Structural Studies on N-(2,4,6-Trimethylphenyl)-methyl/chloro-acetamides, 2,4,6-(CH₃)₃C₆H₂NH-CO-CH_{3-y}X_y (X = CH₃ or Cl and y = 0, 1, 2)

Basavalinganadoddy Thimme Gowda^a, Jozef Kožíšek^b, and Hartmut Fuess^c

- ^a Department of Studies in Chemistry, Mangalore University, Mangalagangotri-574199, India
- b Department of Physical Chemistry, Slovak University of Technology, Bratislava, Slovak Republic
- ^c Institute of Materials Science, Darmstadt University of Technology, D-64287 Darmstadt, Germany

Reprint requests to Prof. B. T. G.; E-mail: gowdabt@yahoo.com

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The effect of substitutions in the ring and in the side chain on the crystal structure of N-(2,4,6-trimethylphenyl)-methyl/chloro-acetamides of the configuration 2,4,6-(CH₃)₃C₆H₂NH-CO- $CH_{3-\nu}X_{\nu}$ (X = CH₃ or Cl and $\nu = 0,1,2$) has been studied by determining the crystal structures of N-(2,4,6-trimethylphenyl)-acetamide, 2,4,6-(CH₃)₃C₆H₂NH-CO-CH₃ (TMPA); N-(2,4,6trimethylphenyl)-2-methylacetamide, 2,4,6-(CH₃)₃C₆H₂NH-CO-CH₂CH₃ (**TMPMA**); N-(2,4,6trimethylphenyl)-2,2-dimethylacetamide, 2,4,6-(CH₃)₃C₆H₂NH-CO-CH(CH₃)₂ (TMPDMA) and $N-(2,4,6-\text{trimethylphenyl})-2,2-\text{dichloroacetamide}, 2,4,6-(CH_3)_3C_6H_2NH-CO-CHCl_2$ (TMPDCA). The crystallographic system, space group, formula units and lattice constants in Å are: TMPA: monoclinic, $Pn, Z = 2, a = 8.142(3), b = 8.469(3), c = 8.223(3), \beta = 113.61(2)^{\circ}$; **TMPMA**: monoclinic, $P2_1/n$, Z=8, a=9.103(1), b=15.812(2), c=16.4787(19), $\alpha=89.974(10)^{\circ}$, $\beta=96.951(10)^{\circ}$, $\gamma = 89.967(10)^{\circ}$; **TMPDMA**: monoclinic, $P2_1/c$, Z = 4, a = 4.757(1), b = 24.644(4), c = 10.785(2), $\vec{\beta} = 99.647(17)^{\circ}$; **TMPDCA**: triclinic, $P\bar{1}$, Z = 2, a = 4.652(1), b = 11.006(1), c = 12.369(1), $\alpha = 82.521(7)^{\circ}$, $\beta = 83.09(1)^{\circ}$, $\gamma = 79.84(1)^{\circ}$. The results are analyzed along with the structural data of N-phenylacetamide, C₆H₅NH-CO-CH₃; N-(2,4,6-trimethylphenyl)-2-chloroacetamide, 2,4,6-(CH₃)₃C₆H₂NH-CO-CH₂Cl; N-(2,4,6-trichlorophenyl)-acetamide, 2,4,6-Cl₃C₆H₂NH-CO-CH₃; N-(2,4,6-trichlorophenyl)-2-chloroacetamide, 2,4,6-Cl₃C₆H₂NH-CO-CH₂Cl; N-(2,4,6-trichlorophenyl)-2,2-dichloroacetamide, 2,4,6-Cl₃C₆H₂NH-CO-CHCl₂ and N-(2,4,6-trichlorophenyl)-2,2,2-trichloroacetamide, 2,4,6-Cl₃C₆H₂NH-CO-CCl₃. **TMPA**, **TMPMA** and **TMPDCA** have one molecule each in their asymmetric units, while TMPDMA has two molecules in its asymmetric unit. Changes in the mean ring distances are smaller on substitution as the effect has to be transmitted through the peptide linkage. The comparison of the other bond parameters reveal that there are significant changes in them on substitution.

Key words: Crystal Structures; *N*-(2,4,6-Trimethylphenyl)-methyl/chloro-acetamides.