R-phenylethylamine (*R*-PEA), formed an interdigitated trilayer film (*R*-C_{15}-MA, *R*-PEA), which is crystalline, but for the alkyl *p*-$C_{15}H_{31}$ chains at the top surface of the film. By comparison, the amphiphile *R*-C_{15}-MA over an *S*-PEA solution formed, on compression, a (*R*-C_{15}-MA, *S*-PEA) bilayer which is neither crystalline nor interdigitated. An analogous result was obtained for the bimolecular system in which the hydrocabon chain was attached to phenylethylamine only. The formation and packing arrangements of these multilayers will be discussed.(3)

The major tools applied for structure elucidation were grazing incidence X-ray diffraction and atomic force microscopy.

1.J. L. Slater, C. H. Huang, *Prog.Lipid.Res.* **27**, 325 (1988).
2.M. C. Brianso, M. Leclercq, J. Jacques, *Acta Cryst.* **B35**, 2751 (1979); S. Larsen, H. L. Diego, *Acta Cryst.* **B49**, 303 (1993).
3.I. Kuzmenko, R. Buller, K. Kjaer, J. Als-Nielsen, M. Lahav, L.Leiserowitz, to be submitted for publication, (1996).

MS16.04.03 MORPHOLOGY CONTROL PER COMPUTER: PRESENT AND FUTURE. F.J.J. Leusen, Molecular Simulations Inc., 240/250 The Quorum, Barnwell Road, Cambridge CB5 8RE, United Kingdom

Although the ability to predict crystal morphology was established several decades ago, there is still no reliable and generally applicable computational approach to predict, quantitatively, the effects of the growth medium on crystal morphology (e.g., effects of solvents, additives, impurities, etc.).

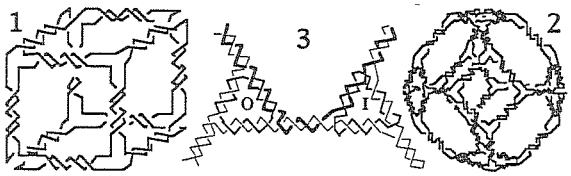
Procedures to accurately evaluate the effect of a solvent or additive on morphology exist [e.g., 1], but they are extremely complicated and not yet automated; application requires a lot of time and expertise. Some of these procedures will be discussed and illustrated with application examples.

The incorporation of these procedures into existing computational approaches to predict morphology is now becoming feasible due to the compute power of modern computers and the development of new algorithms. An automated computational tool to predict the effect of solvents and additives on the morphology of both organic and inorganic crystalline solids can thus be envisioned - possible approaches and pitfalls will be discussed.

[1] X.Y. Liu, E.S. Boek, W.J. Briels and P. Bennema, *Nature*, 374:342 (1995)

MS16.04.04 THE DESIGN OF LATTICES FROM DNA BRANCHED JUNCTIONS: PRINCIPLES AND PROBLEMS. N.C. Seeman, J. Qi, X. Li, X. Yang, B. Liu and H. Qiu, Chemistry Dept., New York University, New York, NY 10003, USA.

A significant goal of crystallography is 3-D structural control that enables the construction of both individual objects and periodic matter. There are at least three elements necessary for the control of 3-D structure: [1] The predictable specificity of interactions between components; [2] the structural predictability of intermolecular products; and [3] the structural rigidity of the components. The first two of these elements allow for topological control over the products of assembly, in the senses both of the connectivity of the molecular graph and of the linking of plectonemic substructures. The third element, structural rigidity, appears to be needed to fabricate targets that contain symmetry; hence it seems to be particularly important for the construction of periodic networks, whose components exhibit translational symmetry. We are pursuing these ends with synthetic DNA branched junctions. Ligating branched structures generates stick-figures whose edges are duplex DNA, and whose vertices are branch points. Control of topology (elements [1] and [2] above) in this system is strong, and it has allowed us to build DNA molecules whose helix axes have the connectivities of a cube (**1** below) and of a truncated octahedron (**2** below). To construct lattices, we have sought rigid components, by using DNA triangles whose branches are bulged junctions. By alternating triangles with the bulges on the inside (**I**) and outside (**O**) strands, one generates a module with a reporter strand (dark strand in **3** below), whose fate reflects the rigidity of the complex in ligation closure experiments. We have performed such experiments with the components of **3**, and find that this system does not satisfy criterion [3]. The search for rigid DNA components continues.



This work has been supported by grants from the NIH and ONR.

MS16.04.05 CHAINS, PLANES AND FRAMES - HOW THE DIMENSIONALITY OF HYDROGEN BONDED OR COORDINATION POLYMER NETWORKS INFLUENCES CRYSTAL MORPHOLOGY Michael J. Zaworotko, Donald C. MacQuarrie, Pierre Losier and C.V.K. Sharma, Department of Chemistry, Saint Mary's University, Halifax, Nova Scotia, B3H 3C3, Canada.

Recent work in our group has concentrated upon the development of strategies for controlling the dimensionality of network structures in the solid state. As such, we have characterized numerous examples of 3-D (diamondoid,[1] octahedral[2]), 2-D (honeycomb grid, square grid) and 1-D (strand) networks. The chemical nature of the compounds that we have investigated is diverse and encompasses hydrogen bonded cocrystals, organic salts and coordination polymers. It has become clear that judicious choice of molecular modules for their symmetry (linear, trigonal, tetrahedral or octahedral) and functionality (complementarity of hydrogen bonding, π–π stacking or metal/ligand coordinate bonding sites) at the molecular level can afford a high degree of control over the nature of the crystal packing, i.e. many of the crystals we have investigated can be regarded as *de facto* manifestations of supramolecular chemistry.

The presentation will concentrate upon an overview of how the symmetry and dimensionality of the hydrogen bonded or coordination polymer frameworks correlates with space group and crystal morphology.

[1] M.J. Zaworotko, *Chem. Soc. Rev.*, 283 (1994)
[2] S. Subramanian and M.J. Zaworotko, *Angew. Chem. Int. Ed. Engl.*, 34, 2127 (1995).

MS16.04.06 MORPHOLOGY OF BULK RBCO SINGLE CRYSTALS. E.V.Sokol[a], L.P.Kozeeva[b], M.Yu.Kameneva[b]; [a]Joint Inst. of Geology, [b]Inst. of Inorganic Chemistry, Novosibirsk, 630090, Russia

Understanding of the forms of crystallization of 123 cuprate superconductors is vital for controlling their properties. Morphological analysis of more than 100 well-shaped individuals and crystal aggregates of RBCO (R= Y, Tm, Ho, Lu) obtained by the flux method in alumina crucibles in different conditions showed 3 stages of crystallization. The nucleation of crystals could be: multicentre two-dimensional one forming the crystal base, and the skeleton growth of different relief roughness with tops and (or) edges between {001} and {100} faces of tetragonal prism as generating points. The second stage was layer-to-layer growth of {001} plane. Heterogeneous aggregates of microcrystals from the first stage may be overlapped by {001} layers, producing monocrystal-like specimens. The crystals of clearly thick platy habit usually had shiny {001} facets and sufficiently smooth of {100} ones. With increasing sizes of {100} facets different types of relief roughening were observed: so-called slice- and hooper-like forms and overhanging of {001} facets. Side faces {011} are presented in the habit of the most perfect crystals with smooth {100} faces. Bulk crystals took their final form at the third stage. The basal faces developed to smooth mirror surfaces sometimes

with growth spirals. At the same time clear microblock features due to of impurity poisoning of growth surface were observed. Thin platelets with smooth {001} crystallized at this stage too. Summary: {001} and {0$\bar{1}$1} faces are growth forms of crystals of RBCO, {100} faces - passive ones. The real symmetry of as-grown bulk crystals is lower than P4/mmm - the horizontal plane of symmetry (001) is usually absent.

MS16.04.07 MORPHOLOGY OF THE EXPLOSIVE COMPOUND RDX. J.H. ter Horst, R.M. Geertman, A.E. van der Heijden*, G.M. van Rosmalen. Delft University of Technology, Laboratory for Process Equipment, Leeghwaterstraat 44, 2628 CA Delft, The Netherlands; *TNO Prins Maurits Laboratory, Pyrotechnics and Energetic Materials, Post office box 45, 2280 AA Rijswijk, The Netherlands

Small scale cooling crystallization experiments in stagnant media show (figure 1 and 2) that the solvent has a strong influence on the crystal morphology of RDX (cyclotrimethylene trinitramine). It is the objective of this study to find an explanation for this behavior.

A PBC (Periodic Bond Chain) Analysis is carried out in order to determine the crystal forms that may contribute to the crystal morphology. Furthermore the growth rates of all geometrically possible faces are calculated by assuming that they are proportional to the attachment energies of these faces. The combination of the PBC analysis and the attachment energy calculations results in an RDX crystal morphology prediction neglecting the influence of the solvent (figure 3). All forms observed experimentally are also present on the calculated morphology.

This calculated morphology gives information about the surface structure on a molecular level and allows an estimation of the influence of the solvents on the crystal morphology e.g. by means of the sorption module of the computer program Cerius^2.

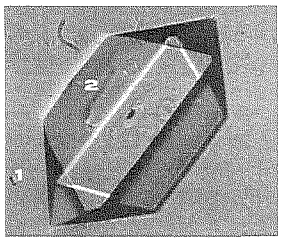


Figure 1: RDX crystal from g-butyrolactone, Σ=0.4

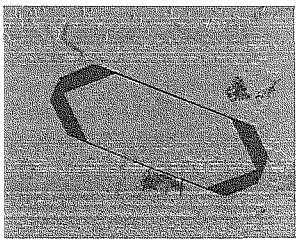


Figure 2: RDX crystal from water waturated cyclohexanon, Σ=0.3

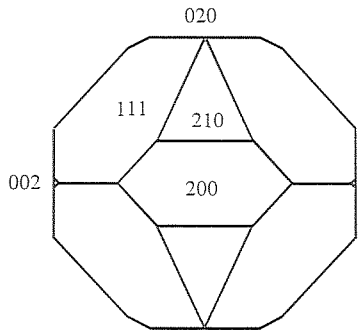


Figure 3: Calculated RDX crystal morphology

Macromolecular Crystal Growth Under Microgravity

PS16.05.01 RECENT ACTIVITIES OF SPACE PROTEIN CRYSTALLIZATION IN CHINA. Ru-Chang Bi, Institute of Biophysics, Academia Sinica, Beijing 100101, P.R.China

Based on encouraging results obtained on the first mission in 1992, the second Chinese mission of protein crystallization was conducted in 1994 using tube-like vapor diffusion apparatus on a Chinese re-entry satellite. More than 14 different proteins have been tested on the two missions. In comparison with the first mission, much better results were acquired on the second mission. Besides hen egg-white lysozyme, an acidic phospholipase A2 from snake venom and hemoglobin from bareheaded goose have produced good- quality crystals. The positive effects of microgravity on protein crystal growth and even results of protein crystallization in space can be reproducible. As an important factor affecting protein crystal growth, the microgravity may display its role in different degree depending on the protein crystallized and the crystallization conditions used.

Our first attempt to grow protein crystals with the liquid-liquid diffusion method was carried out on the August 1995 flight of the US space shuttle, STS-69. The hardware, MDA Minilab developed by the Instrumentation Technology Associates in US, was employed in this space experiment. Although the experiment was restrained by some conditions, the three proteins which we supplied to use six diffusion cells in a MDA unit, were crystallized on this mission. An important finding of our experiments is that in contrast with the case of vapor diffusion technique, the optimized conditions for growing good protein crystals on Earth may be different remarkably from those to be optimized in space. These differences could be caused by the density-driven convection and will be discussed in this report.

PS16.05.02 MULTI-USER FACILITY FOR PROTEIN CRYSTAL GROWTH IN MICROGRAVITY: RESULTS FROM PCAM AND DCAM. Daniel C. Carter, Pam D. Twigg, Brenda Wright, Joseph X. Ho, Kapp Lim, Jenny Chapman, Teresa Miller, NASA ES76 Laboratory for Structural Biology, Marshall Space Flight Center, Huntsville, Alabama, USA

Two newly developed microgravity multi-user facility-based hardwares for protein crystal growth will be described. Both hardwares feature disposable interfaces for improved logistics and handling. PCAM (Protein Crystallization Apparatus for Microgravity) is a high capacity device which closely approximates a common laboratory vapor diffusion method to grow crystals. DCAM (Diffusion-controlled Crystallization Apparatus for Microgravity) is a unique multi-user dialysis device which offers passive control of the diffusion profiles for each individual experiment. DCAM was specifically designed for long duration microgravity opportunities. The hardware is operated as government facility and access is provided through peer reviewed proposals. Significant improvements in crystal size and perfection obtained from flight experiments conducted over the course of less than a year will be described.