Synthetic, Infrared and NMR (^{1}H and ^{13}C) Spectral Studies of N-(Substituted Phenyl)-Methanesulphonamides

K. L. Jayalakshmi 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

Z. Naturforsch. **59a,** 491 – 500 (2004); received February 19, 2004

Twenty two N-(substituted phenyl)-methanesulphonamides of the general formula, CH_3SO_2NHR, where R = 4-XC_6H_4(X = H, CH_3, F, Cl, Br or NO_2), *i*-XC_6H_4(X = CH_3, Cl or NO_2 and $i = 2$ or 3) and *i*, *j*-$X_2C_6H_3$(*i*, *j*-X_2 = 2,3-$(CH_3)_2$, 2,4-$(CH_3)_2$, 2,5-$(CH_3)_2$, 2,6-$(CH_3)_2$, 3,5-$(CH_3)_2$, 2,3-Cl_2, 2,4-Cl_2, 2,5-Cl_2, 2,6-Cl_2 or 3,4-Cl_2) were prepared, characterized and their infrared spectra in the solid state and the NMR (^{1}H and ^{13}C) spectra in solution studied. The N-H stretching vibrations absorb in the range, 3298 – 3232 cm^{-1}. Asymmetric and symmetric SO_2 stretching vibrations appear as strong absorptions in the ranges, 1331 – 1317 cm^{-1} and 1157 – 1139 cm^{-1}, respectively. The sulphonamides exhibit S-N stretching vibrations in the range, 926 – 833 cm^{-1}. The effect of substitution in the phenyl ring in terms of electron withdrawing and electron donating groups is non-systematic. The ^{1}H and ^{13}C chemical shifts of N-(substituted phenyl)-methanesulphonamides are assigned to various protons and carbons of the compounds. Further, incremental shifts of the ring protons and carbons due to CH_3SO_2- and CH_3SO_2NH- groups in the N-(phenyl)-methanesulphonamide are computed and used to calculate the ^{1}H and ^{13}C chemical shifts of various protons and carbons of N-(substituted phenyl)-methanesulphonamides, by adding substituent contributions to the corresponding aromatic proton or carbon chemical shifts of either aniline, substituted anilines, benzene or substituted benzenes, in different ways, as per the principle of substituent addition. The computed values by different procedures agree well with each other and with the experimental chemical shifts. The correlation of these incremental shifts with the Hammett substituent parameters is poor.

Key words: Infrared; ^{1}H and ^{13}C NMR; N-(substituted phenyl)-methanesulphonamides.