

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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LETTER FROM THE PRESIDENT

Letter from the President



Yuji Ohashi

The activities of the IUCr are divided into three parts. The first concerns the activities of the National Committees (39 Adhering Bodies) and the three Regional Associates (ACA, AsCA and ECA). The second involves publication of the journals, International Tables and the IUCr/OUP Book Series. The third part is the activities of the 16 non-publishing scientific Commissions.

In order to foster the growth of crystallography, it is very important to welcome membership from the developing countries. The number of 39 is too small, although many non-member countries do participate in the activities of the Regional Associates. In Florence, we welcomed the Hellenic Crystallographic Association but lost the Adhering Bodies for Ukraine and Bulgaria. Of course, the IUCr supports not only crystallographers in member countries but also those in non-member countries. We must remember, however, that IUCr activities depend on those of the member countries. To increase the number of members, the IUCr, in cooperation with the Regional Associates, will support efforts of crystallographers in non-member countries to organize seminars or schools and will help them to form national crystallographic societies.

For publishing activities, the launch of the new online journal *Acta Crystallographica* Section F, combined with *Acta Crystallographica* Section D, should contribute significantly to promoting research in biological crystallography. Furthermore, the online version of the International Tables for Crystallography will be available in the near future. I hope crystallography will thus become more familiar to students and young scientists.

In order to cultivate new areas of crystallography, the activities of the scientific Commissions are important. Since crystallography is based on a variety of scientific fields, we must always be on the lookout for a seed or germ of new areas of research. At the Florence General Assembly we accepted the new Commission on Mathematical and Theoretical Crystallography. More Commissions may become necessary to cover such scientific fields as the development of new apparatus, including detectors, and research on surfaces and interfaces. Since current IUCr Commissions covers only 16 scientific fields, we are ready to accept new ones. Moreover, it is important that not only experienced scientists but also young scientists should serve as members of each Commission. I expect that the Chairs of Commissions will take this into account when recommending new members, also taking into consideration geographical, age and gender balance.

In addition to management of the above activities, the Executive Committee is discussing new nomination procedures for its membership to reflect new expectations within the crystallographic community. In the discussion we must remember that the IUCr consists of Adhering Bodies from member countries whose valuable input is always highly appreciated. We will report on the new plan after the summer meeting of the Executive Committee.

Yuji Ohashi, yohashi@spring8.or.jp

LETTER TO THE EDITOR

Letter to the Editor

Dear Judy

I have just read your Editorial in Volume 13, Number 3, 2005 concerning the lack of women on the IUCr Executive Committee and as officers over the years. It was a very considered and constructive piece, and I hope that some of the newly elected Committee will resonate with what you say. In the sciences, the IUCr is unique in having such a massive participation and contribution from women. At the same time, the number of female representatives in the higher offices of the Union has been pitiful. This is ironic when set against official requests for gender and geographical balance in inviting speakers for scientific microsymposia. Since I had to leave Florence a day or so before the election I hadn't heard Maria Carrondo's exact words before. They are both dignified and true, and I believe that the vast majority of crystallographers would agree.

Frank Allen

LETTER TO THE EDITOR

Letter to the Editor

Dear Judith,

I could not afford to go to Florence but I fully agree with all your comments concerning the election process. I am an 'adopted' citizen of the USA and I value tremendously the democratic ways of conduct. However sometimes it seems to me that what is loudly described as 'a democratic process' in reality reminds me of what we experienced under the totalitarian system where elections were 'doctored'. By all means we should fight against any such trends. Also, nothing irritates me more personally than separate societies for women in science, special awards for female scientists, etc. Is it not the time to realize that there is no such thing as a second category in science? As in every profession the only divisions should be for GOOD and BAD which should have NOTHING to do with gender! In this respect I am reminded of a few facts from our own crystallographic background. The "...experimental determination of the structure of the benzene ring by X-ray diffraction, which showed that all the ring C-C bonds were of the same lengths and all the internal C-C-C bond angles were 120 degrees, had an enormous impact on organic chemistry" - this is a comment made by K.N. Trueblood about work done by Kathleen Yardley Lonsdale, who happened to be a female crystallographer. Needless to say the benzene ring is still depicted as three single and three double bonds in many textbooks and elsewhere. It was Rosalind Franklin and her ingenious mind and - first of all - her meticulous work that made possible the description of DNA structure. Let us not forget that it was Maurice Wilkins who, without her knowledge, showed her unpublished results to Watson (DNA form B), who in his own words described it as follows ("The Double Helix"): "The instant I saw the picture my mouth fell open and my pulse began to race...the black cross of reflections which dominated the picture could arise only from a helical structure...mere inspection of the X-ray picture gave several of the vital helical parameters". Let us not forget that it was also Rosalind Franklin who insisted that the base pairs are inside and the sugar-phosphate backbone is on the outside of the molecule. As Watson put it in his book "Her past uncompromising statements on this matter thus reflected first-rate science, not the outpourings of a misguided feminist." And how about Dorothy Crowfoot-Hodgkin who single-handedly provided structures of vitamins, human hormones, penicillin and insulin - an enormous impact on medicine as we know it! She was a scientific role model for many young people who were lucky enough to get to know her (that includes me). Not too many scientists measure up to her in terms of being unpretentious, humble, unselfish, eager to help and always showing a truly deep and genuine interest in the work of others, including students in the infancy of their profession. Such personal qualities are extremely rare and once again let it be stressed that gender has nothing to do with it. She served on many committees (including Pugwash). I am sure she would be neither impressed with nor able to approve the way EC is acting. Thank you for speaking up.

Ewa Skrzypczak-Jankun

EDITORIAL

XXIUCr is over! - Arrivederci to Osaka



Based on comments from a number of participants, the XX IUCr Congress was a huge success. As organizers, we are proud to say that in spite of the record numbers of participants everything ran very smoothly. The general consensus was that the quality of both the scientific program and the social events was exceptional.

We hosted approximately 3000 participants from 62 countries. About 200 of the total were accompanying persons. Of the remaining 2800 attendees, one fourth were students. As many as 450 bursaries were distributed, thanks to the generous contributions of the Marie-Curie Actions (European Commission), the Organization for the Prohibition of Chemical Weapons (OPCW), the IUCr, the British and Italian Crystallographic Associations, and the local student support organization (ARDSU), which arranged for economic yet comfortable accommodations. A number of individual countries also sponsored student travel.

We wish to thank all the chairs and speakers for deferring any kind of financial support which made it possible for us to assist younger or under privileged participants and to focus spending on the services that were appreciated by all attendees. In this respect, we made an unprecedented experiment at an IUCr Congress by including the cost of lunch in the registration fee. Having lunch on site also favored the programs taking place during the midday breaks which were particularly hectic (open commission meetings, reunions of various councils, poster sessions, computer fayre, etc). Serving quick and high quality lunches increased participation in these activities and created an extremely friendly environment that was carried over to the various nightly events. The Congress banquet at the Boboli Garden which required only a symbolic booking fee provided the perfect atmosphere for an electric and memorable event.

Also contributing to the success of the Congress was the tailored combination of frontier scientific research (brought to Florence by the multidisciplinary crystallographic community) and art, for which Florence is a cradle. Initiatives in this area such as the Microsymposia on Art and Crystallography and on Crystallography and Cultural Heritage were very successful. The latter was so stimulating that a group of participants agreed to form a homonymous commission within the IUCr to study the topic. Also along the artistic line, the musical events (during the Opening Ceremony and the Concert of Aug. 27th) were both quite appreciated and acclaimed.

The scientific program, assembled thanks to the cooperation and competence of the international committee, was a great success. It started with the excellent presentation by the winner of the 7th Ewald Prize (Philip Coppens) during the opening ceremony. At this time, the first IUCr prize for exceptional service to Crystallography was also announced and the winner, Lodovico Riva di Sanseverino, received the award during the banquet. Overall the program consisted of 527 lectures, among which were three by Nobel Laureates (R. Hoffmann, H. Kroto and A. Zewail). It would be no surprise if some other distinguished speaker at this Congress is awarded the Nobel Prize in the future.



Andrea Ienco, Patrizia Rossi, Paola Paoli, Annalisa Guerri, and Carlo Mealli.

Of the 98 microsymposia we have already mentioned those having artistic themes, but essentially all of the others were of such high quality that it would be impossible to establish an order of merit. It suffices to point out that 22 MS dealt with biological macromolecules, 14 with structural chemistry, 9 with crystallographic computing, and 9 with powder diffraction. Topics such as mineralogy, high pressure, neutron diffraction, aperiodic crystals and small angle scattering were also well represented. About 230 different posters per day were on display, their high quality being testified to by the continuous overcrowding in the poster area. Several poster prizes were issued by different institutions and companies. It is certain that the judges faced a very difficult task in selecting the winners. Last but not least it is important to mention the relevance of the exhibition which attracted many interested visitors. The exhibitors were also appreciative of the large spaces allotted to them and of the arrangement of the stands. The congress held its audience until the last moment as seen by a large number of people at the closing ceremony, during which the poster prizes were awarded. An ideal bridge was built between Florence 2005 and Osaka 2008 thanks to the presence of the newly elected IUCr President Yuji Ohashi, to whom we wish a fruitful mandate. Our warmest thanks also go Past President William Duax, who always trusted and encouraged us, for help in making a success of the XX IUCr Congress. Since the Congress, we have received many messages of appreciation and congratulations. One of them (quoted) was particularly touching for us because it reflects the feelings of someone who was active in both the scientific programme and the commercial exhibition.

Our most sincere thanks go to all the people who helped us in this endeavour. Beside our own institutions, CNR and the U. of Florence, we wish to mention our closest collaborators (Andrea Ienco, Patrizia Rossi and Annalisa Guerri), the members of the local organizing committee, the institutional and commercial sponsors and the organizing secretariat (Newtours SpA).

Carlo Mealli and Paola Paoli

Comments

..."When things go badly, people can be very quick to criticise. When things go well, rather fewer people take time to say well done. I know this because we run a service industry at the CCDC!! I want to say that the Firenze Meeting was a huge success. It was very well organised at an excellent site. It was smooth, and everyone I spoke to was full of praise. Your colleagues and staff were helpful and friendly. You have performed a service to crystallography in all its aspects. Please tell your colleagues and the staff of the conference bureau that it was much appreciated (by CCDC at least!). Thanks."

Frank H. Allen, Executive Director of the Cambridge Crystallographic Data Centre

..."On behalf of the Spanish Crystallography Committee, I would like to thank you for the enormous efforts that you have made, together with Paola Paoli, which enabled the 20th UICr Congress in Florence to be such a total success. All the Spanish crystallographers felt very much at home at the conference..."

C.Miravittles

"I would like to thanks everything for all! I was very happy in Firenze. Thank you the bursary, this was the only chance for me to be at the Congress. This meeting was absolutely useful to keep in contact and to find a post doc position for me. So thank you again your helpful works! Firenze is really a diamond in Italy..."

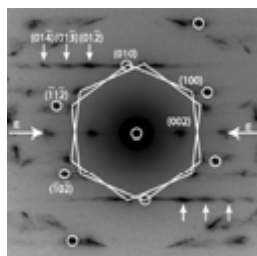
Niki Bathori

I very much enjoyed the IUCr2005 congress in the beautiful city of Florence. The participants, lectures, posters, discussions, the opening ceremony (parade and welcome cocktail), the Art and Crystallography exhibition and the concert were all most interesting and stimulating...

Chava Brender

Double-helix structure in multiwall boron nitride nanotubes

***Acta Cryst.* (2005). A61, 533–541 [doi:10.1107/S0108767305026723]**



Diffraction pattern recorded from a 50 nm section of BN nanotube, which shows evidence of both faceted and circular tube.

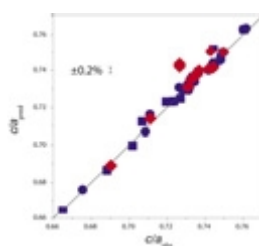
Electron diffraction patterns can be recorded from individual nanostructures for their structure determination. A study of multiwall, chiral, boron nitride nanotubes is reported. The combination of diffraction information (obtained using a 50 nm parallel electron beam along different tube sections) and electron imaging shows that the tube structure consists of two helices, one highly crystalline and faceted and the other circular and less ordered. This type of structure is present in BN tubes exhibiting similar chirality among its different walls.

A. Celik-Aktas, J.-M. Zuo, J. F. Stubbins, C. Tang and Y. Bando

Geometrical parameterization of the crystal chemistry of $P6_3/m$ apatites: comparison with experimental data and *ab initio* results

Geometrical parameterization of the crystal chemistry of $P6_3/m$ apatites: comparison with experimental data and *ab initio* results

Acta Cryst. (2005). B61, 635–655 [doi:10.1107/S0108768105031125]



Model predictions made from crystal-chemical parameters as a function of the observed c/a . Legend for symbols: red= single-crystal refinements; blue= *ab initio* optimizations.

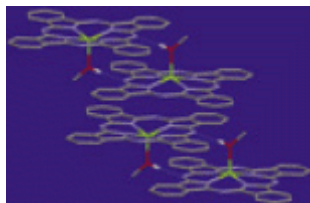
Experimental single-crystal and Rietveld analysis results of apatite materials are compared with *ab initio* simulations using a geometric crystal-chemical model involving 10 parameters and 4 constraints equivalent to unit-cell parameters (a and c) and 12 independent atom coordinates. From crystal-chemical parameters representing polyhedral distortions, the magnitude of a and c is reproduced to $\pm 0.025\text{\AA}$ accuracy whereas the c/a ratio is predicted to $\pm 0.2\%$. Comparison of *ab initio* optimized structures with experimental ones shows good agreement (within ± 0.5 – 2.0%) with only the most reliable single-crystal refinements.

P. H. J. Mercier, Y. Le Page, P. S. Whitfield, L. D. Mitchell, I. J. Davidson and T. J. White

IUCR JOURNALS NEWS

Why magnesium is five-coordinate in methanol(phthalocyaninato)magnesium(II)

***Acta Cryst.* (2005). C61, m472-m475 [doi:10.1107/S0108270105029732]**



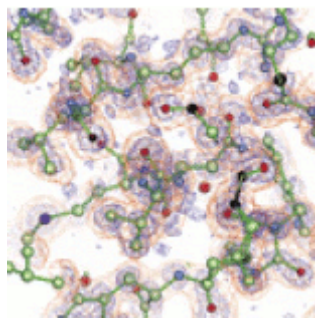
Packing of methanol(phthalocyaninato)magnesium(II). (Mg: green, O: red, N: blue, C: grey, H: white.) The metallophthalocyanines exhibit a wide array of physical and chemical properties that can be profoundly affected by subtle changes in their structures. Shown here is methanol(η^4 -phthalocyaninato)magnesium(II), a recent addition to the list of compounds that fit this classification. Two types of intermolecular interactions drive the crystallization of this chemical: π - π dimerization and O-H $\cdots$ N hydrogen bonding. One interesting subtlety of the structure is that the phthalocyaninate ligand adopts a “hat visor” shape, a description put forth for the first time in describing this structure.

I. A. Guzei, R. W. McGaff and H. M. Kieler

IUCR JOURNALS NEWS

A modified ACORN to solve protein structures at resolutions of 1.7 Å or better

***Acta Cryst.* (2005). D61, 1465-1475 [doi:10.1107/S090744490502576X]**



ACORN *F* map with observed data to 1.5 Å (red) and *E* map with data artificially extended to 1.0 Å (blue) for 1uuq.

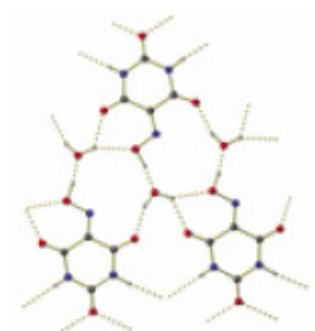
ACORN is a procedure for determining protein structures from small fragments with data to better than 1.3 Å resolution. A modified *ACORN* now gives atomic-resolution protein solutions with observed data resolution as low as 1.7 Å. Data are artificially extended to 1 Å resolution, assuming that all extended data have $|E| = 1$. Additionally, improved density modification techniques are employed that are particularly effective in developing weak, but true, density. *ACORN* gives atomic-resolution maps that are easily traced and can be used to build structures automatically.

Yao Jia-xing, M. M. Woolfson, K. S. Wilson and E. J. Dodson

IUCR JOURNALS NEWS

Violuric acid monohydrate: a definitive redetermination at 150 K

***Acta Cryst.* (2005). E61, o3788–o3790 [doi:10.1107/S160053680503343X]**



The hydrogen-bonded sheet structure of violuric acid monohydrate.

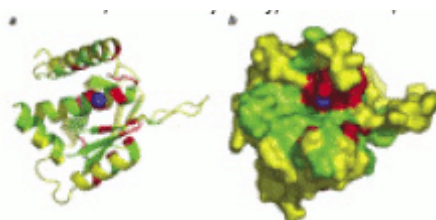
The crystal structure of violuric acid monohydrate was originally determined over 40 years ago in 1964 from X-ray and neutron data. A number of issues concerning potential pseudo-symmetry and disorder caused by abnormally high thermal atomic motion were raised in the original reports and could not be resolved. Re-collection of data at 150 K allows confirmation that the structure is indeed in the noncentrosymmetric space group $Cmc2_1$ and is disorder-free, despite the presence of pseudo-symmetry. All atoms lie on a crystallographic mirror plane, leading to hydrogen-bonded planar sheets.

G. S. Nichol and W. Clegg

IUCR JOURNALS NEWS

The ybeY protein from *Escherichia coli* is a metalloprotein

***Acta Cryst.* (2005). F61, 959-963 [doi:10.1107/S1744309105031131]**



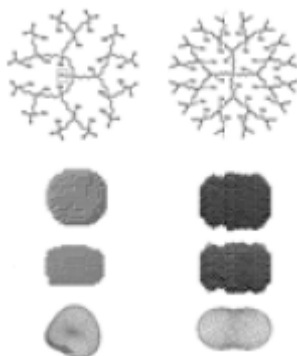
Evolutionary conservation is mapped onto the ybeY structure in a) ribbon and b) surface representation. Identical, conserved and less conserved residues are marked red, green and yellow, respectively. The metal ion is represented by a blue sphere.

The ybeY protein is a hypothetical *Escherichia coli* protein in the UPF0054 family with no functional annotation. The structure reported here reveals that the protein has an α/β fold and binds a metal ion with tetrahedral coordination. Bioinformatics analysis suggests that ybeY is a member of a family of metal-dependent hydrolases. This report was prepared using a semi-automated tool, termed the *Autopublish* server, which represents a first step towards enabling the rapid publication of crystallographic structures that result from worldwide Structural Genomics efforts.

C. Zhan, E. V. Fedorov, W. Shi, U. A. Ramagopal, R. Thirumuruhan, B. A. Manjasetty, S. C. Almo, A. Fiser, M. R. Chance and A. A. Fedorov

The spatial structure of dendritic macromolecules

***J. Appl. Cryst.* (2005). 38, 996–1003 [doi:10.1107/S0021889805032115]**

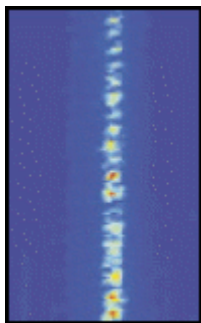


Shape determination for polycarbosilane dendrimers with the three- (left) and four-functional branching center (right) topology. *Ab initio* models are displayed as beads and envelopes in orthogonal orientations. Structural characterization of tree-like dendrimer macromolecules is very important for practical applications. This paper presents low-resolution shapes of polycarbosilane dendrimers in solution reconstructed *ab initio* from SAXS and SANS data. The bead and envelope models reveal anisometric shapes but also pronounced heterogeneity of the internal dendrimer structure allowing for penetration of solvent molecules. The *ab initio* models agree astonishingly well with the recent independent results of molecular dynamics simulations on dendrimers.

Alexander N. Ozerin, Dmitri I. Svergun, Vladimir V. Volkov, Alexander I. Kuklin, Valentin I. Gordelyi, Akmed Kh. Islamov, Lyudmila A. Ozerina and Denis S. Zavorotnyuk

Grazing-incidence scattering of coherent X-rays from a liquid surface

J. Synchrotron Rad. (2005). **12**, 786–794 [doi:10.1107/S0909049505022065]



When a partially coherent X-ray beam is scattered from disorder, a random diffraction image ('speckle pattern') is generated, which contains information about both the incoming radiation and the scattering sample. Here, the X-ray beam is applied under grazing incidence (GISAXS) to study a glycerol surface as it is cooled towards its glass transition. The temporal fluctuations of the speckle pattern are characterized by time-correlation spectroscopy (XPCS), and a slowing down of surface dynamics upon cooling is evident. We show that the appearance of the 'frozen-in' speckle pattern (figure) obtained in the glassy phase depends crucially on the scattering geometry, and the differences between SAXS and GISAXS geometries are discussed.

A. Madsen, T. Seydel, M. Tolan and G. Grübel

MEETING REPORT

XX Congress and general assembly

KEYNOTE LECTURES

Ion pumping by Ca^{2+} -ATPase of sarcoplasmic reticulum



In the keynote lecture by Chikashi Toyoshima, he presented, using several movies, how the Ca^{2+} -pump (ATPase) works based on their crystallographic and molecular dynamics studies. His group has been successful in determining 6 intermediate state structures, covering the whole reaction cycle. In this lecture, he presented a new 2.4 Å structure of the E2 state stabilized with two potent inhibitors that bind to the transmembrane region. He addressed why such large and complicated domain movements are necessary, what ATP and phosphorylation do, and why H^{+} -countertransport is necessary. He stressed that ion pumps are vigorously fluctuating by thermal energy, which is utilized efficiently for structural changes. Large domain motions are necessary for the mechanism of the pump, and protonation of specific acidic residues is required for structural integrity. These proposals were sustained by molecular dynamics studies, which certainly provide a new dimension to the work of Toyoshima's group.

Giuseppe Ines

KN07 structure analysis of modulated crystals



Vaclav Petricek, through his development and continual improvement of the “industry standard” JANA suite of programs, has made an enormous contribution to the rapidly growing area of aperiodic crystallography. He gave a presentation of the application of the superspace approach introduced by de Wolff, Janssen and Janner to higher dimensional crystal structure determination, focussing on atomic modulation functions and their determination in conventional as well as composite modulated structures. The broad range of crystal structure types in which modulated structures have nowadays been found, including inorganic and organic protein crystals, was highlighted. The efficiency of methods used for the solution and refinement of such modulated structures were discussed along with more recent methods including maximum entropy and charge flipping methods. The introduction of discontinuous atomic modulation functions and the use of the superspace approach to systematize the structural characterization of whole families of closely related structure types were highlighted.

Ray Withers

High throughput technologies in structural biology



The explosive growth of biological macromolecular crystallography in the genomics era has necessitated many technological innovations to facilitate high throughput operations. The plenary lecture by Raymond Stevens dealt with these innovations. Recurring themes of the innovations introduced by Stevens and his collaborators have been miniaturization and automation. Miniaturization has been achieved in NMR, thermodynamic measurements, electron microscopy and high throughput crystallization. He described the application of the new technologies to structural genomics of enzyme pathways, studies of biophysical properties, structure-based drug discovery and structure-based enzyme replacement therapy. He provided glimpses of future technology developments including the crystallization of membrane proteins, total synthesis of genes, crystal engineering via surface mutagenesis, *in situ* X-ray diffraction data collection and the development of miniaturized, compact X-ray sources for intensity data collection.

M. Vijayan

Protein kinase inhibition and substrate recognition



Louise Johnson brings incredible experience to the understanding of the structure and function of the human kinome. There are 518 protein kinases that make up the human kinome and which are key components of cell signalling pathways. Defects in these processes lead to diseases such as cancer, diabetes and arthritis and hence protein kinases have become targets for drug design and therapy. Louise's research team in Oxford has concentrated on the structures of the cell cycle protein kinases and in particular CDK2/cyclin A, CDK2/cyclin E, CDK7 and polo-like kinase. In addition to these studies she and her colleagues recently published a high impact review in *Science* surveying progress in this field with special reference to kinase inhibitors that are in clinical trials or in the clinic, and for which structural information is available^[1]. Louise has co-authored an excellent text on crystallography with Tom Blundell, is a Fellow of The Royal Society of London, and was made a Dame of the British Empire ('DBE') by The Queen for her services to biophysics. Louise is Sir David Phillips Professor of Molecular Biophysics at Oxford U. and she is also Life Sciences Director at the new UK Diamond Light Source being constructed at the Rutherford Appleton Laboratory at Chilton near Oxford.

John R. Helliiwell

Reference

[1] Noble M.E., Endicott J.A., Johnson L.N., *Science*, 2004, **303**, 1800.



Audience at the Opening Ceremony

The importance of structure in the design of lithium battery materials



Climate change is now recognized as the greatest threat facing humanity in the 21st Century. Transportation accounts for more than 30% of CO₂ emissions. The solution for the next 20-40 years is likely to be the hybrid electric vehicle, combining an internal combustion engine, or later a fuel cell, with a rechargeable battery. The battery of choice is the rechargeable lithium-ion battery. Mike Thackeray demonstrated how crystallography has played a key role in the discovery and understanding of new electrode materials essential for the operation of the rechargeable lithium-ion battery.



Figure 1

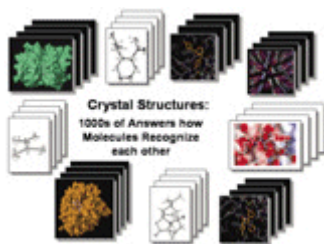
The positive electrode material used in the current generation of lithium-ion batteries is the lithium intercalation host LiCoO₂ (R3m). The capacity to store lithium is limited by the stability range of the solid solution Li_xCoO₂; 0.5 < x < 1. Crystallography has revealed that it is possible to insert Li₂O into compounds such as α-MnO₂ (hollandite structure). The presence of oxygen in the centre of the hollandite tunnels significantly enhances the ability to insert and remove lithium. Crystallography has also revealed a new concept in lithium intercalation materials, in which the compound consists of an intimate intergrowth between a stabilising compound, such as L₂MnO₃, and an electrochemically active component, such as LiNiO₂. Such intergrowths open the way to a higher capacity to store lithium than conventional materials. Turning attention to the negative electrode, Thackeray has demonstrated, using crystallography, that it is possible to understand new and unusual mechanisms by which lithium reacts with intermetallic compounds. For example, one of the metal components may be extruded from the crystal structure but can then re-enter the structure on lithium extraction. The remarkable correspondence between compounds that are sufficiently stable to act as electrodes in lithium-ion batteries and those that exist in the world of gem stones was highlighted in the talk (Figure 1). Some of the most promising lithium battery materials are based on the structure of spinel, olivine and garnet, all of which are being actively pursued as electrodes for the batteries.

The demand for lithium ion batteries will grow substantially over the next 10 years and crystallography will continue to play a vital role in both the fundamental science needed to understand the materials and for their technological exploitation.

Peter G. Bruce, Chair

Molecular recognition principles in protein-ligand interactions





More than 300 people gathered in the Michelangelo lecture hall to listen to Gerhard Klebe's fascinating exposition on the design of bioactive compounds. He turned the approach to science of many of his listeners topsy-turvy by pointing out that the published literature has many answers ready to be discovered, if only we can find the appropriate questions! To achieve this goal the published information needs to be preprocessed into databases. Gerhard has met this challenge for protein-ligand complexes, structural water in biomolecules, the shapes of binding pockets with respect to the prediction of their functional properties and for the relationship between protein structure and ligand binding data, without overlooking, however, the problems of substrate promiscuity. He showed the importance of filling the pockets and subpockets of protein active sites for achieving selectivity. Virtual screening of ligands in the computer, synthesis of promising lead compounds and determination of their binding were demonstrated for aspartyl proteases. The chiral nature of proteins implies the disconcerting problem that one enantiomer of an active compound may have a beneficial effect while the other one damages the organism. In such cases knowing their binding characteristics is as important as determining their crystal structures. Interestingly enough, calorimetric experiments allow determination of the thermodynamic parameters without prior resolution of the racemate, as was demonstrated for some inhibitors of trypsin and thrombin. The talk displayed the rich toolbox available today to developers of new bioactive compounds.

Hans-Beat Bürgi

Structural studies of macromolecular complexes: cytochrome b_6f



Janet Smith's lecture highlighted two aspects of her recent work. She opened her lecture with a dedication to two giants of macromolecular crystallography, Carl-Ivar Brändén and Muttaiya Sundaralingam, who had recently passed away. Janet then took us on a fascinating journey through the complex life of the cytochrome b_6f complex, which functions in the electron transfer chain between the two photosystems in the photosynthetic apparatus of plants, blue green algae and cyanobacteria. Despite years of previous biochemical work in other laboratories, the structure of the large complex which includes two copies of each of eight different polypeptides, unexpectedly revealed the presence of an additional haem cofactor, located close to the putative binding site for the electron donor, plastoquinone. Janet speculated that this haem may play a role in short-circuiting electron flow, which is known to occur in the complex. Janet concluded her presentation with a description of the new protein crystallography facility, GM/CA-CAT, being constructed on behalf of the NIH at the Advanced Photon Source at the Argonne National Labs near Chicago. The suite of three beamlines, two on novel canted undulators and the third on a bending magnet, promises to be one of the finest protein crystallography facilities in the world. The three lines are all completely independent and one offers an extraordinary energy range of 3 to 35 keV. Operations are intended to be fully automated with crystal-mounting robots at each station. The Blu-Ice software from SSRL has been adapted for use at GM/CA-CAT. Janet Smith provided the audience with a fascinating, beautifully told story of some of her recent work and a glimpse into facilities promised for the near future.

Mitchell Guss

CIMS SESSIONS AND OCM

The Commission on Inorganic and Mineral Structures (CIMS) sponsored two Keynote Lectures (Lynne Mc Cusker, “Elucidating the structures of nanoporous microcrystals” and Tim White, “Crystallographic basis of synthetic mineral immobilisation”), an Open Commission Meeting (OCM) and five microsymposia, as well as four other microsymposia co-sponsored with other Commissions. Attendance dealing with inorganic structures, particularly in materials science, was higher at IUCr-XX in comparison with previous IUCr congresses.

Crystal chemistry of inorganic and mineral compounds



A. Vegas



C. Ferraris

Angel Vegas' (Spain) proposal to apply the Zintl-Klemm concept to the cation positions in some oxides, especially silicates, set the stage for a series of well-prepared lectures. Sergey Krivovichev (Russia, Austria) reported on his fascinating findings in the field of uranyl selenates. His most important finding is that these materials form various kinds of nano-structures which have the potential to open up new fields in both basic and applied research. Charles Geiger (Germany) emphasized the importance of vibrational spectroscopy for clarifying the nature of molecule – mineral inner-surface interactions in natural microporous silicates. Obviously, X-ray studies with their averaging effect in space and time are less suited for unravelling local phenomena and structures. Cristiano Ferraris (Singapore, France) clearly demonstrated the difficulties encountered in the investigation of Oxygen/Fluorine ordering in niobium oxyfluorides. By studying several rare minerals Natalia Zubkova (Russia) was able to derive a systematic of the topologies of arsenates. The microsymposium was attended by 80 – 100 delegates on average and was accompanied by lively discussions.

Wulf Depmeier, Herta Effenberger

Modularity and modulation in inorganic and mineral structures



L. Cario



G. Ferraris



D. Charkin

This session took place in a hall with an auspicious name, the Donatello Hall, introducing perhaps a new renaissance of the subject. The topics selected covered practically the entire field of modular structures and modulation. Laurent Cario (France) presented a generalization of the modular approach to 2D-misfit layered chalcogenides. It leads to a design of new commensurate and noncommensurate 2D layered compounds using the 2D building blocs observed in known structures. Giovanni Ferraris (Italy) spoke about recurrent modules in modular structures. He described a plethora of modules observed in oxides and silicates and showed how they can be used in modelling hitherto unknown structures of polysomatic series, interpreting topotactic reactions and defects, as well as tuning the properties of new synthetic materials. Jirí Hybler (Czech Republic), discussed the problems of structure refinement of partially disordered OD structures. They demonstrated the importance of separate scaling of so-called “family reflections”, common to all polytypic sequences, and the “polytype reflections”, characteristic for a given polytype. Improper scaling produces “ghost peaks” in the Fourier syntheses. Luca Bindi (Italy), treated the incommensurately modulated structure of natural melilite (a disilicate of Ca, Al and Mg) by means of a five-dimensional refinement. It confirmed that the modulation is primarily related to the variation in the Ca coordination but demonstrated substantial differences between the natural and synthetic specimens. The last speaker of the session, Dmitri O. Charkin (Russia) demonstrated a modular approach to the tailoring of bismuth-containing layered perovskites. Instead of simple doping of various compounds of this type, they introduce additional 2D structural moduli, building in this way complicated mixed-layer structures. They prepared more than 20 new structure types and a range of new ferroelectrics.

Giovanni Ferraris

Structure/property relationships of technologically relevant inorganic and mineral compounds



F. Taulelle



M. Delgado



Moreton Moore

Although minerals have been investigated for many years, it has become increasingly evident that the study of their formation, crystal structure and reactivity is an endless source of inspiration for designing novel materials. The knowledge of the structure of a given material is an important step forward towards understanding its properties. It is at this point that much chemistry begins: new experiments, which may yield related materials with improved properties, may be proposed.

The session began with a talk by Bernard Grobety (Switzerland) on nanotubes of chrysotile, an asbestos (carcinogenic) material, the use of which deserves careful safety consideration. He reported research on the behavior of chrysotile fibers in the environment and suggested that new applications requiring only small amounts of chrysotile should be targeted.

Francis Taulelle (France) presented a stimulating talk on solidstate Nuclear Magnetic Resonance (NMR) crystallography of inorganic materials. He explained the principles of NMR crystallography on powders (giving special emphasis to the use of Wyckoff spectra) and summarized major recent advances towards that goal. NMR and X-ray crystallography are complementary techniques, extremely powerful when used in tandem.

Carlo Lamberti (Italy) showed the importance of combining synchrotron powder X-ray diffraction and spectroscopic methods in the study of guest molecules in microporous (zeolitic) hosts. Zeolites are heterogeneous catalysts and their active sites are located within the internal cavities of the structures. The reactivity of the active sites is analyzed via the adsorption of probe molecules monitored by infrared and Raman spectroscopies. Miguel Delgado (Venezuela) discussed semiconductor materials, with application in solar cells, based upon chalcopyrite using powder XRD.

The symposium was closed by Moreton Moore (UK) with a talk on the growth and morphology of diamonds. Some 80% of natural diamonds are used in industry because they contain defects or impurities that result in poor optical properties. However, industry uses mostly synthetic diamonds. Based on X-ray topography, he discussed the growth modes of natural and synthetic diamonds grown by high-pressure/high-temperature methods.

João Rocha, Alessandro Gualtieri

MS35: polytypism and twinning



A. Arakcheeva



C. Viti



R. Herbst-Irmer

This microsymposium attracted theoreticians studying crystal symmetry and users of software packages for automatic solution and refinement of crystal structures. Twinning or polytypism is less common in organic than in inorganic structures, but the statistics can be biased by different approaches taken to the problem. Typically, polytypes can coexist in the same crystal and often only an average structure is reported in these cases. A nice example was presented by Daniela Pinto (Italy) for the case of the new mineral vurroite, a complex sulfosalt whose structure has been solved by the application of modular theory of homologous series. Thanks to OD theory, it has been shown that vurroite includes two polytypes: thus, the new minerals are actually two and not just one! A relationship between the crystal

structure of incommensurately modulated layer compounds and the family of polytypes according to which the layers can be stacked has been shown for the first time by Alla Arakcheeva (Switzerland) who illustrated the case of $\beta\text{-K}_5\text{Yb}(\text{MoO}_4)_4$. Cecilia Viti (Italy) discussed the structure of polygonal serpentine. New HRTEM results provide an explanation of puzzling features of the XRPD pattern of this mineral. Massimo Nespolo (France) and Regine Herbst-Irmer (Germany) devoted their contributions to theoretical and experimental aspects of the twinning problem, respectively. Nespolo discussed the case of large-index twins and showed that often such twins actually have a lower *effective twin* index because, besides the subset of (quasi)overlapped lattice points accounted for by the classical twin cell, the contributions of other quasi-overlapped nodes must also be included; thus *hybrid twins* have been defined. Herbst-Irmer presented a strategy to measure the full contribution to the diffraction pattern from the different individuals of a twin when the diffracted spots do not exactly overlap because of non-zero obliquity twinning. The procedure has been implemented in SHELXL and also tested for structures of proteins.

Giovanni Ferraris

Inorganic and mineral structures solved and refined by powder diffraction data



H. Gies



J. Kaduk



D. Argyriou



K. Vidal



V. Ting

Most of the contributions in this session complemented powder diffraction with other techniques such as electron diffraction, electron microscopy or solid-state NMR spectrometry. Hermann Gies (Germany) described the characterisation of a new hydrous layer silicate, RUB-39 which condenses, when heated, to

a framework silicate with zeolitic pores. One interesting feature of RUB-39 is that the layers are held together by extremely short inter-layer H bonds (2.4Å), also detected by solid-state ^1H NMR data. This is in contrast to other layer silicates which only form short intra-layer H bonds. James Kaduk (USA) described the synthesis and characterization of the molecular solid insulator $\text{Pd}(\text{NO}_3)_2$ and the hygroscopic layered sulphate $(\text{Mg,V})\text{O}_{0.63}(\text{SO}_4)(\text{H}_2\text{O})_{1.5}$. Particularly interesting was the description of the new compound NaGe_4 possessing a zeolite-like Ge framework. This compound resulted from the systematic search for new more efficient thermoelectric materials. Here the Na atoms occupy ordered sites but some residual Na atoms can also be found in the large 24-ring channels. At the end of his talk he presented the new and rather complex silicate mineral 'charoite'. The presentation by Dimitri Argyriou (Germany) concerned the superconducting layered cobaltate $\text{Na}_x\text{CoO}_2 \cdot y\text{D}_2\text{O}$ studied using electron and neutron powder diffraction data. One of the principal difficulties in the study of this material is the refinement of the water molecules which requires the location of the hydrogen atoms. Thanks to a convenient combination of H and D in the compound, only the O of the water molecule needed to be refined. This allowed determination of the Na arrangement and provided an explanation of why the water amount remains constant and the Na content can vary. In her talk, Karmele Vidal (Spain) summarized her results on new cathodes for solid oxide fuel cells using powder diffraction techniques which constitute part of her doctoral thesis work. These cathodes are based on a new family of iron oxide perovskites. The last contribution by Valeska Ting (Australia) was on the modelling of stacking faults in ordered perovskites by refining the amount of two stacking faulted variants in addition to the main variant.

Jordi Rius-Palleiro

Open commission meeting on inorganic and mineral structures (CIMS)



S. Merlino



E. Makovicky

A short introduction by the chairperson on the activity of CIMS during its first triennium preceded six oral contributions that touched different fields of interest for CIMS: from modular aspects of inorganic crystal structures to databases of structures, single structures, graph theory and pressure calibration. A number of polytypes can coexist in the same crystal and often only an average structure is reported, as shown by Stefano Merlino (Italy) who illustrated basic examples of applying Object Discover (OD) theory. Even undiscovered new forms of a compound can be predicted after unravelling OD polytypes. Emil Makovicky (Denmark) reported on a series of crystal structures based on the same modules which incrementally increase their size. The problem of identifying structure type included in the Inorganic Crystal Structure Database (ICSD) was discussed by Rudolf Allmann (Germany). The crystal structures of iron-containing minerals recently characterized in collaboration with different European laboratories were efficaciously illustrated by Dmitry Pushcharovsky (Russia). In connection with his well known theory on bond-strength/bond-length correlations, David Brown (Canada) showed examples of graph theory application which provides better models for structures with deformed coordination polyhedra. Masanori Matsu (Japan) presented his results on T-P-V equations of state obtained by applying his breathing shell model to molecular dynamics methods in order to establish better pressure calibration standards at high T and P.

Giovanni Ferraris

MICROSYMPOSIA

Chiral and non-centrosymmetric structures



P. Mentrangolo



A. Persoons



M. Strumpel



J. Bernstein

Presentations in this microsymposium ranged from organic materials to nonlinear optical (NLO) properties of polymers. P. Mentrangolo (Italy) discussed ways to self-assemble perfluorocarbons (PFC's). As these compounds are insoluble in H_2O , it was shown that cocrystallizing these materials with hydrocarbons (HC's) resulted in hybrid PFC-HC systems. The spontaneous self-assembly of these systems resulted in strongly directed hydrogen bonding in addition to chiral resolution. Continuing with the theme of chirality, A. Persoons (Belgium and USA) discussed nonlinear optical properties of chiral polymers. The NLO effects indicated connections between magnetic hypersusceptibilities and chirality. Thus it is possible to observe these types of NLO phenomena even in a centrosymmetric environment. Also, helical assemblies that exhibited NLO-CD (circular dichroism) effects were discussed. These crystalline liquid state assemblies could be switched by the application of an electric field. M. Strumpel (Germany) discussed invariom modeling, specifically how to determine the absolute configuration of a structure with light atoms. This model uses aspherical electron density and works well with structures in chiral space groups. Pioneering research on chiro-optical imaging using a circular extinction imaging microscope was discussed by W. Kaminsky (USA). With this technique it is possible to examine heterogeneously organized media via intrinsic CD and anomalous circular extinction. In the final talk, J. Bernstein (Israel) discussed organic non-centrosymmetric structures, by referring to Kitaigorodskii's famous comment 'centrosymmetric molecules are not expected to crystallize in non-centrosymmetric space groups.' Bernstein discussed some examples of polymorphs that crystallize in both chiral and achiral space groups.

P. Shiv Halasyamani

Polymorphism



S. Reutzel-Edens



K. Sato



C. Pulham

The talks in the Polymorphism microsymposium ranged from theoretical to applied and well represented this highly charged field, including prediction, thermodynamics, control, and design of polymorphs. By far the most represented industry was the pharmaceutical industry, perhaps due to the high interest generated by recent patent cases which hinged on polymorphism. Susan Reutzel-Edens (USA) discussed the pharmaceutical industry's need for total understanding and control of the solid state of active pharmaceutical ingredients (APIs). She highlighted the need to carefully evaluate the thermodynamics and stability relationships in development of crystallizing processes.

Frank Leusen's (UK) discussion moved from experimental realities and control to the state-of-the-art in predicting polymorphism. While much progress has been made, it was clear that rational control and design of polymorphs from first principles is not likely any time soon!

Kiyotaka Sato (Japan) and Colin Pulham (UK) provided insight into efforts to control and modify polymorphism via conditions of crystallization. Sato discussed emulsions which, despite their complexity, could be used to crystallize desired polymorphs. Pulham went to another extreme in the study of polymorphism at high pressure, where access to new polymorphs is possible.

Mike Zaworotko (USA) managed to meld crystal engineering with polymorph control with the innovative concept of forming co-crystals of polymorphic APIs with readily available, pharmaceutically acceptable, molecules with complimentary intermolecular interactions. Co-crystals provides a level of solid state control not available for pure compounds. The field appears to have huge practical application and likely will lead to many new APIs with improved properties. As brought out in his talk, the field of co-crystals has long been known, but has been little studied, especially given the huge practical implications. It is also clear that the term 'co-crystals' will be the subject of continuing debate!

All in all, the message of the microsymposium was clear; the control and prediction of very high value crystalline solids remains an elusive, yet incredibly important field which should provide fundamental insight and practical application. Time will tell how soon the crystallographic community can rise to the challenge!

Elias Vlieg and Robin D. Rogers

Controlled building of crystals from non-covalent interactions



R. Davey



W. Hossein



C. Ruiz-Pérez



A. Comotti



C.-H. Görbitz

Presentations in this microsymposia covered three complementary aspects of supramolecular solid-state chemistry; nucleation, crystal building, and structureproperty correlations.

Roger Davey (UK) presented a thoughtful and instructive lecture on the use of UV/vis spectroscopy; vibrational spectroscopies; NMR; and neutron scattering in understanding the key interactions in highly concentrated solutions of five different organic molecular compounds. In many cases a clear link between solvent mediated self-assembly and the resulting crystal structures could be determined.

Wais Hossein (France) described the use of molecular tectonics for the rational design and formation of molecular networks with predefined connectivity. The precise metrics and dimensionality of many 1-D and 2-D networks can be controlled by careful design of the nature and position of recognition sites within each tecton.

Catalina Ruiz-Pérez (Spain) focused on the design and assembly of extended transition-metal containing networks. The syntheses, crystal structures and magnetic properties of a range of malonate-based copper(II) complexes were described in detail.

Angiolina Comotti (Italy) discussed weak interactions at the gassolid interface and was able to provide considerable insight into the nature of specific $\text{CH}\cdots\pi$ and $\pi\cdots\pi$ interactions that were present between hexagonal porous hosts and a variety of guests, such as carbon dioxide and methane, using NMR spectroscopy.

Finally, Carl-Henrik Görbitz (Norway) demonstrated how small peptides can act as building blocks for the deliberate assembly of tubular porous structures. Through suitable, and very deliberate, covalent modifications to the hydrogen-bonding capacity of individual peptides, 2-D assemblies can be replaced with microporous architectures with considerable strength.

Christer Aakeroy

Packing of organic molecular compounds

The speakers in this session reflected the dynamic and diverse nature of research in organic solid state crystallography in academic and industrial laboratories. Symposium sponsorship from the RSC journal *CrystEngComm* allowed for extended discussions among the speakers over dinner.



L. Barbour

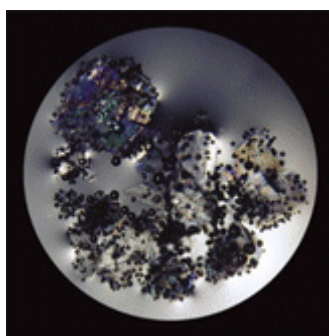


Figure 1: The replacement of enclathrated air with nitrobenzene guest in a non-porous calixarene. The Symposium was kicked off by Len Barbour (South Africa), who showed how well known calixarenes can be made to perform new tricks. By subliming *p*-*t*-butylcalix[4]arene, empty cavity-containing materials are obtained that are capable of absorbing small guest molecules such as vinyl bromide and gases such as CO₂ even though there is no pore or channel in the structure to admit them. The work poses difficult to address questions about the nature of diffusion through close packed organic solids. The phenomenon was delightfully illustrated by a video sequence showing the replacement of calixarene-included air with a more favoured guest, nitrobenzene. When a drop of nitrobenzene is placed on the crystal, bubbles of included air are rapidly evolved as oxygen and nitrogen molecules in the cavities are replaced by the aromatic guest (Figure 1). The integrity of the single crystal is preserved throughout. Exciting discussion was provided by Stan Nyburg concerning the pressures of H₂ gas required to put hydrogen as a guest in related systems.



C. Gervais

Claire Gervais (Switzerland) outlined her new approach to polymorph prediction based on a 'derived crystal packing model'. Taking layers or slices of known polymorphs, Claire derives a series of daughter phases based on common packing motifs and symmetry operations. Comparison with the powder patterns of unknown polymorphs, particularly patterns of poor quality that do not admit *ab initio* structure solution and Rietveld refinement, can yield the structure of inaccessible polymorphs. To illustrate, she derived a model for an unsolved phase of the pharmaceutical Modenafinil. Vigorous

discussion was led by Luigi Nassimbeni.



A. Gillon

The pharmaceutical polymorphism theme was continued by Amy Gillon (UK). Amy showed how a very wide range of techniques are applied to screening and characterizing drug polymorphic forms. A key question she addressed concerned when is it appropriate to stop looking for polymorphs with reasonable confidence that no new forms will subsequently be identified – a formulation and intellectual property nightmare.



M. Kubicki

Maciej Kubicki (Poland) provided a thoughtful look at the poorly understood world of compounds with $Z' > 1$, i.e. crystals with more than one molecule (however we might define it) in the crystallographic asymmetric unit, including crystals where there are two independent half molecules using examples from his own work on nitroimidazole derivatives.



L. MacGillivray

The final speaker, Len MacGillivray (USA), illustrated the profound control over solid state reactivity that can be gained through the use of 1,3-dihydroxy benzene as a template to position reactive double bonds. The work has resulted in the highly efficient synthesis of exotic structures such as ladderanes. What was particularly pleasing about Len's talk was the systematic use of increasingly bulky substituents on the diol template in order to bring about the desired, convergent crystal packing arrangements, representing a clear case of crystal structure design and control with immediate application.

Given the tender age profile of the researchers, many more interesting results can be expected in IUCr meetings to come.

Jonathan W. Steed and Carolyn P. Brock

Crystallography and forensic science



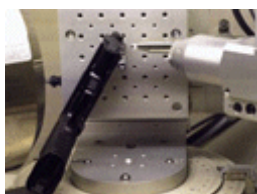
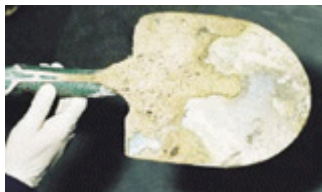
W. Kugler



R. Fitzpatrick



W. Heijinen



Contact traces at the muzzle of the barrel of a Police Officer's pistol



Y. Terada



I. Nakai

The advent of DNA profiling evolutionized forensic science. In the absence of material leading to the recovery of DNA, however, the forensic scientist has to rely upon chemical analysis of classical trace materials in order to establish or eliminate links between suspect and crime scene. X-ray powder diffraction (XRD) and X-ray fluorescence (XRF) are two valuable non-destructive analytical methods available for this purpose, and recent developments of these methods were illustrated by the speakers through practical applications at interesting crime scenes. Werner Kugler (Germany) described a case in which the analysis, by *in situ* powder diffractometry, of traces of material on the barrel of a police officer's hand gun exonerated the officer of the murder of a suspected bank robber. The gun had discharged accidentally after having been dropped on the sidewalk and traces of quartz and calcite on the barrel confirmed the officer's account of the incident. Soil is potentially one of the most useful evidence types, and Rob Fitzpatrick (Australia) outlined the systematic sequence used in its analysis. In a double murder case, XRD was used to identify and compare clay minerals in soils on a shovel belonging to the suspect, with those in the soil of a quarry where the bodies were buried. Paper used to write threatening letters was analysed by Wim Heijnen (The Netherlands). XRD identified the fillers (talc, chlorite and kaolinite) present and also provided a measure of the cellulose crystallinity. The use of

synchrotron radiation in forensic analysis has been pioneered by Yasuko Terada (Japan). She described cases in which the light source was used for XRD and XRF analysis of trace amounts of material including fluorescent powders used as markers when thrown at robbers. Use of portable XRD/XRF equipment for *in situ* analyses at crime scenes may become routine in the future, and in the final presentation, Izumi Nakai (Japan) illustrated his talk with pictures of a compact, portable diffractometer currently used at archaeological sites for mineral identification.

David Rendle and Izumi Nakai

Crystallography and environmental science

Multiple connections between environmental science and crystallography were highlighted by this microsymposium, with topics ranging from geomicrobiology to materials research, from basic science to industrial applications.



A. Gualtieri

In the opening lecture, Alessandro Gualtieri (Italy) documented that structural differences among zeolites (NH_4 -substituted chabazite and phillipsite) affect their potential as „slow-release” fertilizers.



F. Guyot

François Guyot (France) showed some exotic cases of carbonate biomineralization. Spatial distributions of various carbonaceous species, including proteins, carbonates, and polysaccharides can be mapped using scanning transmission X-ray microscopy; energy-filtered images reveal how microorganisms induce the precipitation of calcite, aragonite, or amorphous calcium carbonate.



G. Jordan

The environmental importance of mineral dissolution was emphasized by Guntram Jordan (Germany), who presented results of atomic force microscopy studies on mineral/water interface processes. A variety of dissolution mechanisms were illustrated by the examples of carbonates, plagioclase feldspars, and apophyllite.

The final two lectures focused on crystallographic problems related to the production and properties of materials that are used in environmentally friendly industrial applications. K. Byrappa (India) discussed the methods and results of the hydrothermal synthesis of nanocrystalline TiO_2 on an amorphous carbon substrate, a composite that is used as a photocatalyst. Katsuhito Mori (Japan) presented a study on polyhydroxybutyrate thin films. Film thickness, surface roughness, and crystallographic orientation were characterized using X-ray reflectivity; the environmental significance of the study comes from the fact that such films are biodegradable.

Mihaly Posfai



FEATURE ARTICLE

A new IUCr commission: commission on mathematical and theoretical crystallography



Far from having exhausted its research potential, Mathematical and Theoretical Crystallography (MaThCryst) is facing new challenges, not only in the very classical field of group theory (magnetic groups, chromatic groups, N -dimensional groups) and its applications (phase transitions, polymorphism and polytypism, twinning, biocrystallography, ferroic crystals), but also in several directions that previously were less strongly perceived as being directly related to crystallography and crystal-chemistry, such as graph theory, combinatorial topology, number theory, discrete geometry, diffraction theory, etc. The development of mathematical and theoretical crystallography will strengthen the interaction between crystallographers, mathematicians and materials scientists and will definitely contribute to the recognition of crystallography as an interdisciplinary science.

The outstanding success that applied crystallography has experienced in recent years has transformed a common structural investigation into a routine task, often performed by researchers with no specific background in crystallography. Moreover, the success of automated structure solutions, whose results are persistently accepted without sufficient criticism, has contributed to the spread of the pernicious impression that a specific education in crystallography is no longer necessary in order to perform crystallographic tasks on a daily basis. The result is that nowadays crystallography is increasingly perceived as a technique, if not just as a tool, rather than an interdisciplinary science strongly interacting with fundamental and applied disciplines like mathematics, chemistry, physics, materials science, geosciences and biosciences. As a consequence, the time devoted to crystallographic education in undergraduate and graduate courses is continuously shrinking, and a solid background in crystallography is disappearing from the requirements of many positions that involve a considerable amount of crystallographic work.

The IUCr-MaThCryst Commission was started in September 2002 as an informal workgroup by a nucleus of researchers who felt the necessity of trying to reverse the current trend towards “crystallography as a black-box tool”. The aims of the new commission can be summarized in the following points.

- To strengthen links and interactions among crystallographers, mathematicians and theoretical physicists and chemists, and to promote a common language in these fields.
- To promote the presence at IUCr meetings of scientists working in the fields of mathematics, geometry, topology, and symmetry.
- To strengthen the recognition of crystallography as an interdisciplinary science in those fields where it is now considered only to be a technique.
- To promote the publication of mathematical and theoretical papers in the journals of the Union.
- To encourage the development and dissemination of mathematical and theoretical methods, software and databases for the solution of crystallographic problems.
- To promote and organize symposia of interest to mathematical and theoretical crystallographers during IUCr congresses and meetings of the regional associates, in cooperation with other Commissions of the Union.

- To promote and organize meetings, workshops and schools in collaboration with other Commissions particularly targeting post-graduate students and young scientists needing and willing to complete their education in crystallography.

The MaThCryst Commission has already organized a satellite conference (Budapest, August 2004) and a Summer School (Nancy, June 2005). Forthcoming activities include:

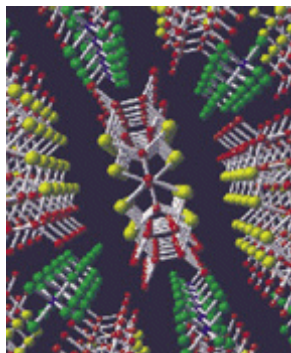
- Satellite conference of the ECM-23 meeting, Leuven (Belgium), August 4-6, 2006
- Satellite conference of the AsCA'06 meeting, Tsukuba (Japan), November 18-19, 2006
- Winter School at Havana (Cuba), January 14-19, 2007
- Satellite conference of the ECM-24 meeting, Marrakech (Morocco), August 20-22, 2007
- Summer School on the Garda Lake (Italy), May 2008 Up-to-date information can be obtained on the MaThCryst website (www.lcm3b.uhp-nancy.fr/mathcryst/)

MEETING REPORT

Croatian-Slovenian meeting

Vrsar, Croatia, June 15-18, 2005

The 14th Croatian-Slovenian Crystallographic Meeting was held in Vrsar, a famous tourist resort on the western coast of the Istria peninsula, pointing far into the Adriatic.



There were five plenary lectures. Nina Lah (Ljubljana) presented the extraordinary structural diversity and possibilities in copper coordination compounds. Len MacGillivray (Iowa City) gave a molecular architecture story - namely how to construct molecules in the solid state using UV radiation instead of wet chemistry. Radovan Cerny (Geneva) explained how it is possible to extract 3D information if the data is accumulated in 1D only - a survey was given on how crystal structures are obtained from powder diffraction patterns. Milorad Milun (Zagreb) gave us an educational overview of atomic structures of surfaces and thin films - we were thrilled with his description of a terrace with a step of only one atom height. The last lecture was given by Eugen Libowitzky (Vienna) on dynamics of crystal structures and the interplay between diffraction and spectroscopy - comparing how to make fruit brandy from apples and pears. There were 50 short oral contributions by 144 authors (48 contributing authors). Beside Croatians and Slovenians, there were representatives from 13 other countries, which is quite an achievement.



Deep silence in the lecture hall

B. Kamenar (Zagreb) and Lj. Golic (Ljubljana) were the honorary Chairs of the meeting, while S. Popovic (Zagreb) and I. Leban (Ljubljana) were the program co-Chairs; due to their stamina these meetings are so successful and regular. Special thanks to A. Tonejc (Zagreb) as the Chair of the Organizing Committee and to the colleagues who actually performed the job - Mario Cetina, Željko Skoko, Zoran Štefanic and Aleksandar Višnjevac. We shall proceed with this concept for future meetings and we shall also try to have the meetings without a registration fee. This is the 14th meeting in a row of this sort which is good proof that this is possible.



Plenary lecturers, from the left Radovan Cerny, Nina Lah, Eugen Libowitzky

Therefore we thank the sponsors and donors: Ministry of Science, Education and Sport of the Republic of Croatia; RENACON, Zagreb, representative of PANalytical; Rigaku, UK; SCAN, Preddvor, Slovenia; Marresearch GmbH, Germany; Oxford Diffraction Ltd, UK; Micro-Polo, Slovenia, representative of Bruker-Nonius; Physics Dept., Faculty of Science, U. of Zagreb, Croatia; Tourist Enterprise Maistra dd, Rovinj, Croatia; Croatian Tourist Assn; Školska Knjiga (School Books Publisher), Zagreb, Croatia. Only with their help was all this possible.



The Local Organizing Committee (from left: Z. Stefanic, A. Visnjevac, Z. Skoko, M. Cetina, B. Kamenar, A. Tonejc, S. Popovic)

The participants enjoyed a crystallographic trip inside the Istria peninsula, where they admired the Baredine cave (the forming and crystallization of calcite and aragonite in action, having long range order, of course). The trip also included Eufirius basilica in Porec, a UNESCO protected monument, where we saw nice mosaic patterns (which are also connected with crystallography; stone pieces forming a mosaic show of short range order and a long range disorder). The participants also experienced some practical work (of a workshop type) in a nearby wine cellar. During wine and cheese tasting they listened to secrets of wine producing (organoleptic group analysis of various samples of biotechnological origins; it did not matter that tasting different sorts of wine might result in a long-term disorder). One may be sure that the text in brackets will only appear in the report to the Ministry of Science, Education and Sport. For more information please visit www.hazu.hr/kristallografi .

The next meeting will be held in Slovenia in June 2006. We would like to welcome again all participants of our previous meetings as well as others who would like to experience a gathering of crystallographers in very friendly and familiar circumstances, in a resort of natural beauty, somewhere in Slovenia. For more information please contact: Ivan Leban, Ljubljana, ivan.leban@fkkt.uni-lj.si or Stanko Popovic, Zagreb, spopovic@phy.hr

Stanko Popovic

Secretary, Croatian Crystallographic Assn

MEETING REPORT

Practical workshops for young biocrystallographers at the Poznan BioXHIT TID Centre

Poznan, Poland, November 27 - December 9, 2005



A TID cake with a sweet puzzle for the participants

For two weeks, the Center for Biocrystallographic Research (CBB, www.man.poznan.pl/CBB) at the Inst. of Bioorganic Chemistry, Polish Academy of Sciences in Poznan, Poland, was swarming with young people from different European countries, bustling about performing protein purification and crystallization, collecting and processing X-ray diffraction data, and trying to solve and model protein structures. In this fashion, the Poznan Training, Implementation and Dissemination (TID) Centre of the European BioXHIT Project (icarus.embl-hamburg.de/bioxhit) inaugurated its operation. BioXHIT is a unique project in the field of structural genomics, funded by the European Union, with a mission to consolidate the efforts of the existing European facilities and software developers for high-throughput structure determination. The results are disseminated through its TID Centres. By targeting young people, the TID Centres should ensure that there will be qualified cadres for researchers for structural genomics efforts in all European regions. In the two TID Workshops held in Poznan, all participants were at a graduate or postgraduate level. In the first workshop, there were participants from Poland (9), Lithuania (1), Russia (3), Ukraine (1), Slovakia (2), Czech Republic (2), Germany (1), Sweden (1), France (2), Spain (1), and Portugal (1). The 24 places in the second workshop were filled by a group of Ph.D. students from the European doctoral training network called ADOPT and from the International Max-Planck Research School, both coordinated from Cologne. The training program consisted of nine lectures and six practical sessions in which the students, divided into small groups, could gain hands-on experience with all the essential experimental steps leading from a crude protein preparation to the most refined product – its crystal structure. In addition to the local staff (Grzegorz Bujacz, Wojtek Rypniewski, Michal Sikorski), the teaching team included some of the best European experts in structural genomics. A contingent of instructors from the EMBL Hamburg Outstation included Paul Tucker (overview of structural genomics with synchrotron radiation), Jochen Mueller-Dieckmann (high-throughput crystallization), Sasha Popov (the BEST data collection strategy), and Santosh Panjikar and Venkataraman Parthasarathy (the AutoRickshaw pipeline). There were two instructors from Warsaw, Michal Dadlez overseeing the applications of mass spectrometry for structural genomics and Matthias Bochtler teaching about molecular replacement and

model building. A great help in the crystallization tutorials was our young colleague, Robert Kolodziejczyk. It was a real pleasure to host, as a special guest, Zbyszek Dauter, who was able to donate two weeks out of his busy schedule at the APS synchrotron center in Chicago to teach about optimal data processing and extraction of phasing signals. The students were housed and instructed under one roof, and they seemed to enjoy the workshops and the practical aspects, skillfully arranged by Joanna Stepkowska. One evening of each workshop was reserved for a cultural program (concert of organ music) and for a gala dinner. For the instructors, it was a gratifying experience to work with highly motivated and enthusiastic young people. We hope that the efforts will have a lasting effect, both for the education of a new generation of biocrystallographers and for their integration into our community. The Poznan TID Centre will continue its training mission, with workshops planned for 2006 and 2007.

Mariusz Jaskolski, Poznan

MEETING REPORT

8th Heart of Europe meeting

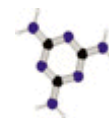
Karlovy Vary, Czech Rep., September 29 - October 1, 2005 It has become a tradition that the “Heart of Europe Crystallography (HEC)” meetings bring crystallographers from Central Europe together for three days. This year, the meeting was organized by Juraj Sedlacek under the auspices of the Czech and Slovak Crystallographic Assn and held in Karlovy Vary. As in previous meetings, the purpose was to give Ph.D. students and younger scientists a forum to discuss their results and ideas. In line with HEC traditions, group leaders were banned from giving presentations, except for heads of newly participating groups. This year, the HEC community welcomed the first group from Austria, when Kristina Djinovic Carugo introduced her team from the U. of Vienna. Altogether, about 100 people took part in the meeting and over 30 participants presented 15 minute lectures. Most talks focused on new crystal structures, but there were also two sessions devoted to methods development and instrumentation. Zbiginiew Dauter (Argonne, IL) presented the keynote lecture and emphasized the jolly sides of SAD, and Thomas Wollert (Braunschweig) won the award for best lecture. All participants will have happy memories of the charming location of the meeting. Karlovy Vary has preserved much of its old glory, and the conference centre was no exception. The place felt like a luxury mansion from the 19th century, and participants were impressed to learn that this was the place where Dvorák’s “From the New World” was first publicly performed. Thanks are due to the European Crystallographic Assn, the Czech and Slovak Crystallographic Assn, and the company sponsors (www.img.cas.cz/hec/) for financial support, and of course particularly to Juraj Sedlacek for organizing such a nice meeting in such a splendid location!

Matthias Bochtler and Roman Szczepanowski

MEETING REPORT

Belgian Crystallography Symposium BCS-4

Brussels, Belgium, October 19, 2005



Speakers, poster prize winners and organizers of the 4th Belgian Crystallography Symposium BCS-4. The Belgian National Committee for Crystallography organized the 4th Belgian Crystallography Symposium BCS-4, which was held at the Academy House in Brussels. About 85 Belgian crystallographers attended this biannual meeting. The morning session consisted of three invited lectures. Frank H. Allen (Cambridge) presented some applications of the Cambridge Structural Database in the field of structural chemistry, drug design and pharmaceutical development. The second talk by Alain Jonas (Louvain-la-Neuve) concentrated on self-assembly and self-organization as studied by scattering and microscopy techniques. Claude Lecomte (Nancy) illustrated the use of ultra high resolution X-ray diffraction in the study of protein-ligand interactions. A poster session and commercial exhibition were organized during lunchtime. The afternoon session consisted of three oral presentations selected from the submitted abstracts (H. Novoa de Armas (Leuven), F. Hatert (Liège), and J. Burton (Namur)). At the end of the meeting two poster prizes were awarded to W. Tirry and Y. Boland. The BCS-4 meeting was sponsored by the Royal Academies of Sciences and Art of Belgium, and by the firms Bruker AXS, PANalytical, FEI and JEOL.

Luc Van Meervelt

OBITUARY

Oksana Ivanivna Bodak (1942-2005)

Oksana Ivanivna Bodak, an outstanding figure in the field of intermetallic compounds, passed away at the age of 63 on October 25, 2005, after a terrible illness. She was the Director of the Department of Inorganic Chemistry at Ivan Franko National U. of Lviv (Ukraine).

Oksana Bodak obtained her PhD in Chemistry at Lviv University under the guidance of E. Gladyshevskii. During her 40-year career at Lviv U., she progressively became a docent, a professor (1984) and the head of the Dept. of Inorganic Chemistry (1989). Motivated by her devotion to teaching and the research on intermetallic compounds, she led the department through periods of difficult economic conditions and managed to build up a worldwide network of scientific collaborations. Under her direction, the Dept. of Inorganic Chemistry prepared 280 masters in chemistry, every sixth master pursuing further studies to obtain a PhD title.

At an early stage in her career, Oksana Bodak joined *Lviv School on Crystal Chemistry of Intermetallic Compounds*. Her works on binary and ternary compounds containing rare-earth metals have greatly contributed to our knowledge of intermetallic compounds, and earned her respect in the scientific community, in several cases rewarded by prizes and medals. During her long and prolific scientific career, she studied more than 180 chemical systems, determining the conditions of formation and the crystal structures of more than 1800 compounds, and discovered 130 new structure types. The results of her works have been published in some 800 scientific papers and she co-authored two monographs. She characterized a number of important crystal chemical anomalies, and collaborated on the development of generalization concerning the relationships between intermetallic structure types.

Oksana Bodak enjoyed sharing her deep scientific knowledge and experience with students and young scientists and was an inspiring teacher. Trustworthiness, intelligence and kindness were evident in all the actions of her everyday life and she will be greatly missed by those who had the good fortune to know her.

R. Gladyshevskii, B. Belan

OBITUARY

Robinson D. Burbank (1921-2006)

Robinson Derry Burbank, president of the American Crystallographic Assn in 1975 and Bell Labs scientist who worked on the Manhattan Project, died February 9, 2006 at home in Summit, NJ following a brief illness.

Rob was born October 3, 1921 in Berlin, NH, graduated Phi Beta Kappa from Colby College in 1942 and received his PhD in inorganic chemistry from MIT in 1950. He performed spectrochemical analysis on uranium and thorium at MIT during World War II as part of the Manhattan Project. Upon completing his doctorate, he joined the Gaseous Diffusion Plant in Oak Ridge, Tennessee as a senior physicist before coming to Bell Laboratories in Murray Hill, NJ in 1955. His contributions to greater accuracy in structural investigations included his early demonstration of the value of cooling the crystal under investigation to low temperatures, his recognition of the geometric conditions under which intrinsic multiple diffraction occurs and his comparisons of the use of ω and 2θ scans for integrated intensity measurements. Materials of unusual chemistry and physical properties, including noble gas and interhalogen compounds such as $\text{XeF}_2 \cdot \text{IF}_5$ and XeF_6 , the structures of which he determined, were also among his interests as were the mechanisms of phase transitions.

He was a charter member of the American Crystallographic Assn, a member of the the American Physical Society and the American Assn for the Advancement of Science. He served on the executive committee of the Governing Board of the American Institute of Physics. He was a U.S. delegate to the IUCr in 1975.

A ski-jumper in his youth, Rob Burbank was an avid skier, hiker, and mountain climber. He was a longtime patron of the arts, especially the Metropolitan Opera. He is survived by a son, Paul R. Burbank of Ozone Park, NY, a daughter, Claudia Burbank of Bernardsville, NJ, and two granddaughters, Christine and Joy Burbank of Kew Gardens, NY. Contributions in his memory may be made to the Mount Washington Observatory, P.O. Box 2310, North Conway, NH 03860, or to the Metropolitan Opera Company in New York.

Claudia Burbank and Sidney Abrahams

OBITUARY

Reuben Rudman (1937 - 2006)

Professor Reuben Rudman died suddenly on February 15 in Jerusalem, Israel. He was born in New York and received an M.A. degree from Columbia U. (1957) and rabbinic ordination as well as M.H.L. from Yeshiva U. (1959). He was awarded a Ph.D. in 1966 from the Polytechnic Inst. of Brooklyn under the guidance of Ben Post. Reuben devoted his scientific career to crystallography: research, teaching and serving the crystallographic community. His research interest included the systematic study of phase transitions exhibited by pseudo-spherical molecules supplemented by differential calorimetric investigations; instrumentation for low temperature X-ray diffraction both for single crystal and powder methods. He has published more than 70 scientific papers in these fields. He served as chairman and member of a number of committees of IUCr, ACA and Gordfon Research Conferences. He was professor of chemistry at Adelphi U., Garden City, NY, for 35 years, where he taught general and inorganic chemistry, solid state chemistry and crystallography until his retirement in 2003.

His book, "Low-temperature X-ray diffraction. Apparatus and Techniques" published by Plenum Press, N.Y, was written during his sabbatical in Israel 1973-74, where he served as a visiting professor at the Inst. of Chemistry of the Hebrew U. Jerusalem. He returned to the Hebrew U. again after his retirement and volunteered to teach X-ray crystallography to graduate students of chemistry until his sudden death.

Reuben was beloved by his many friends and colleagues, he was an excellent teacher highly appreciated by his students. He is survived by his wife Idelle, five children, grandchildren and great-granddaughter.

Mayer Itzchak and Shmuel Cohen