

Synthetic and ^1H and ^{13}C NMR Spectral Studies on *N*-(Mono-substituted-phenyl)-acetamides and Substituted Acetamides, 2/3/4- $\text{Y}\text{C}_6\text{H}_4\text{NH-CO-CH}_{3-i}\text{X}_i$ ($\text{Y} = \text{CH}_3, \text{F}, \text{Cl}, \text{Br}, \text{NO}_2$; $\text{X} = \text{Cl}, \text{CH}_3$; $i = 0, 1, 2, 3$)

Basavalinganadoddy Thimme Gowda, Shilpa, and Jayalakshmi K. Lakshmipathy

Department of Post-Graduate Studies and Research in Chemistry, Mangalore University, Mangalagangothri-574 199, Mangalore, India

Reprint requests to Prof. B. T. G.; Fax: 91 824 2287 367; E-mail: gowdabt@yahoo.com

Z. Naturforsch. **61a**, 595 – 599 (2006); received July 19, 2006

Nineteen *N*-(2/3/4-methyl/halo/nitro-phenyl)-acetamides and substituted acetamides, 2/3/4- $\text{Y}\text{C}_6\text{H}_4\text{NH-CO-CH}_{3-i}\text{X}_i$ ($\text{Y} = \text{CH}_3, \text{F}, \text{Cl}, \text{Br}$ or NO_2 ; $\text{X} = \text{Cl}$ or CH_3 and $i = 0, 1, 2$ or 3), have been prepared, characterized, and their ^1H and ^{13}C NMR spectra in solution measured and correlated. ^1H and ^{13}C NMR chemical shifts were assigned to the protons and carbon atoms, respectively, in line with those for similar compounds. Since the chemical shifts are dependent on the electron density around the nucleus or associated with the atom to which it is bound, the incremental shifts of the aromatic protons or carbon atoms due to $-\text{NH-CO-CH}_{3-i}\text{X}_i$ and $-\text{CO-CH}_{3-i}\text{X}_i$ ($\text{X} = \text{Cl}$ or CH_3 and $i = 0, 1, 2, 3$) in all the *N*-phenyl-substituted acetamides, $\text{C}_6\text{H}_5\text{NH-CO-CH}_{3-i}\text{X}_i$, are calculated by comparing the proton or carbon chemical shifts of these compounds with those of benzene or aniline. The incremental shifts due to the groups in the parent compounds have also been computed by comparing the chemical shifts of the protons or carbon atoms in these compounds with those of benzene or aniline, respectively. The computed incremental shifts and other data were used to calculate the ^1H and ^{13}C NMR chemical shifts of the substituted compounds in three different ways. The calculated chemical shifts by the three methods compared well with each other and with the observed chemical shifts, testing the validity of the principle of additivity of the substituent effects in these compounds. The variation of ^1H NMR chemical shifts of either the aromatic or *N*-H protons, with the substituents in *N*-(phenyl)- and *N*-(2/3/4-chloro/methylphenyl)-acetamides and substituted acetamides did not follow the same trend, while the variation of the ^{13}C NMR chemical shifts of C-1 and C=O carbon atoms and those of alkyl carbon atoms of these compounds followed more or less the same trend.

Key words: ^1H and ^{13}C NMR Spectra; *N*-Aryl-acetamides; *N*-Aryl-substituted Acetamides.