# Structural Studies on Substituted *N*-(phenyl)-2,2-Dichloroacetamides, 2/4-$XC_6H_4$·NHCO·$CHCl_2$ (X = H, Cl or $CH_3$)

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The effect of substitution in the phenyl ring on the crystal systems of amides of the type, 2/4-$XC_6H_4$-NHCO-$CHCl_2$ (X = H, Cl or $CH_3$), has been studied by determining the crystal structures of the compounds, *N*-(phenyl)-2,2-dichloroacetamide, $C_6H_5$-NHCO-$CHCl_2$ (PhDCA); *N*-(2-chlorophenyl)-2,2-dichloroacetamide, 2-$ClC_6H_4$-NHCO-$CHCl_2$ (*o*-ClPhDCA), *N*-(4-chlorophenyl)-2,2-dichloroacetamide, 4-$ClC_6H_4$-NHCO-$CHCl_2$ (*p*-ClPhDCA) and *N*-(4-methylphenyl)-2,2-dichloroacetamide, 4-$CH_3C_6H_4$-NHCO-$CHCl_2$ (*p*-$CH_3$PhDCA) and analysed the data along with our earlier crystal structures of the compounds, *N*-(phenyl)-2,2,2-trichloroacetamide (PhTCA), *N*-(2-chlorophenyl)-2,2,2-trichloroacetamide (*o*-ClPhTCA), *N*-(4-chlorophenyl)-2,2,2-trichloroacetamide (*p*-ClPhTCA), *N*-(4-methylphenyl)-2,2,2-trichloroacetamide (*p*-$CH_3$PhTCA); *N*-chloro-*N*-(phenyl)-2,2-dichloroacetamide (NClPhDCA), *N*-chloro-*N*-(phenyl)-2,2,2-trichloroacetamide (NClPhTCA) and *N*-(phenyl) acetamide (PhA). The crystal type, space group, formula units and lattice constants in Å of the new structures are; PhDCA: monoclinic, $P2_1/c$, $Z = 4$, $a = 8.785(3)$, $b = 11.139(4)$, $c = 9.521(3)$, $\beta = 97.47(2)^\circ$; *o*-ClPhDCA: monoclinic, $P2_1/c$, $Z = 4$, $a = 4.711(2)$, $b = 11.234(6)$, $c = 19.191(8)$, $\beta = 98.12(2)^\circ$; *p*-ClPhDCA: monoclinic, $P2_1/c$, $Z = 8$, $a = 18.627(5)$, $b = 11.533(3)$, $c = 9.583(3)$, $\beta = 102.43(2)^\circ$, and *p*-$CH_3$PhDCA: orthorhombic, Pbca, $Z = 8$, $a = 9.464(3)$, $b = 9.894(3)$, $c = 21.973(7)$. The compound *p*-ClPhDCA 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 crystal systems of the chlorosubstituted and methyl substituted chloroacetamides get interchanged on replacement of the side chain -$CHCl_2$ by -$CCl_3$. C(i)-C(j) ring distances show no significant variations with the substitution either at the side chain or in the phenyl ring. C(ring)-N and C(O)-N bond distances are also not much affected by either ring or side chain substitution, but are affected by *N*-chlorination, while the C-O bond length is slightly shortened by the replacement of the -$CH_3$ group by -$CCl_3$, the introduction of electron withdrawing group into the phenyl ring or by *N*-chlorination. Deviations of C2(ring)-C1(ring)-N, C6(ring)-C1(ring)-N and C(ring)-N-C(O) bond angles from 120° narrow down on substitution either in the phenyl ring or in the side chain, but the latter increases on *N*-chlorination of the compounds.

*Key words:* Crystal Structures; Substituted *N*-phenyldichloroacetamides.