Synthetic and Spectroscopic Studies on N-(i,j-Disubstituted Phenyl)-4-Substituted Benzenesulphonamides, 4-X’C₆H₄SO₂NH(i,j-X₂C₆H₃), where X’ = H, CH₃, C₂H₅, F, Cl or Br; i, j = 2, 3; 2, 4; 2, 5; 2, 6 or 3, 4; and X = CH₃ or Cl

Mahesha Shetty and B. Thimme Gowda
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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Fifty four N-(i,j-disubstituted phenyl)-4-substituted benzenesulphonamides of the general formula 4-X’C₆H₄SO₂NH(i,j-X₂C₆H₃), where X’ = H, CH₃, C₂H₅, F, Cl or Br; i, j = 2, 3; 2, 4; 2, 5; 2, 6 or 3, 4; and X = CH₃ or Cl, are prepared and characterized and their infrared, ¹H and ¹³C NMR spectra in solution are studied. The N-H stretching vibrations νN–H absorb in the range 3305 – 3205 cm⁻¹, while the asymmetric and symmetric SO₂ vibrations vary in the ranges 1377 – 1307 cm⁻¹ and 1184 – 1128 cm⁻¹, respectively. The N-(i,j-disubstituted phenyl)-4-substituted benzenesulphonamides show C-S, S-N and C-N stretching vibrations in the ranges 844 – 800 cm⁻¹, 945 – 891 cm⁻¹ and 1309 – 1170 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 ¹H and ¹³C chemical shifts of

![Chemical Structure]

are assigned to protons and carbon atoms of the two benzene rings. Incremental shifts of the ring protons and carbon atoms due to –SO₂NH(i,j-X₂C₆H₃) groups in C₆H₅SO₂NH(i,j-X₂C₆H₃) and 4-X’C₆H₄SO₂NH– groups in 4-X’C₆H₄SO₂NH(C₆H₅) are computed and employed to calculate the chemical shifts of the ring protons and carbon atoms in the substituted compounds 4-X’C₆H₄SO₂NH(i,j-X₂C₆H₃). The different methods of calculation lead to almost the same values in most cases and agree well with the observed chemical shifts, indicating the validity of the principle of additivity of the substituent effects with chemical shifts in these compounds.

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