

Infrared and NMR (^1H & ^{13}C) Spectra of Sodium Salts of N-Bromo-Mono and Di-Substituted-Benzenesulphonamides

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Fifteen sodium salts of mono and di-substituted N-bromobenzene-sulphonamides of the configuration, 4-X-C₆H₄SO₂NaNBr (where X = H; CH₃; C₂H₅; F; Cl; Br; or NO₂) and i-X,j-YC₆H₃SO₂NaNBr (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) are prepared and characterised by measuring their infrared spectra in the solid state and NMR spectra in solution. The N-Br vibrational frequencies, $\nu_{\text{N-Br}}$ of N-bromoarylsulphonamides vary in the range, 945 – 925 cm⁻¹, while the N-Cl vibrational frequencies, $\nu_{\text{N-Cl}}$, are observed in the range 950 – 927 cm⁻¹ for the corresponding N-chloroarylsulphonamides. Asymmetric and symmetric SO₂ stretching vibrations appear in the ranges, 1391 – 1352 cm⁻¹ and 1148 – 1131 cm⁻¹ for the monosubstituted N-bromoarylsulphonamides, while for the disubstituted N-bromocompounds they absorb in the ranges 1391 – 1331 cm⁻¹ and 1149 – 1121 cm⁻¹, respectively. The chemical shifts of aromatic protons and carbon-13 in all the N-bromoarylsulphonamides have been calculated by adding substituent contributions to the shift of benzene and compared with the observed values. The agreement between the calculated and experimental chemical shifts for different protons or carbon-13 is quite good.

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