^{35}Cl NQR Spectra of N-(substitutedphenyl)-2,2-dichloroacetamides and Correlation of ^{35}Cl NQR γCl(ω) of Substituted N-Phenyl-Chloroacetamides $X_yC_6H_{5-y}NHCOR$ (X = Cl or CH_3, y = 1 or 2, R = CH_2Cl, $CHCl_2$ or CCl_3)

B. Thimme Gowda, B. H. Arun Kumar, and Hartmut Fuess[a]

Department of Studies in Chemistry, Mangalore University,
Mangalagangothri 574199, Mangalore, India
[a] Institute of Materials Science, Darmstadt University of Technology,
Petersenstrasse 23, D-64287 Darmstadt

Reprint requests to Prof. B. T. G.; Fax: 0091 824 742367; e-mail: gowdabt@yahoo.com

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To study the effect of electron donating or repelling group substitution in the phenyl ring on the γ(^{35}Cl NQR of Cl(ω)) of the dichloroacetyl group, several N-(methylsubstituted-phenyl)-2,2-dichloroacetamides have been synthesised, characterised and their ^{35}Cl NQR frequencies measured at 77 K. All the substituted amides, except N-(2,5-dimethylphenyl)-2,2-dichloro-acetamide, show two ω-C-Cl frequencies in the range of 37.009 - 38.014 MHz. N-(2,5-dimethylphenyl)-2,2-dichloroacetamide shows one ω-C-Cl NQR frequency at 37.50 MHz for the two chlorine atoms present. The two atoms may be crystallographically equivalent. The frequencies of all the methyl-substituted dichloroacetamides have been compared and correlated alongwith the corresponding chloro substituted-phenyl dichloroacetamides. The γ(^{35}Cl NQR) of Cl(ω) of all the N-(substituted-phenyl)-2,2-dichloroacetamides have been correlated with the NQR substituent parameters (κ), assuming additivity of the substituent effects. The frequencies are also correlated with Hammett σ. The effect of ring substitution on the average ^{35}Cl NQR Cl(ω) frequencies of the dichloroacetyl group is not substantial, but it affects the crystal structures of the substituted compounds. Using the κ_i values for various groups and ω-C-Cl NQR frequencies of N-(phenyl)-2,2-dichloroacetamide (37.195 and 37.596 MHz), γ(^{35}Cl NQR) of all the N-(methyl and chlorosubstitutedphenyl)-2,2-dichloroacetamides have been estimated. Similar calculations are extended to all the N-(methyl and chlorosubstitutedphenyl)-2-chloroacetamides and -2,2,2-trichloroacetamides. There is a reasonably good agreement between the computed and the experimental values for all the three groups of compounds. Further, γ(^{35}Cl NQR of Cl(ω)) of all the substituted N-phenyl-chloroacetamides represented by the general formula $X_yC_6H_{5-y}NHCOR$ (where X = Cl, or CH_3, y = 1 or 2 and R = CH_2Cl, $CHCl_2$ or CCl_3) are compared. The γ(^{35}Cl NQR of Cl(ω)) of the substituted N-(phenyl)-2,2-dichloroacetamides lie between the frequencies of the corresponding substituted N-(phenyl)-2-chloroacetamides and substituted N-(phenyl)-2,2,2-trichloroacetamides.

Key words: Nuclear Quadrupole Resonance; Aryl Dichloroacetamides.