^{35}Cl NQR Spectra of Substituted N-(Phenyl)-2,2,2-Trichloroacetamides

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Several substituted acetamides, $X_yC_6H_{5-y}NHCOCCl_3$ (X=CH_3, NO_2, or Br and y=1 or 2) have been synthesized and studied by NQR. The effect of ring substitution on the average $\nu(^{35}Cl)$ NQR of the trichloroacetyl group is not substantial, but it affects the crystal structure of the substituted compounds. The NQR spectra of $X_yC_6H_{5-y}NHCOCCl_3$ (where X_y=4–CH_3, 4–NO_2, and 2,3–$(CH_3)_2$) show six ^{35}Cl NQR frequencies, each indicating the presence of two molecules in their respective asymmetric units. The temperature dependence of $\nu(^{35}Cl)$ NQR of N-(4-methylphenyl)-2,2,2-trichloroacetamide reveals that it undergoes a first order phase transition around 205 K. Its spectrum shows six lines up to 205 K and three lines thereafter. The latter triplet part of the spectrum fades out around 250 K due to librational motions in the crystal lattice, as the torsional motions of the CCl_3 group are easily excited. The ^{35}Cl NQR spectra of all the methylsubstituted amides have been compared with those of the corresponding chlorosubstituted compounds. Generally there is no systematic variation of the mean values of $\nu(^{35}Cl)$ NQR or the trichloroacetyl group with the substituents in the phenyl ring. The ω C-Cl frequencies of the trichloroacetyl group of all the ν-substituted N-(phenyl)-2,2,2-trichloroacetamides have been estimated using NQR substituent parameters (k) and the frequencies of N-(phenyl)-2,2,2-trichloroacetamide. Agreement between these values and the experimental frequencies is quite good. The $\nu(^{35}Cl)$ NQR of these amides has also been correlated with Σk_i of the substituents. Further $\nu(^{35}Cl)$ NQR spectra of mono- and trichloroacetamides have been correlated.

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