

than optimal" [1]. Nevertheless, it is important to appreciate the preferred arrangement of functional groups within a non-covalent interaction if a crystal is to be engineered. An understanding of the relative energetics of different interaction motifs as well as the effect of changes in the geometry on the interaction energy is also crucial when designing or analysing crystal structures. Towards this goal a number of intermolecular interaction types have been investigated based on energy and geometry, including cyano...cyano contacts and hydrogen bonds to C=S acceptors. A combination of approaches has been used in this study to investigate the changes in the non-covalent interactions. Firstly, a study of structures available in the Cambridge Structural Database [2] has been performed to determine the relative directionalities of the interactions and their preferred geometries in the solid state. Intermolecular interaction energy calculations have then been carried out using intermolecular perturbation theory as implemented in the CADPAC 6.5 program package [3].

[1] Dunitz, J. D., Schweizer, W. B. (2007). *CrystEngComm*, 9, 266-269.

[2] Allen, F. H. (2002). *Acta Crystallographica*, Section B58, 380-388.

[3] Amos, R. D. et al. (1998). CADPAC 6.5, The Cambridge Analytic Derivatives Package.

Keywords: intermolecular interactions, energy calculations, cambridge structural database

P09.07.47

Acta Cryst. (2008). A64, C488

Controlling the formation of co-crystal polymorphs

Craig R Martin, Adam Jibson, Craig Wales, Andrew Parkin

University of Glasgow, Chemistry, A5-22a Joseph Black Building, Glasgow, West Lanarkshire, G12 8QQ, UK, E-mail : craima@chem.gla.ac.uk

Crystal engineering as a concept is approaching its 20th birthday, since first defined by Desiraju¹ in 1989. This area of chemistry has been of increasing importance, as our knowledge of the solid-state has developed. Crystal engineers have tended to focus solely on the single crystal products of their co-crystallisation experiments, although increasingly polymorphism is being observed in these products grown under different conditions². It seems, therefore, that as with traditional chemical synthesis and the crystallization of single-component systems, the method of synthesis can greatly affect the observed product. Polymorphism adds a new level to the challenge facing crystal engineers; not only is it necessary to understand the co-crystal (we use the term here in its broadest sense, encompassing all "multi-component" crystals) in terms of the supramolecular synthon, but to successfully predict and synthesise new co-crystal complexes it is also necessary to investigate the method of co-crystal formation. Our aim has been to prepare, characterise and control new co-crystal complexes by varying the physical conditions under which they are grown. This poster will present some results of our investigations into the control of polymorphism in co-crystals by using a range of solvents, and will illustrate how the combined use of a number of analytical techniques – including single crystal diffraction, powder diffraction, Differential Scanning Calorimetry and Infra-Red Spectroscopy – is necessary to fully investigate the compounds observed.

1. Desiraju, G.R. (1989). "Crystal Engineering: The design of Organic Solids." Amsterdam: Elsevier Academic Press.

2. Sreekanth, B.R., Vishweshwar, P and Vyas, K. (2007). *Chem. Comm.* 2375-2377.

Keywords: polymorphs, solvent effects, crystal engineering

P09.07.48

Acta Cryst. (2008). A64, C488

Comparing entire crystal structures: Structural genetic fingerprinting

Andrew Parkin¹, Gordon Barr¹, Wei Dong¹, Christopher J Gilmore¹, Dylan Jayatilaka², Joshua J McKinnon², Mark A Spackman², Chick C Wilson¹

¹University of Glasgow, Department of Chemistry, University Avenue, Glasgow, Lanarkshire, G12 8QQ, UK, ²Chemistry M313, School of Biomedical, Biomolecular & Chemical Sciences, University of Western Australia, Crawley, WA 6009, Australia., E-mail : a.parkin@chem.gla.ac.uk

A method is described that is both robust and generally applicable, which allows the calculation of a similarity index between whole molecular crystal structures [1]. It is based on the use of fingerprint plots derived from Hirshfeld surfaces coupled with cluster analysis and associated multivariate statistics. Using this formalism, it is possible to show quantitatively that naphthalene is more similar to anthracene than to benzene, and moreover that benzodicyclopentene is more similar to anthracene than naphthalene is to anthracene. Whereas the correlation coefficients themselves obtained say nothing about the ways in which the patterns of intermolecular interactions are similar or different for two different structures, the fingerprint plots do contain such information. For the first time structural analysts have a robust method for quantifying structural similarities of whole molecular crystal structures; this has been termed 'Structural Genetic Fingerprinting'. Developments of this method, including the use of partial fingerprints, will be presented. A number of examples will be used to illustrate the broad applicability of the method, including a comparison of predicted crystal structures and a comparison of intermolecular interactions in apparently dissimilar structures. The method will be shown to be suitable for large datasets of hundreds or even thousands of structures.

1. A. Parkin, G. Barr, W. Dong, C. J. Gilmore, D. Jayatilaka, J. J. McKinnon, M. A. Spackman and C. C. Wilson, *CrystEngComm.*, 2007, pp 648-652.

Keywords: structure comparison, hirshfeld surface, structural genetic fingerprinting

P09.06.49

Acta Cryst. (2008). A64, C488-489

Mixed crystal of bidentate and tridentate perfluoro-phenylmercury Lewis acids with organic molecules

Mikhail Yu. Antipin^{1,2}, Fedor M. Dolgushin², Andrey A. Yakovenko², Jose H. Gallegos¹, Tatiana V. Timofeeva¹

¹New Mexico Highlands University, Department of Natural Sciences, Diamond Ave., Las Vegas, NM, 87701, USA, ²Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow, 119991, Russia, E-mail : m_antipin@yahoo.com

At present a number of studied organic/organic mixed crystals (co-crystals) is quite significant, however not many mixed organic/organometallic crystals have been synthesised and described till now. Our group collected a large array of experimental data that have shown affinity of Lewis acids, such as cyclic tridentate perfluoro-o-phenylmercury, o-C₆F₄(Hg)₃ (I) and bidentate 1,2-bis(chloromercurio) tetrafluorobenzene o-(C₆F₄)(HgCl)₂ (II), to formation of mixed crystals with numerous neutral and ionic organic molecules. Formation of mixed crystals can influence catalytic activity, solid state polymerization, prevent decomposition of unstable guest-molecules, transform spectral behaviour of guest,