

Infrared, ^1H and ^{13}C NMR Spectra of N,N-Dichloroarylsulphonamides, 4-X-C₆H₄SO₂NCl₂ (X = H, CH₃, C₂H₅, F, Cl or Br) and *i*-X, *j*-YC₆H₃SO₂NCl₂ (*i*-X, *j*-Y = 2,3-(CH₃)₂, 2,4-(CH₃)₂, 2,5-(CH₃)₂, 2-CH₃, 4-Cl, 2-CH₃, 5-Cl, 3-CH₃, 4-Cl, 2,4-Cl₂ or 3,4-Cl₂)

B. Thimme Gowda, K. Jyothi, and N. Damodara

Department of Post-Graduate Studies and Research in Chemistry, Mangalore University,
Mangalagangothri- 574 199, Mangalore, India

Reprint requests to Prof. B. Th. G. Fax: 0091 824 287 367; E-mail: gowdabt@yahoo.com

Z. Naturforsch. **58a**, 563 – 568 (2003); received November 25, 2002

Several mono- and di-substituted N,N-dichloroarylsulphonamides of the configuration, 4-X-C₆H₄SO₂NCl₂ (where X = H, CH₃, C₂H₅, F, Cl or Br) and *i*-X, *j*-YC₆H₃SO₂NCl₂ (where *i*-X, *j*-Y = 2,3-(CH₃)₂, 2,4-(CH₃)₂, 2,5-(CH₃)₂, 2-CH₃, 4-Cl, 2-CH₃, 5-Cl, 3-CH₃, 4-Cl, 2,4-Cl₂ or 3,4-Cl₂), respectively, were prepared, characterised and their infrared spectra in the solid state and NMR spectra in solution state were measured and correlated. Comparison of the infrared spectra of the N,N-dichloroarylsulphonamides with the corresponding arylsulphonamides and N-chloroarylsulphonamides revealed that the infrared absorption bands in the ranges, 790 – 735 cm⁻¹ and 595 – 546 cm⁻¹ are due to N-Cl asymmetric and symmetric stretching vibrations, respectively, and that the effect of ring substitution on the N-Cl frequencies is not consistent. The frequencies in the ranges 1384 – 1333 cm⁻¹ and 1181 – 1143 cm⁻¹ are, respectively, assigned to S=O asymmetric and symmetric modes of vibration. The effect of substitution in the phenyl ring in terms of electron withdrawing and electron donating groups is non-systematic. Since the chemical shift depends on the electron density around the nucleus, empirical correlations relating the chemical shifts to the structures have been considered. The chemical shifts of aromatic protons and carbons in all the N,N-dichloroarylsulphonamides have been calculated by adding substituent contributions to the shift of benzene. Considering the approximation made, the agreement between the calculated and experimental chemical shifts is good.

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