

**Infrared and NMR Spectra of Arylsulphonamides,
4-X-C₆H₄SO₂NH₂ and *i*-X, *j*-YC₆H₃SO₂NH₂ (X = H; CH₃; C₂H₅;
F; Cl; Br; I or NO₂ and *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 J. D. D'Souza

Department of Post-Graduate Studies and Research in Chemistry, Mangalore University,
Mangalagangothri-574199, Mangalore, India

Reprint requests to Prof. B. T. G.; Fax: +91 824 287 367; e-mail: gowdabt@yahoo.com

Z. Naturforsch. **57a**, 967–973 (2002); received August 14, 2002

Several arylsulphonamides of the configuration, 4-X-C₆H₄SO₂NH₂ (where X = H; CH₃; C₂H₅; F; Cl; Br; I or NO₂) and *i*-X, *j*-YC₆H₃SO₂NH₂ (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) were prepared, and their infrared spectra were measured in the solid state. The NMR spectra were recorded in solution. N–H asymmetric and symmetric stretching vibrations absorb in the ranges, 3390–3323 cm⁻¹ and 3279–3229 cm⁻¹, respectively. Asymmetric and symmetric SO₂ stretching vibrations appear as strong absorption lines in the ranges, 1344–1317 cm⁻¹ and 1187–1147 cm⁻¹, respectively. Sulphonamides exhibit S–N stretching vibrational absorptions in the range, 924–906 cm⁻¹. The effect of substitution in the phenyl ring in terms of electron withdrawing and electron donating groups could not be generalised, as the effect is non-systematic. The chemical shift is highly dependent on the electron density around the nucleus or associated with the atom to which it is bonded. Hence empirical correlations relating the chemical shifts to the structures have been discussed. The chemical shifts of aromatic protons and carbons in all the arylsulphonamides have been calculated by adding substituent contributions to the shift of benzene, the principle of substituent addition. Considering the approximation made, the agreement between the calculated and experimental chemical shift values is reasonably good. Generally, electron-withdrawing groups shows high chemical shifts compared to electron-donating groups.

Key words: Infrared; Nuclear Magnetic Resonance; Arylsulphonamides.