Effect of Substituent on Crystal Structures of N-(Substituted-phenyl)-2,2,2-Trichloroacetamides, 2/3/4-$XC_6H_4.NHCO.CCl_3$ (X = Cl, NO_2 or CH_3)

B. Thimme Gowda*, Helmut Paulus, 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: 0091 824 742367; e-mail: gowdabt@yahoo.com or Prof. H. F.; Fax: 0049 6151 166023; e-mail: hfuess@tu-darmstadt.de

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The crystal structures of N-(substitutedphenyl)-2,2,2-trichloroacetamides of the type 2/3/4-$XC_6H_4.NHCO.CCl_3$ (X = Cl, NO_2 or CH_3), namely, N-(3-nitrophenyl)-2,2,2-trichloroacetamide, 3-$NO_2C_6H_4.NHCO.CCl_3$ (**m-NO_2PhTCA**); N-(4-nitrophenyl)-2,2,2-trichloroacetamide, 4-$NO_2C_6H_4.NHCO.CCl_3$ (**p-NO_2PhTCA**); N-(2-chlorophenyl)-2,2,2-trichloroacetamide, 2-$ClC_6H_4.NHCO.CCl_3$ (**o-ClPhTCA**) and N-(4-chlorophenyl)-2,2,2-trichloroacetamide, 4-$ClC_6H_4.NHCO.CCl_3$ (**p-ClPhTCA**) have been determined at room temperature. The present data are analysed along with our earlier crystal structures of N-(2-nitrophenyl)-2,2,2-trichloroacetamide, 2-$NO_2C_6H_4.NHCO.CCl_3$ (**o-NO_2PhTCA**); N-(4-methylphenyl)-2,2,2-trichloroacetamide, 4-$CH_3C_6H_4$. $NHCO.CCl_3$ (**p-CH_3PhTCA**); N-(phenyl)-2,2,2-trichloroacetamide, $C_6H_5.NHCO.CCl_3$ (**PhTCA**); N-chloro-N-(phenyl)-2,2,2-trichloroacetamide, $C_6H_5.NClCO.CCl_3$ (**NClPhTCA**); and finally with N-(phenyl) acetamide, $C_6H_5.NHCO.CH_3$ (**PhA**). The crystal type, space group, formula units and lattice constants in Å of the new structures are; **m-NO_2PhTCA**: triclinic, P1, Z = 4, a = 7.493(3), b = 9.992(3), c = 15.225(5), α = 84.16(2)°, β = 82.59(2)°, γ = 84.92(2); **p-NO_2PhTCA**: monoclinic, $P2_1/n$, Z = 4, a = 5.807(2), b = 15.354(6), c = 12.475(5), β = 92.28(2)°; **o-ClPhTCA**: orthorhombic, $Pna2_1$, Z = 4, a = 8.769(2), b = 12.838(3), c = 9.578(2) and **p-ClPhTCA**: orthorhombic, Pbca, Z = 8, a = 9.742(4), b = 10.031(4), c = 23.110(9). The compounds, **m-NO_2PhTCA**, **o-NO_2PhTCA** and **p-CH_3PhTCA** show two molecules each in their asymmetric units. This is in agreement with the multiple lines observed in the ^{35}Cl NQR spectra of the latter two compounds. But the presence of two molecules in the asymmetric unit of **m-NO_2PhTCA** indicates that it may undergoe a phase transition below room temperature. The bond lengths and bond angles are normal except for some deviations. The presence of strong electron withdrawing group at the ortho position of the phenyl ring and N-chlorination of the amide will have significant effect on some bond distances and bond angles.

Key words: Substituent Effect; Crystal Structures; N-phenyltrichloroacetamides.