Spectroscopic Studies with N-Chloroarylsulphonamides: IR and  $^{1}$ H,  $^{13}$ C and  $^{23}$ Na NMR Spectra of Sodium Salts of N-Chloro-Mono- and Di-Substituted-Benzenesulphonamides, 4-X-C $_{6}$ H $_{4}$ SO $_{2}$ NaNCl (X = H; CH $_{3}$ ; C $_{2}$ H $_{5}$ ; F; Cl; Br; I or NO $_{2}$ ) and i-X, j-YC $_{6}$ H $_{3}$ SO $_{2}$ NaNCl (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 $_{2}$ )

B. Thimme Gowda, J. D. D'Souza, and B. H. Arun Kumar

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

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

Z. Naturforsch. **58a.** 51 – 56 (2003); received October 25, 2002

In an effort to introduce N-chloroarylsulphonamides of different oxydising strengths, sixteen sodium salts of N-chloro-mono- and di-substituted benzenesulphonamides of the configuration, 4-X-C<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>NaNCl (where X = H; CH<sub>3</sub>; C<sub>2</sub>H<sub>5</sub>; F; Cl; Br; I or NO<sub>2</sub>) and i-X, j-YC<sub>6</sub>H<sub>3</sub>SO<sub>2</sub>NaNCl (where i-X, j-Y = 2,3-(CH<sub>3</sub>)<sub>2</sub>; 2,4-(CH<sub>3</sub>)<sub>2</sub>; 2,5-(CH<sub>3</sub>)<sub>2</sub>; 2-CH<sub>3</sub>,4-Cl; 2-CH<sub>3</sub>,5-Cl; 3-CH<sub>3</sub>,4-Cl; 2,4-Cl<sub>2</sub> or 3,4-Cl<sub>2</sub>) are prepared, characterized through their infrared spectra in the solid state and NMR spectra in solution. The  $v_{N$ —Cl frequencies vary in the range 950–927 cm<sup>-1</sup>. Effects of substitution in the benzene ring in terms of electron donating and electron withdrawing groups have been considered, and conclusions drawn. The chemical shifts of aromatic protons and carbon-13 in all the N-chloroarylsulphonamides have been calculated by adding substituent contributions to the shift of benzene. Considering the approximation employed the agreement between the calculated and experimental chemical shift values for different protons or carbon-13 is quite good. Effects of phenyl ring substitution on chemical shift values of both <sup>1</sup>H and <sup>13</sup>C are also graphically represented in terms of line diagrams.

Key words: Infrared; Nuclear Magnetic Resonance; N-Chloroarylsulphonamides.