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Phosphorus, Sulfur, and Silicon and the Related Elements

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713618290>

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

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To cite this Article Klasinc, L. , Lisini, A. , Novak, I. , Pellizer, G. , Pitacco, G. , Srzič, D. and Valentin, E.(1979) 'NMR, PE AND MASS SPECTROSCOPY OF 2-ALKYL- AND 2-ARYL-CARBAMYL- AND THIOCARBAMYL-CYCLOHEXANONES', Phosphorus, Sulfur, and Silicon and the Related Elements, 6: 1, 371 — 372

To link to this Article: DOI: 10.1080/03086647908080459

URL: <http://dx.doi.org/10.1080/03086647908080459>

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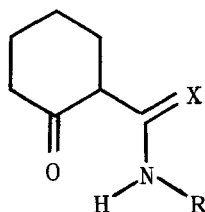
NMR, PE AND MASS SPECTROSCOPY OF 2-ALKYL- AND 2-ARYL-CARBAMYL-
AND THIOCARBAMYL-CYCLOHEXANONES

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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 ¹H 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 CCl₄ to CD₃CN 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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