

**MS11.07.06 INVESTIGATION OF THE SOLID STATE CRYSTAL STRUCTURES OF CONJUGATED RIGID-ROD COMPOUNDS: PRELIMINARY ATTEMPTS TO CORRELATE PACKING WITH LIQUID CRYSTALLINE PHASE BEHAVIOUR.** A.J. Scott, W. Clegg, Department of Chemistry, University of Newcastle upon Tyne, Newcastle upon Tyne, NE1 7RU, UK.; C Dai, P. Nguyen, G. Lesley, F. Somera, M.P. Hirsch, N.J. Taylor, T.B. Marder, Department of Chemistry, University of Waterloo, Waterloo, Ontario, NL2 3G1, Canada; C. Viney, Department of Materials, University of Oxford, Parks Road, Oxford, OX1 3PH, UK; V.Chu, Department of Bioengineering, University of Washington, Seattle, WA, 98195, USA.

Rigid-rod shaped molecules are well-known for their tendency to form liquid crystalline phases. In order to probe the effect of substituents with differing electronic properties on liquid crystalline phase behaviour, a series of conjugated symmetric and unsymmetric ( $\pi$ -donor/ acceptor), rigid-rod compounds composed of alternating aryl and alkynyl groups have been prepared. The solid state single crystal structures of these bis(phenylethynyl)benzenes (BPEB's) and diphenyl acetylenes (tolans) have been determined with a view to understanding the relationship between packing in single crystals and thermotropic liquid crystalline phase behaviour.

**PS11.07.07 NITRO OXYGEN...HALOGEN INTERACTIONS: A COMBINED CRYSTALLOGRAPHIC DATABASE AND AB INITIO MOLECULAR ORBITAL STUDY.** Vanessa J. Hoy[a], Judith A. K. Howard[a], Frank H. Allen[b], Jos P. M., Lommerse[b] and Gautam R. Desiraju[c], [a] Department of Chemistry, University of Durham, South Rd., DURHAM, DH1, 3LE, U.K.; [b] C.C.D.C, 12 Union Rd., CAMBRIDGE, CB2 1EZ, U.K.; [c] School of Chemistry, University of Hyderabad, Central University PO, Hyderabad, 500046, India.

Recently it has been observed that the halogens, Cl, Br and I form mutual recognition motifs with nitro groups[1-3]. Interactions of this type are of interest because of their potential to act as substructural building blocks in crystal engineering applications[4]. The usefulness of X...O<sub>2</sub>N interactions for this purpose is critically dependant on our ability to predict their occurrence. In order to do that we must have some understanding of the nature and strength of the interaction.

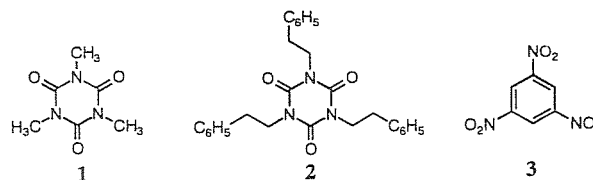
A previous crystallographic database study of X...O<sub>2</sub>N interactions[1] revealed that there are three X...O<sub>2</sub>N bonding modes; a symmetric P type, a skew Q type and an asymmetric R type. However, the precise geometric and energetic differences between these three were not investigated further.

In view of the limited scope of the previous study and the recent improvements in the Cambridge Crystallographic Database System's[5] three dimensional search software we felt that it was appropriate to perform a more complete analysis of the crystallographic results relating to X...O<sub>2</sub>N interactions and additionally, to obtain quantitative estimates of the interaction energies involved. The results of this study, together with relevant new structural data, will be presented.

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- 5 - Allen, F. H., Davies, J. E., Galloy, J. J., Johnson, O., Kennard, O., Macrae, C. F., Mitchell, E. M., Watson, D. G., *J. Chem. Inf. Comput. Sci.*, 1991, 31, 204.

**PS11.07.08 C-H...O BASED SOLID STATE SUPRAMOLECULAR ASSEMBLY:CRYSTAL STRUCTURE OF THE 1:2 COMPLEX OF TRIS (2PHENETHYL)-ISOCYANURATE-1,3,5-TRINITROBENZENE.** Venkat R.Thalladi,<sup>a</sup> Amy K.Katz,<sup>b</sup> H.L.Carrell<sup>b</sup> and Gautam R.Desiraju.<sup>a</sup> a.School of Chemistry, University of Hyderabad, Hyderabad 500 046, India b. Fox Chase Cancer Center, 7701 Burholme Avenue, Philadelphia, PA 19111, USA

Use of weak intermolecular interactions, especially C-H...O hydrogen bonds in the deliberate design of utilitarian crystal structures is a continuing challenge in crystal engineering.<sup>1</sup> We have shown that C-H...O hydrogen bonds play a vital role in stabilising the crystal structure of the 1:1 complex formed by trimethylisocyanurate, **1** and 1,3,5-trinitrobenzene, **3**.<sup>2</sup> This observation lead us to investigate structures governed solely by C-H...O hydrogen bonds. Accordingly, we crystallised the 1:2 complex of tris-(2-phenethyl)isocyanurate, **2** and **3**. In this structure, molecules of **2** and **3** form distinct stepwise linear supramolecular chains, assembled with C-H...O hydrogen bonds.



References:

- 1 G.R.Desiraju, *Crystal Engineering. The Design of Organic Solids*, Elsevier, Amsterdam, 1989; G.R.Desiraju, *Angew.Chem.Int.Ed. Engl.*, 1995, 34, 2311.
- 2 V.R.Thalladi, K.Panneerselvam, C.J.Carrell, H.L.Carrell and G.R.Desiraju, *J.Chem.Soc., Chem.Commun.*, 1995, 341.

**PS11.07.09 HYDROGEN BONDING IN BETAINE:PHENOL COCRYSTALS.** G.Buczak, A.Katrusiak, M.Szafran, Z.Dega-Szafran, Faculty of Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznan, Poland

Formation of hydrogen bonds in cocrystals built of betaine (BET) or its pyridine derivative (PBET) with pentachloro- or dichloronitrophenols has been studied. In these cocrystals short hydrogen bonds are formed between carboxyl groups of betaine and the hydroxyl groups of the phenols, linking these molecules into aggregates at 1:1 or 1:2 stoichiometries. The position of the H-atoms in these hydrogen bonds depends primarily on the proton-donor and acceptor properties of these molecules, however this study is also aimed at investigating the geometrical factors which may influence the hydrogen bond structure. The following cocrystals have been studied and their structures determined by X-ray diffraction:

- (i) BET:dichloronitrophenol 1:1 cocrystal; space group  $P\bar{1}$ ,  $R=0.0332$ ;
- (ii) PBET:dichloronitrophenol 1:1 cocrystal; space group  $P2_1/c$ ,  $R=0.0381$ ;
- (iii) PBET:dichloronitrophenol 1:2 cocrystal; space group  $P2_1/c$ ,  $R=0.0335$ ;
- (iv) PBET:pentachlorophenol 1:2 cocrystal; space group  $P\bar{1}$ ,  $R=0.0487$ ;

The O...O distances in the hydrogen bonds in these substances range from 2.419(3)Å in (i), to 2.623(4)Å in (ii). The structural data obtained for these compounds indicate that the geometrical and angular criteria described previously for chemically equivalent donor and acceptor groups [A.Katrusiak, *J.Mol.Struct.*269 (1992) 329; *Phys.Rev.* B48 (1993) 2992] can be also applied to the hydrogen bonds between the donor and acceptor groups which are chemically different.