the β-ketothioamides; change of solvent from CCl_4 to CD_3CN has just minor effects on its chemical shift. This suggests that enethiolic forms, if at all present, are just minor components.[7]

The electronic structure of these compounds in the gas phase has been studied through photoelectron spectroscopy; data are re-

ported. Moreover, deuterium exchange studied by mass spectroscopy has shown that two hydrogen atoms can be exchanged in these compounds.

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