

# **$^1\text{H}$ and $^{13}\text{C}$ NMR Spectral Studies on N-(Aryl)-Substituted Acetamides, $\text{C}_6\text{H}_5\text{NHCOCH}_{3-i}\text{X}_i$ and 2/4- $\text{XC}_6\text{H}_4\text{NHCOCH}_{3-i}\text{X}_i$ (where X = Cl or $\text{CH}_3$ and $i = 0, 1, 2$ or $3$ )**

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35 N-(Phenyl)-, N-(2/4-chlorophenyl)- and N-(2/4-methylphenyl)-substituted acetamides are prepared, characterised and their NMR spectra studied in solution state. The variation of the chemical shifts of the aromatic protons in these compounds follow more or less the same trend with changes in the side chain. The chemical shifts remain almost the same on introduction of Cl substituent to the benzene ring, while that of methyl group lowers the chemical shifts of the aromatic protons. But only  $^{13}\text{C}$ -1 and  $^{13}\text{C}$ -4 chemical shifts in these compounds are sensitive to variations of the side chain. The incremental shifts in the chemical shifts of the aromatic protons and carbons due to  $-\text{COCH}_{3-i}\text{X}_i$  or  $\text{NHCOCH}_{3-i}\text{X}_i$  groups in all the N-(phenyl)-substituted acetamides,  $\text{C}_6\text{H}_5\text{NHCOCH}_{3-i}\text{X}_i$  (where X = Cl or  $\text{CH}_3$  and  $i = 0, 1, 2$  or  $3$ ) are calculated. These incremental chemical shifts are used to calculate the chemical shifts of the aromatic protons and carbons in all the N-(2/4-chlorophenyl)- and N-(2/4-methylphenyl)-substituted acetamides, in two ways. In the first way, the chemical shifts of aromatic protons or carbons are computed by adding the incremental shifts due to  $-\text{COCH}_{3-i}\text{X}_i$  groups and the substituents at the 2<sup>nd</sup> or 4<sup>th</sup> position in the benzene ring to the chemical shifts of the corresponding aromatic protons or carbons of the parent aniline. In the second way, the chemical shifts are calculated by adding the incremental shifts due to  $-\text{NHCOCH}_{3-i}\text{X}_i$  groups and the substituents at the 2<sup>nd</sup> or 4<sup>th</sup> position in the benzene ring to the chemical shift of a benzene proton or carbon, respectively. Comparison of the two sets of calculated chemical shifts of the aromatic protons or carbons of all the compounds revealed that the two procedures of calculation lead to almost the same values in most cases and agree well with the experimental chemical shifts.

*Key words:* Nuclear Magnetic Resonance; N-Aryl Substituted Acetamides.