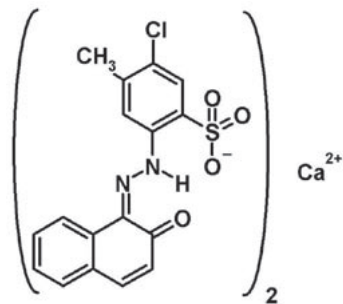


colours. All polymorphs were characterised by X-ray powder diffraction, DSC and DTA/TG. Additionally, temperature-dependent X-ray powder diffraction was used to determine the phase transitions, which occur upon heating.

[1] W. Herbst, K. Hunger, *Industrial Organic Pigments*, 3rd ed., Wiley-VCH, Weinheim, 269-270 (2004).



Keywords: polymorphism, organic compound, X-ray powder diffraction

P06.07.58

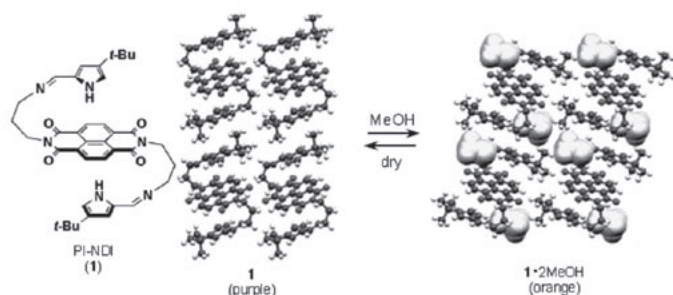
Acta Cryst. (2008). A64, C640

Development of Vapochromic Organic Crystals for Monitoring Systems of Sick-House Syndrome Gases

Eiji Takahashi¹, Hikaru Takaya^{1,2}, Takeshi Naota¹

¹Graduate School of Engineering Science, Osaka University, Department of Chemistry, Machikaneyama, Toyonaka, Osaka, 560-8531, Japan, ²PRESTO, Japan Science and Technology Agency (JST), E-mail : takahashi@soc.chem.es.osaka-u.ac.jp

Growing public awareness of the potential risk from exposure to volatile organic compounds (VOCs) in ordinary environment has prompted us to develop organic sensing materials by crystal engineering. Of particular interest are vapochromic materials that show reversible color change in visible spectral regions upon exposure to VOCs. Porous organic crystal of PI-NDI (**1**) was obtained by recrystallization from MeOH and subsequent removal of the solvent *in vacuo*. These purple crystals exhibit vapochromic behavior upon exposure to a variety of organic vapor such as MeOH (orange), acetone (orange), toluene (red) and triethylamine (yellow). It is noteworthy that sick-house gases such as formaldehyde can be also absorbed efficiently with irreversible color change to yellow. Powder structure analysis using synchrotron X-ray at SPring-8 (BL19B2) revealed that controlled intensity of D-A interaction between the PI and NDI units is a key for the vapochromism.



Keywords: solid-state gas-sensors, powder structure determination, inclusion complexes

P09.05.54

Acta Cryst. (2008). A64, C640

Crystal engineering Intermolecular Hydrogen bond

Johnson A Young

Cement Technology Institute, Engineering Dept, 20 Lawson Crescent, Ibadan, Oyo- State, 23402, Nigeria, E-mail : johnsonbravo1980@yahoo.com

Crystal Engineering:

The rational design of supramolecular structure can be realized through crystal engineering based on relatively weak intermolecular forces. Among these forces, hydrogen bonding is the most common; however, other interactions including halogen-halogen or halogen-nitrogen have been used to organize molecules within the crystal. In particular, it is possible to define a supramolecular synthon as a structural unit within a supermolecule which can be formed and/or assembled by known or conceivable synthetic operations involving intermolecular interactions, by analogy with Corey's definition of a synthon in traditional organic synthesis. To understand the design of crystal packing of substituted benzene compounds, we look to different supramolecular synthons, to determine if there is a relationship between the role of substitution pattern and different types of intermolecular interactions.

Intermolecular:

Intermolecular forces are forces that act between stable molecules or between functional groups of macromolecules. Intermolecular forces include momentary attractions between molecules, diatomic free elements, and individual atoms. They differ from covalent and ionic bonding in that they are not stable, but are caused by momentary polarization of particles. Because electrons have no fixed position in the structure of an atom or molecule, but rather are distributed in a probabilistic fashion based on quantum probability, there is a positive chance that the electrons are not evenly distributed and thus their electrical charges are not evenly distributed.

Young Johnson

Cement Technology Institute
Engineering Dept

Keywords: Crystal engineering, Intermolecular, Hydrogen bond

P10.01.56

Acta Cryst. (2008). A64, C640-641

Inorganic crystallography Geosciences

Nurudeen A Ajeigbe

University Of Ilorin, Geology, P.O.Box 12934 Dugbe General Post Office, Ibadan, Oyo, 23402, Nigeria, E-mail : abiodun1st@yahoo.com

Geosciences are the sciences of the earth, its stones, minerals and waterways. Geologists examine the history of minerals back to the origins of the planet, look at the development of the environment in recent decades, study the evolution of climate since the last Ice Age or deal with the question of why the dinosaurs died out. Geologists understand the process of sediment movement, how minerals are created, and the mineralogical constitution of the earth in the past, present and future. They are able to explain the origins of volcanoes and to forecast eruptions. Geosciences are a field study that deals with a great variety of topics. Geologists must understand the chemical composition of the waters, the physics of earthquakes and continental shifts, the evolution of life, the structures of precious stones but also the components of which the earth is made. Moreover, they must understand the impact of rain and snow on the mountains. In our society, the profession of geoscientist is a very important one,

covering, for example, the utilisation and protection of ground water, the foundations of skyscrapers, the sealing of waste deposits, canalisation systems, railway and road construction, and the redevelopment of waterways and the soil. The determination of the crystal structure of senaite has progressed to the point where a trial model consisting of all atoms has been defined. Plumboferrite has been examined and found to have the magnetoplumbite substructure. The structure of CoGeO₃ has been refined in detail and the occurrence of polytypism in this compound is readily explained by the approximation to closest packing.

Ajeigbe Nurudeen Abiodun
University of Ilorin
Department of Geology

Keywords: General Geoscience, Inorganic crystallography, Geosciences

P12.12.51

Acta Cryst. (2008). A64, C641

Thickness dependent crystallographic transition in Fe/Ni superlattices

Saeed Kamali^{1,2,3}

¹Uppsala University, Physics, Box 530, Uppsala, Uppland, 751 21, Sweden, ²Nanotechnology Research Center, Amirkabir University of Technology (Tehran Polytechnic), Tehran 15914, Iran, ³Japan Synchrotron Radiation Research Institute (JASRI), SPring8, 679-5198 Japan, E-mail : kamali@spring8.or.jp

The 3d transition metals have historically got a huge attention due to both interesting physical properties as well as the applications of systems containing such elements. FeNi alloys, in all concentration ranges, are of particular interest due to industrial applications with emphasis on the so called Invar [1]. While body centered cubic (bcc) Fe is ferromagnetic at room temperature, face centered cubic (fcc) Fe can possess rich variety of magnetic phases. Mossbauer spectroscopy, due to its sensitivity to magnetic and structural environment, is a powerful technique for studying such systems and also because it can isolate Fe magnetism. In contrast to previous studies, where a thick Ni layer has been used as buffer layer and then a thin Fe layer has been established as fcc structure on that, here another approach has been tried. By starting with higher thickness of Fe than Ni, a bcc structure is established. By increasing the Ni thickness, the structure should transit gradually from bcc to fcc. This transition is however smooth, i.e. there will be coexistence of both faces. Several sample series of Fe/Ni superlattices with varied x ML of Fe and y ML of Ni were grown by dc magnetron sputtering method onto MgO substrate. In the first sample series the ratio x/y was kept constant, while the bilayer thickness was changed. In the second sample series, the ratio x/y was also changed. The study of the first series showed that the bcc structure persisted and was almost insensitive to changes of the interface density. The result from the study of the second sample series, where the ratio x/y was changed, i.e. thickness of the Ni layer increased while the thickness of Fe layer was unchanged, showed a gradual transition from bcc to fcc.

[1] B. Window, *J. Appl. Phys.* 44 (1973) 2853.

Keywords: Mossbauer Spectroscopy, Fe/Ni Superlattices, Magnetism

P25.10.14

Acta Cryst. (2008). A64, C641

Combined use of crystallography and mass spectrometry for ligand characterization and drug design

Jean-Paul Renaud^{1,2}, Denis Zeyer², Valerie Vivat²,
Dominique Roecklin², Pascal Muller²

¹IGBMC, Structural Biology and Genomics Department, 1 rue Laurent Fries - BP 10142, Illkirch, Alsace, 67404, France, ²AliX, boulevard Sebastien Brant, Illkirch, Alsace, 67400, France, E-mail: jpr@igbmc.fr

AliX has developed FAMASS (Fragment Analysis by MASS Spectrometry), a proprietary approach for structure-based drug discovery combining X-ray crystallography and non-covalent mass spectrometry. We routinely use non-covalent electrospray ionization mass spectrometry to check the purity and the functionality of proteins used in [protein-ligand] complex crystallization, and also to screen ligands for binding to given targets. This is especially interesting when a functional assay is not available, as in the case of orphan nuclear receptors. Non-covalent mass spectrometry is an efficient secondary screening method to discard false positives from a high-throughput primary screening. We have now extended this approach to fragment-based drug discovery. Fragments selected by *in silico* screening are validated for physical binding to the target by non-covalent mass spectrometry. Validated fragments are then co-crystallized with the target and their mode of binding elucidated by crystallography, paving the way toward the design of new scaffolds.

Keywords: protein-ligand complex, mass spectrometry, fragment-based drug discovery

P26.01.03

Acta Cryst. (2008). A64, C641-642

Teaching how to simply replace the independent atom model - the example of Bergenin

Peter Luger¹, Manuela Weber¹, Roman Kalinowski¹,
Simon Grabowsky¹, Birger Dittrich², Christian B. Huebschle²

¹Freie Universitaet Berlin, Chemistry and Biochemistry/Crystallography, Fabeckstrasse 36a, Berlin, Berlin, 14195, Germany, ²Georg-August-Universitaet Goettingen, Tammanstr. 4, 37077 Goettingen, Germany, E-mail: luger@chemie.fu-berlin.de

In four years the crystallographic community will celebrate 100 years of X-ray diffraction. While in the first 50 years the method was applicable only in exceptional cases, the developments in the second half of the last century increased the number of published X-ray structures dramatically, so that the number of CCDC entries is quickly approaching half a million. Nevertheless, in almost all cases the independent atom model (IAM) was applied that uses spherical scattering factors which do not allow a proper description of chemical bonding. To replace the IAM with an aspherical scattering model we recently introduced the concept of Invarioms, generated an Invariom library and corresponding software for a straightforward application [1]. Since the needed X-ray and computer equipment is far from expensive up-to-date standard and since we will show that the use of the Invariom model can easily be taught, the aspherical Invariom model is best suited to be used by groups also in less developed countries. This is demonstrated by the example of Bergenin, a compound of traditional Asian medicine, which is known for anti-HIV and other biological activities. On a more than 20 years old diffractometer a low resolution ($\sin(\theta)/\lambda = 0.60 \text{ \AA}^{-1}$) data set was measured at room temperature that was properly suited to obtain an improved molecular geometry compared to the IAM and a variety