

# Structural Studies on N-(2,4,5-trichlorophenyl)-2-Chloro- and 2,2,2-trichloroacetamides and N-Chloro-N-(2,4,5-trichlorophenyl)-2-Chloroacetamide

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The effect of N-chloro, side chain and sites of ring substitutions on the crystal structure of N-(trichlorophenyl)-2-chloro and 2,2,2-trichloroacetamides has been studied by determining the crystal structure of N-(2,4,5-trichlorophenyl)-2-chloroacetamide,  $2,4,5\text{-Cl}_3\text{C}_6\text{H}_2\text{.NHCO.CH}_2\text{Cl}$  (N245TCPCA), N-chloro-N-(2,4,5-trichlorophenyl)-2-chloroacetamide,  $2,4,5\text{-Cl}_3\text{C}_6\text{H}_2\text{.NCICO.CH}_2\text{Cl}$  (NC245TCPCA) and N-(2,4,5-trichlorophenyl)-2,2,2-trichloroacetamide,  $2,4,5\text{-Cl}_3\text{C}_6\text{H}_2\text{.NHCO.CCl}_3$  (N245TCPTCA). The crystal type, space group, formula units and lattice constants in Å are: **N245TCPCA**: monoclinic,  $P2_1/n$ ,  $Z = 4$ ,  $a = 4.732(1)$ ,  $b = 29.522(3)$ ,  $c = 7.734(1)$ ,  $\beta = 108.33(1)^\circ$ ; **NC245TCPCA**: monoclinic,  $P2_1/c$ ,  $Z = 4$ ,  $a = 15.965(3)$ ,  $b = 9.398(1)$ ,  $c = 7.352(2)$ ,  $\beta = 91.51(2)^\circ$ ; **N245TCPTCA**: orthorhombic,  $Pmc2_1$ ,  $Z = 4$ ,  $a = 6.945(1)$ ,  $b = 11.370(3)$ ,  $c = 15.555(3)$ . The results are compared with the structure of N-(phenyl)-acetamide, N-(phenyl)-2,2,2-trichloroacetamide, N-(2-chlorophenyl)-2,2,2-trichloroacetamide, N-(4-chlorophenyl)-2,2,2-trichloroacetamide, N-(2,6-dichlorophenyl)-2,2,2-trichloroacetamide, N-(2,4,6-trichlorophenyl)-acetamide, N-(2,4,6-trichlorophenyl)-2-chloroacetamide and N-(2,4,6-trichlorophenyl)-2,2,2-trichloroacetamide. The comparison of the bond parameters reveal that there are significant changes by substitution in both the ring and side chain of the amides and by N-chlorination. But to draw general conclusions further, substantial work is needed with varying substitutions.

*Key words:* Crystal Structures; N-(2,4,5-trichlorophenyl)-chloroacetamides;  
N-chloro-N-(2,4,5-trichlorophenyl)-2-chloroacetamide.