# Structural Studies of N-(2,4,6-trisubstitutedphenyl)-Chloroacetamides, 2,4,6-$X_3C_6H_2$-NHCO-$CH_{3-y}Cl_y$ (X = $CH_3$ or Cl and $y$ = 1 - 3).

B. Thimme Gowda*, I. Svoboda, and Hartmut Fuess

Darmstadt University of Technology, Institute of Materials Science,
Petersenstr.23, D-64287 Darmstadt
*Permanent Address:* Mangalore University Department of Chemistry,
Mangalagangotri-574 199, India

Reprint requests to Prof. B. T. G.; Fax: +91 824 742 367; E-mail: gowdabt@yahoO-Com
or Prof. H. F.; Fax: +49 6151 166023; E-mail: hfuess@tu-darmstadt.de

Z. Naturforsch. **55 a,** 779–790 (2000); received July 6, 2000

The effect of side chain and ring substitutions on the crystal structures of N-(2,4,6-substituted-phenyl)-chloroacetamides of the type, 2,4,6-$X_3C_6H_2$-NHCO-$CH_{3-y}Cl_y$ (X = $CH_3$ or Cl and $1 \leq y \leq 3$), has been studied by determining the crystal structures of N-(2,4,6-trimethylphenyl)-2-chloroacetamide, 2,4,6-$(CH_3)_3C_6H_2$-NHCO-$CH_2Cl$ (**TMPMCA**); N-(2,4,6-trichlorophenyl)-2-chloroacetamide, 2,4,6-$Cl_3C_6H_2$-NHCO-$CH_2Cl$ (**TCPMCA**); N-(2,4,6-trichlorophenyl)-2,2-dichloroacetamide, 2,4,6-$Cl_3C_6H_2$-NHCO-$CHCl_2$ (**TCPDCA**) and N-(2,4,6-trichlorophenyl)-2,2,2-trichloroacetamide, 2,4,6-$Cl_3C_6H_2$-NHCO-$CCl_3$ (**TCPTCA**). The crystal type, space group, formula units and lattice constants in Å are: (**TMPMCA**); monoclinic, $P2_1/n$, $Z$ = 8, $a$ = 9.029(5), $b$ = 15.688(2), $c$ = 16.150(3), $\beta$ = 96.77(2)°; (**TCPMCA**): orthorhombic, $Pna2_1$, $Z$ = 8, $a$ = 30.708(4), $b$ = 4.685(1), $c$ = 14.506(2); (**TCPDCA**) orthorhombic, $P2_12_12$, $Z$ = 4, $a$ = 16.459(3), $b$ = 15.240(3), $c$ = 4.640(1) and (**TCPTCA**): triclinic, $P\bar{1}$, $Z$ = 4, $a$ = 9.828(2), $b$ = 11.953(2), $c$ = 12.278(2), $\alpha$ = 71.05(1)°, $\beta$ = 75.26(2)°, $\gamma$ = 83.29(1)°. The results have been analysed along with the structures of the ring unsubstituted N-phenylacetamide (**PA**), N-phenyl-2,2,2-trichloro-acetamide, side chain unsubstituted N-(2,4,6-trichlorophenyl)-acetamide, 2,4,6-$Cl_3C_6H_2$-NHCO-$CH_3$ (**TCPA**) and the corresponding di-substituted phenyl acetamides and chloroacetamides. The compounds **TMPMCA, TCPMCA** and **TCPTCA** have 2 molecules each in their asymmetric units. This is in agreement with the multiple lines observed in the $^{35}$Cl NQR spectra of **TCPTCA**. Further, this compound shows disorder as indicated by the multiplicity of the C(side chain) - Cl bonds. The compound **TCPMCA** does not show $^{35}$Cl NQR spectra, while the compound **TMPMCA** shows a single frequency which fades out above 200 K, indicating that it may undergo a phase transition well below room temperature. Conversion of 2,4,6-trichloroaniline into 2,4,6-trichlorophenyl acetamide and gradual replacement of H-atoms in the side chain of the latter decreases slightly the mean ring distances of the compounds, while the replacement of the 3 Cl by 3 $CH_3$ groups in the ring increases it's mean distance. Changes in the mean ring distances are smaller as the effect has to be transmitted through the peptide linkage. The molecules in compounds **TCPDCA** and **TCPTCA** are linked in chains by -NH—O– hydrogen bonds (about 3Å) between the amide groups of the molecules.

*Key words:* Crystal Structures; Trimethylphenyl-, Trichlorophenyl-chloroacetamides.