The Interplay between N-H…O Hydrogen Bonding and Cl…Cl Interactions in Arylformamides

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N-H…O hydrogen bonding occurs in both dichlorophenyl- and dimethylphenyl-formamides, regardless of the substitution pattern around the phenyl group (Fig. 1), forming infinite chains of molecules. We have found that while there are significant differences in the crystal structures of 2,6-dichlorophenyl- (**1**) and 2,6-dimethylphenylformamide (**2**) (Fig. 1), **1** undergoes a phase transformation to a phase isomorphous with that of 2,6-dimethylphenyl-formamide. The differences in these structures are rationalized in terms of the presence (2,6-dichoro) or absence (2,6-dimethyl) of Cl…Cl interactions. In addition the presence of a Me or Cl group in both phenyl ortho positions affects the conformation of the formamide group.

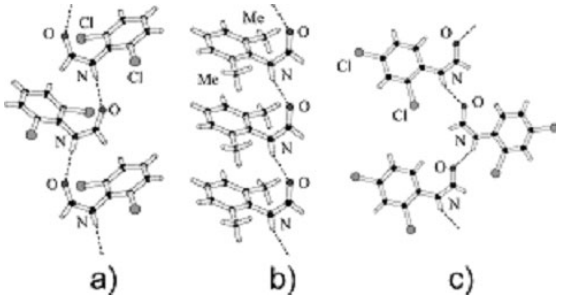

Figure 1. N-H…O hydrogen bonding patterns in (a) **1** (b) **2** (c) 2,4-dichlorophenylformamide.

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