

P.08.13.7*Acta Cryst.* (2005). A61, C340**The Crystal Structure of Tetraformylethane**

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cis-enol arrangement in β -diketones has recently been investigated [1,2]. These compounds prefer the *cis* arrangement with an *intra*-molecular hydrogen bond. When the terminal groups become small, as in the β -dialdehydes, the *trans*-enol form becomes more stable, at least in the solid-state, where the molecules form chains of *inter*-molecular bonds. Tetraformylethane prefers the *trans*-enolic isomer in the solid state, s. g. **Fddd**. $\frac{1}{2} + \frac{1}{4}$ of a molecule constitutes the asymmetric unit. $\frac{2}{3}$ of the molecules crystallize in asymmetric *inter*-molecular hydrogen bonded chains. The pairs of chains formed by centres of inversion comprise an antiferroelectric arrangement of oppositely polarized molecules. Single and double bonds are clearly recognizable but the amount of conjugation is amazingly high. The remaining $\frac{1}{3}$ of the molecules form chains of molecules situated on the intersection of three twofold axes, rendering single and double bonds indistinguishable. These molecules are connected by *inter*-molecular hydrogen bonds across centres of inversion with hydrogen bond distances slightly shorter than that of their asymmetric counterpart. The crystal structure was originally solved in a cell with an *a*-axis $\frac{1}{3}$ of that in the present study (also in **Fddd**). Photographic and diffractometric studies revealed the tripling of the *a*-axis. We venture to call the strange arrangement found "frustrated antiferroelectric".

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Keywords: hydrogen bond, super structure, organic molecule

P.08.13.8*Acta Cryst.* (2005). A61, C340**Computing the Solid-state: Novel Plane-wave DFT Approaches to Hydrogen Bonding**

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Hydrogen bonding is a critical link between crystallography and many physical, chemical and biological processes in condensed matter systems. Much of our recent work on hydrogen bonds has focused on multi-temperature and pressure X-ray and neutron diffraction, indicating often subtle behaviour of the hydrogen bonding present. Some of these effects challenge the limits of current experimental diffraction, and also our theories of hydrogen bond potentials.

As a complementary approach to this issue, we have been developing methods for studying hydrogen bonds in the solid state. These are based on the application of plane-wave (periodic) density functional theory calculations, which we have shown to be far superior in the study of a variety of hydrogen bonding systems. In addition we have developed advanced MD approaches to these calculations allowing us to examine computationally the temperature evolution of molecular structures in the solid state. This leads to a fuller understanding of the hydrogen bond potential and an improved description of structural evolution as observed in experiments.

These approaches will be illustrated by the results of a range of combined experimental and computational studies. Systems studied molecular complexes with short intermolecular hydrogen bonds, intramolecular hydrogen bonded structures, and dimeric systems containing subtle energy asymmetry leading to structural disorder.

Keywords: hydrogen bonds, ab initio periodical calculations, structural change

P.08.13.9*Acta Cryst.* (2005). A61, C340**Conformational and Database Study on the Intramolecular N-H \cdots π Interaction**

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In the last years, much work has been devoted to studying systems characterised by the so-called weak interactions. Between them, the N-H \cdots π interaction has been the subject of several theoretical [1], spectroscopic [2], and structural studies [3], and has been shown to take part in the folding of biological macromolecules [4], competing with the $\pi\cdots\pi$ stacking interactions. In particular, intramolecular X-H \cdots π bond has been found to influence the conformation of compounds containing both X-H and aromatic groups [5], [6].

Considering that several organic compounds, functionalized by aminic and aromatic groups linked by an aliphatic chain, are the parent structure for a variety of biologically important compounds, like dopamine or adrenaline, and have therapeutic potential [7], [8], we have decided to carry out a structural study of the intramolecular N-H \cdots π interaction.

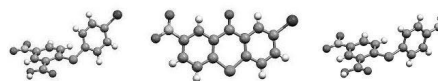
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Keywords: weak interactions, π -cloud, database study

P.08.13.10*Acta Cryst.* (2005). A61, C340**From Carboxylic Precursors to Thioxanthenes: Interplay of Hydrogen Bonds, Br \cdots Nitro, S \cdots Carbonyl and $\pi\cdots\pi$ Stacking Interactions**

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Recently large effort has been set into the synthesis of helical molecular systems, such as sterically overcrowded alkenes. These can be used as photorefractive materials as they allow the presence of measurable dipolar and magnetic contributions to NLO effects[1]. The helical environment is due to the presence of bulky substituents causing sufficient hindrance between the upper and lower half of the alkene to enforce a helical distortion [2]. We present here the results obtained in the precursors and thioxanthene used as basic templates. A systematic study of the intra and inter hydrogen bonds and intermolecular interactions is presented, due to its relevance in the folding and packing of the molecules [3].



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Keywords: hydrogen bond patterns, helical molecules, supramolecular assemblies

P.08.14.1*Acta Cryst.* (2005). A61, C340-C341**Structure Peculiarities of Polydisperse TiO₂ Particles with Metal-Modified Surface**

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