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

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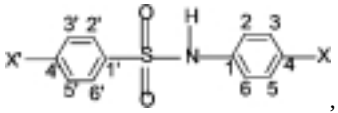
Thirty N-(*p*-substituted phenyl)-*p*-substituted benzenesulphonamides of the general formula, *p*-X'$C_6H_4SO_2NH$(*p*-XC_6H_4), where X' or X = H, CH_3, C_2H_5, F, Cl or Br, are synthesised and their infrared spectra in the solid state and ^{1}H and ^{13}C NMR spectra in solution are measured. The N-H stretching vibrational frequencies, ν_{N-H} vary in the range 3334 – 3219 cm^{-1}, while the asymmetric and symmetric SO_2 vibrations appear in the ranges 1377 – 1311 cm^{-1} and 1182 – 1151 cm^{-1}, respectively. The compounds exhibit S-N and C-N stretching vibrational absorptions in the ranges 937 – 898 cm^{-1} and 1310 – 1180 cm^{-1}, respectively. There are no particular trends in the variation of these frequencies on substitution with either electron withdrawing or electron donating groups. The ^{1}H and ^{13}C chemical shifts of N-(*p*-substituted phenyl)-*p*-substituted benzenesulphonamides,



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are assigned to various protons and carbons of the two benzene rings. Further, incremental shifts of the ring protons and carbons due to –SO_2NH(*p*-XC_6H_4) groups in the compounds of the formula, $C_6H_5SO_2NH$(*p*-XC_6H_4), and *p*-X'$C_6H_4SO_2$- and *p*-X'$C_6H_4SO_2NH$- groups in the compounds of the formula, *p*-X'$C_6H_4SO_2NH(C_6H_5)$ are computed and used to calculate the ^{1}H and ^{13}C chemical shifts of the parallely substituted compounds of the general formula *p*-X'$C_6H_4SO_2NH$(*p*-XC_6H_4). The computed values agree well with the observed chemical shifts. The above incremental shifts are found to correlate with the Hammett substituent parameters.

Key words: IR; ^{1}H and ^{13}C NMR; N-(*p*-substitutedphenyl)-*p*-substitutedbenzenesulphonamides.