Synthetic, Infrared, ^{1}H and ^{13}C NMR Spectral Studies on N-(2-/3-Substituted Phenyl)-4-Substituted Benzenesulphonamides, 4-X'$C_6H_4SO_2NH$(2-/3-XC_6H_4), where X' = H, CH_3, C_2H_5, F, Cl or Br, and X = CH_3 or Cl

B. Thimme Gowda, Mahesha Shetty, and K. L. Jayalakshmi

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.

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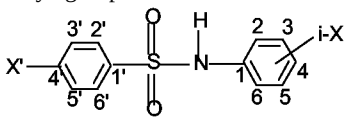
Twenty three N-(2-/3-substituted phenyl)-4-substituted benzenesulphonamides of the general formula, 4-X'$C_6H_4SO_2NH$(2-/3-XC_6H_4), where X' = H, CH_3, C_2H_5, F, Cl or Br and X = CH_3 or Cl have been prepared and characterized, and their infrared spectra in the solid state, ^{1}H and ^{13}C NMR spectra in solution were studied. The N-H stretching vibrations, ν_{N-H}, absorb in the range 3285 – 3199 cm^{-1}, while the asymmetric and symmetric SO_2 vibrations vary in the ranges 1376 – 1309 cm^{-1} and 1177 – 1148 cm^{-1}, respectively. The S-N and C-N stretching vibrations absorb in the ranges 945 – 893 cm^{-1} and 1304 – 1168 cm^{-1}, respectively. The compounds do not exhibit particular trends in the variation of these frequencies on substitution either at *ortho* or *meta* positions with either a methyl group or Cl. The observed ^{1}H and ^{13}C chemical shifts of



are assigned to protons and carbons of the two benzene rings. Incremental shifts of the ring protons and carbons due to –SO_2NH(2-/3-XC_6H_4) groups in $C_6H_5SO_2NH$(2-/3-XC_6H_4), and 4-X'$C_6H_4SO_2$- and 4-X'$C_6H_4SO_2NH$- groups in 4-X'$C_6H_4SO_2NH(C_6H_5)$ are computed and employed to calculate the chemical shifts of the ring protons and carbons in the substituted compounds, 4-X'$C_6H_4SO_2NH$(2-/3-XC_6H_4). The computed values agree well with the observed chemical shifts.

Key words: IR; ^{1}H and ^{13}C NMR; N-(Substituted phenyl)-4-substituted Benzenesulphonamides.