

Infrared, ^1H and ^{13}C NMR Spectral Studies on Di- and Tri-substituted N-Aryl Amides, $2,6\text{-X}_2\text{C}_6\text{H}_3\text{NHCOCH}_{3-i}\text{X}_i$ and $2,4,6\text{-X}_3\text{C}_6\text{H}_2\text{NHCOCH}_{3-i}\text{X}_i$ ($\text{X} = \text{Cl}$ or CH_3 and $i = 0, 1, 2$ or 3)

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Several di- and tri-substituted amides of the general formula, $2,6\text{-X}_2\text{C}_6\text{H}_3\text{NHCOCH}_{3-i}\text{X}_i$ and $2,4,6\text{-X}_3\text{C}_6\text{H}_2\text{NHCOCH}_{3-i}\text{X}_i$ ($\text{X} = \text{Cl}$ or CH_3 and $i = 0, 1, 2$, or 3) are prepared, characterised, and their infrared spectra in the solid state and ^1H and ^{13}C NMR spectra in solution are studied. The $\text{C}=\text{O}$ stretching vibrations of N-(2,6-dichlorophenyl)- and N-(2,6-dimethylphenyl)-amides appear as strong absorptions in the ranges $1707 - 1658\text{ cm}^{-1}$ and $1700 - 1647\text{ cm}^{-1}$, respectively, while the N-H stretching vibrations of N-(2,6-dichlorophenyl)- and N-(2,6-dimethylphenyl)-amides appear as strong vibrations in the ranges $3271 - 3209\text{ cm}^{-1}$ and $3285 - 3214\text{ cm}^{-1}$, respectively. The N-H stretching vibrations of N-(2,4,6-trichlorophenyl)- and N-(2,4,6-trimethylphenyl)- amides also appear as strong absorptions in the ranges $3370 - 3212$ and $3283 - 3225\text{ cm}^{-1}$, respectively, while those of the $\text{C}=\text{O}$ vibrations appear in the ranges $1688 - 1617$ and $1704 - 1647\text{ cm}^{-1}$. The analysis of the $\text{C}=\text{O}$ and N-H absorption frequencies of all amides of the general formula $\text{X}_i\text{C}_6\text{H}_{5-i}\text{NHCOCH}_{3-i}\text{X}_i$ (where $\text{X} = \text{Cl}$ or CH_3 , and $i = 0, 1, 2$ or 3) indicates that their variations do not show regular trends with substitution either in the phenyl ring or in the side chain. The chemical shifts of both the aromatic protons and the aromatic carbons of all the amides are calculated in two ways, either by adding the incremental shifts due to $-\text{COCH}_{3-i}\text{X}_i$ groups and the substituents in the benzene ring to the chemical shifts of the corresponding aromatic protons or carbons of the parent aniline, or by adding the incremental shifts due to $-\text{NHCOCH}_{3-i}\text{X}_i$ groups and the substituents in the benzene ring to the chemical shift of the benzene proton or carbon. The calculated chemical shifts of the aromatic protons and carbons of all the substituted amides by both methods lead to almost the same values in most cases and agree well with the observed chemical shifts, indicating that the principle of additivity of the substituent effects is valid in these compounds.

Key words: Substituted Aryl Acetamides; Infrared; ^1H and ^{13}C NMR Spectra.