Synthetic, Infrared, ^{1}H and ^{13}C NMR Spectral Studies on Potassium Salts of N-Chloroarylsulphonamides

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Several N-chloroarylsulphonamides of the configuration, 4-X-$C_6H_4SO_2(K)NCl\cdot xH_2O$ (where X = H, CH_3, C_2H_5, F, Cl or Br) and *i*-X, *j*-Y$C_6H_3SO_2(K)NCl\cdot xH_2O$ (where *i*-X, *j*-Y = 2,3-$(CH_3)_2$; 2,4-$(CH_3)_2$; 2,5-$(CH_3)_2$; 2-CH_3,4-Cl; 2-CH_3,5-Cl; 3-CH_3,4-Cl; 2,4-Cl_2 or 3,4-Cl_2) are prepared, characterised, and their infrared spectra in the solid state and NMR spectra in solution are measured and correlated. Comparison of the infrared spectra of the potassium salts of N-chloro-arylsulphonamides with the corresponding arylsulphonamides shows that the strong absorptions in the range 947 – 933 cm^{-1} are due to N-Cl stretching vibrations. The effect of ring substitution on the N-Cl frequencies is non-uniform. The frequencies in the ranges 1404 – 1370 cm^{-1} and 1149 – 1125 cm^{-1} are respectively assigned to S=O asymmetric and symmetric vibrations. The effect of substitution in the phenyl ring in terms of electron withdrawing and electron donating groups is non-systematic. Empirical correlations relating the chemical shifts to the structures are considered. The chemical shifts of aromatic protons and carbons in all the N-chloroarylsulphonamides have been calculated by adding substituent contributions to the shift of benzene, as per the principle of substituent addition. Considering the approximation made, the agreement between the calculated and experimental chemical shifts is reasonably good.

Key words: Synthetic, Infrared, ^{1}H and ^{13}C NMR Spectra; N-Chloroarylsulphonamides.