

^{35}Cl NQR and Structural Studies of N-(2,6-Dichlorophenyl)-Amides, 2,6- $\text{Cl}_2\text{C}_6\text{H}_3\text{-NHCO-R}$ (R = H or $\text{CH}_{3-y}\text{X}_y$ and X = CH_3 or Cl; y = 0, 1, 2 or 3)

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The effect of side chain substitution on the ^{35}Cl NQR and crystal structure of amides of the type N-(2,6-dichlorophenyl)-amides, 2,6- $\text{Cl}_2\text{C}_6\text{H}_3\text{-NHCO-R}$ (R = H or $\text{CH}_{3-y}\text{X}_y$ where X = CH_3 or Cl and y = 0, 1, 2 or 3), has been studied by measuring the ^{35}Cl NQR spectra and determining the crystal structures of the compounds N-(2,6-dichlorophenyl)-formamide, 2,6- $\text{Cl}_2\text{C}_6\text{H}_3\text{-NHCO-H}$ (**DCPFA**); N-(2,6-dichlorophenyl)-2-methylacetamide(propionamide), 2,6- $\text{Cl}_2\text{C}_6\text{H}_3\text{-NHCO-CH}_2\text{CH}_3$ (**DCPMA**); N-(2,6-dichlorophenyl)-2,2-dimethylacetamide(isobutyramide), 2,6- $\text{Cl}_2\text{C}_6\text{H}_3\text{-NHCO-CH}(\text{CH}_3)_2$ (**DCPDMA**) and N-(2,6-dichlorophenyl)-2,2,2-trimethylacetamide (neopentylamide), 2,6- $\text{Cl}_2\text{C}_6\text{H}_3\text{-NHCO-C}(\text{CH}_3)_3$ (**DCPTMA**), and by analysing the present data along with the ^{35}Cl NQR spectra and / or crystal structures of the compounds, 2,6-dichloroaniline, 2,6- $\text{Cl}_2\text{C}_6\text{H}_3\text{-NH}_2$ (**DCA**), N-(2,6-dichlorophenyl)-acetamide, 2,6- $\text{Cl}_2\text{C}_6\text{H}_3\text{-NHCO-CH}_3$ (**DCPA**), N-(2,6-dichlorophenyl)-2-chloroacetamide, 2,6- $\text{Cl}_2\text{C}_6\text{H}_3\text{-NHCO-CH}_2\text{Cl}$ (**DCPCA**), N-(2,6-dichlorophenyl)-2,2-dichloroacetamide, 2,6- $\text{Cl}_2\text{C}_6\text{H}_3\text{-NHCO-CHCl}_2$ (**DCPDCA**) and N-(2,6-dichlorophenyl)-2,2,2-trichloroacetamide, 2,6- $\text{Cl}_2\text{C}_6\text{H}_3\text{-NHCO-CCl}_3$ (**DCPTCA**). The crystal type, space group, formula units and lattice constants in Å of the new structures are: **DCPFA**: orthorhombic, Pbc_a, Z = 8, a = 8.593(3), b = 12.728(4), c = 14.376(4); **DCPMA**: orthorhombic, P2₁2₁, Z = 4, a = 4.774(2), b = 10.961(5), c = 19.562(8); **DCPDMA**: monoclinic, P2₁/c, Z = 4, a = 9.901(4), b = 13.785(5), c = 9.060(3), β = 103.58(2) $^\circ$ and **DCPTMA**: monoclinic, P2₁/n, Z = 8, a = 16.047(5), b = 9.882(3), c = 16.270(5) β = 102.12(1) $^\circ$. The compound, **DCPTMA** shows two molecules in its asymmetric unit. This is in agreement with the multiple lines observed in the ^{35}Cl NQR spectra of the compound. The conversion of **DCA** (monoclinic) into its various acid amides **DCPFA**, **DCPA**, **DCPMA**, **DCPDMA**, **DCPTMA**, **DCPCA** and **DCPTCA** affects its crystal symmetry. The replacement of the side chain CH_3 in **DCPA** by the H atom or substitution of either a CH_3 group or a Cl atom for one of the H atoms in the side chain CH_2 or replacement of the two ring Cl atoms by the H atoms changes its crystal symmetry from monoclinic to orthorhombic, while the substitution of 2 or all the 3 H atoms in the CH_2 group of **DCPA** by 2 or 3 CH_3 groups or Cl atoms restores its crystal symmetry back to the monoclinic type. The bond lengths and bond angles are normal except for some deviations.

Key words: ^{35}Cl NQR, Crystal Structures; N-2,6-dichlorophenyl-substituted amides.