³⁵Cl NQR Spectra of Substituted N-(phenyl)-2-chloroacetamides

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Fifteen methyl-, nitro-, or mixed substituted N-(phenyl)-2-chloroacetamides were investigated by 35 Cl NQR. The temperature dependence of the frequencies of the 3-methylphenyl and 2,6-dimethylphenyl derivatives were studied for the range 77 K<T<300 K. Only one ω C–Cl frequency was observed for the compound with the two exceptions. For N-(2-nitro,4-chlorophenyl)-2-chloroacetamide the observed values of 35.623 and 35.350 MHz were assigned to ω C–Cl and ring C–Cl, whereas the corresponding values are 36.254 and 34.815 MHz for N-(2-methyl, 3-chlorophenyl)-2-chloroacetamide. The experimental frequencies of all compounds have been compared with values estimated from NQR substituent parameters 'k' and the frequency of N-(phenyl)-2-chloroacetamide. The agreement is remarkably good with a maximum deviation of 1.64 MHz. Furthermore γ (35 Cl) of all compounds has been correlated with Σ k_i and with the Hammett constants.

Key words: Nuclear Quadrupole Resonance; Chloroacetamide.