Synthetic and Spectroscopic Studies on N-(i,j-Disubstituted Phenyl)-4-Substituted Benzenesulphonamides, 4-X'$C_6H_4SO_2NH$(i,j-$X_2C_6H_3$), where X' = H, CH_3, C_2H_5, F, Cl or Br; i, j = 2, 3; 2, 4; 2, 5; 2, 6 or 3, 4; and X = CH_3 or Cl

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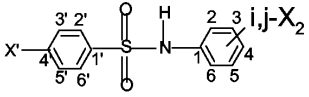
Fifty four N-(i,j-disubstituted phenyl)-4-substituted benzenesulphonamides of the general formula 4-X'$C_6H_4SO_2NH$(i,j-$X_2C_6H_3$), where X' = H, CH_3, C_2H_5, F, Cl or Br; i, j = 2, 3; 2, 4; 2, 5; 2, 6 or 3, 4; and X = CH_3 or Cl, are prepared and characterized and their infrared, ^{1}H and ^{13}C NMR spectra in solution are studied. The N-H stretching vibrations ν_{N-H} absorb in the range 3305 – 3205 cm^{-1}, while the asymmetric and symmetric SO_2 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 ^{1}H and ^{13}C chemical shifts of



are assigned to protons and carbon atoms of the two benzene rings. Incremental shifts of the ring protons and carbon atoms due to –SO_2NH(i,j-$X_2C_6H_3$) groups in $C_6H_5SO_2NH$(i,j-$X_2C_6H_3$) 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 carbon atoms in the substituted compounds 4-X'$C_6H_4SO_2NH$(i,j-$X_2C_6H_3$). 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; ^{1}H and ^{13}C NMR; N-(Disubstituted phenyl)-4-substituted Benzenesulphonamides.