^{35}Cl NQR and Structural Studies on Substituted Amides, $X_yC_6H_{5-y}NHCOR$ (X = H or Cl; y = 0, 1 or 2 and R = $C(CH_3)_3$, $CHClCH_3$, C_6H_5 or 2-ClC_6H_4)

B. Thimme Gowda, K. Jyothi, Helmut Paulus[a], and Hartmut Fuess[a]

Mangalore University Department of Chemistry, Mangalagangotri-574 199, Mangalore, India
[a] Darmstadt University of Technology, Institute of Materials Science, D-64287 Darmstadt, Germany

Reprint requests to Prof. B. T. G.; Fax: +91 824 287367; E-mail: gowdabt@yahoo.com or
Prof. H. Fuess; Fax: +49 6151 166023; E-mail: hfuess@tu-darmstadt.de

Z. Naturforsch. **58a,** 225 – 230 (2003); received January 3, 2003

^{35}Cl NQR frequencies of some N-(substitutedphenyl)-amides represented by the general formula, $X_yC_6H_{5-y}NHCOR$ (where X = H or Cl; y = 0, 1 or 2 and R = H, CH_3, CH_2CH_3, $CH(CH_3)_2$, $C(CH_3)_3$, CH_2Cl, $CHCl_2$ or CCl_3) have been measured and compared with those of other compounds in the family to analyse the effect of substitution in the side chain on the frequencies. Comparison of ^{35}Cl NQR frequencies of all the N-(2-chlorophenyl)- and N-(2,6-dichlorophenyl)-amides reveals that the presence of alkyl groups in the side chain lowers the frequency, while that of aryl or chloro-substituted alkyl groups enhance the frequencies to some extent, when compared to the frequencies of either N-(2-chlorophenyl)-acetamide or N-(2,6-dichlorophenyl)-acetamide. In addition, the crystal structures of N-(phenyl)-2-chloro-2-methylacetamide ($C_6H_5NHCOCHClCH_3$) and N-(phenyl)-2-chloro-benzamide (C_6H_5NHCO-(2-ClC_6H_4)) have been determined and the data analysed along with the crystal structures of related compounds. The data (lattice constants in Å) of the new structures are: C_6H_5NHCO- $CHClCH_3$: monoclinic, $P2_1/c$, $Z = 4$, $a = 10.879(2)$, $b = 9.561(2)$, $c = 10.067(2)$, β = 116.080(10)°; C_6H_5NHCO-(2-ClC_6H_4): tetragonal, P4(3), $Z = 4$, $a = 8.795(4)$, $b = 8.795(4)$, $c = 15.115(6)$, β = 90.0°. It is evident from a comparison, that the side chain substitution influences the C(S)-C(O) bond length, while the effect on the other bond lengths is not significant except for benzanilide. Similarly, only the side chain angles are affected to some extent. The variations do not show definite trends, probably due to the differences in the crystallisations.

Key words: Substituent Effect; ^{35}Cl NQR and Crystal Structures; Substituted Amides.