

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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LETTER FROM THE PRESIDENT

Letter from the President



At the meeting of the Executive Committee held last August, a new initiative was launched to encourage developing countries to be members of the IUCr, as described in a previous issue (Vol. 14, No. 2). According to the initiative, the IUCr strongly recommends crystallographers in developing countries to form a country group and to establish a single Adhering Body to become a member of the IUCr. I am very glad to hear from the Presidents of the three Regional Associates, Professor Bau (ACA), Professor Vijayan (AsCA), and Professor Helliwell (ECA), that discussions to form such groups are progressing in their Associations. I hope a variety of countries will become members of the IUCr at the next General Assembly to be held in Osaka.

The IUCr has supported international schools and seminars on crystallography held in many countries and has provided funds to enable young scientists to attend. A total of USD 125,000 was awarded to 23 schools and seminars last year. This scheme is much appreciated not only by the organizers of the schools and seminars but also by the young scientists, especially from the developing countries. However, there is an important condition to this support, that is, the meetings must be “international”.

In 1991 the Executive Committee recognized that there were many worthwhile schools in developing countries and countries of the former Eastern bloc that were not international but would nevertheless benefit greatly from IUCr support. The IUCr therefore established the Visiting Professor Scheme to support such schools or seminars. According to this Scheme, up to three eminent scientists present a short course at a school or seminar and their travel and insurance costs are met by the IUCr. The local organizers cover the accommodation/subsistence expenses.

The IUCr has provided an annual budget of USD 25,000 for the Scheme. In the past ten years the IUCr has supported Visiting Professorships in Brazil, Cuba, China, India, Indonesia, Kenya, Mexico and Morocco, and these have been very much appreciated by the hosts. However, the Scheme is not well known by crystallographers in many developing countries, compared with the young scientist support. As a matter of fact, the budget has not been fully utilized.

I think it very important that the crystallographic schools and seminars should be held in developing countries to enable crystallographers in these countries to become organised. The IUCr will strongly support such schools or seminars using the above Visiting Professorship Scheme. Those interested in applying for the Visiting Professorship Scheme should contact the Executive Secretary (execsec@iucr.org) for further information.

Yuji Ohashi, yohashi@spring8.or.jp

REGIONAL NEWS

European Crystallographic Association



As current President I have this wonderful feeling of making a British contribution to the European, including African, organisation of our crystallographic science. Furthermore ECA, to be very practical about it, is one of the three regional associates of the IUCr and as such we have reserved some space in the IUCr Newsletter, a most significant point regarding an important channel of communication to our members and the whole world of crystallographers.

My duties thus far have been multi-faceted, and I give you here an overview spanning short, medium and long term matters. Most immediate is to help support our colleagues in Morocco led by Prof Abdelmalek Thalal with their hosting of the ECM24. I visited the Congress Centre in Marrakech in November for helping to finalize the Program and the chance to offer comments on the local facilities. At the ECA website (www.ecanews.org/) I share with you some photos of my visit, including a real collector's item of me in a blue turban! (www.ecanews.org/exc_news.htm). The Marrakech Congress Centre is superb and the attached Hotel also marvellous. I had an afternoon free to visit Marrakech and see some of the sights. From the very positive impression I had of my whole visit one outcome is that my wife and I are now booked on a 2 weeks holiday in several places in Morocco following ECM24! Most importantly the ECM24 scientific programme is advancing very well; for example the number of Microsymposia has been expanded to cope with the diversity of demand and the range of our field. The Chairs of the ECA SIGs especially have done a great job in community consultation and speakers' selection. Further talks will be selected from the submitted abstracts for each Microsymposium.

At the recent ECA Executive Committee meeting held in Manchester we also discussed the planning of ECM25 to be held in Istanbul in August 2009; and yes it is the 25th ECM, clearly a cause for a special celebration. The ECA Executive also reviewed in detail the ECA SIG structure; my Committee colleague Prof Garcia-Granda will expand on this below. Another item of business included the establishment of a 'risks management folder' for the ECA. Also we initiated the setting up of an ECA archive, to be based at IUCr in Chester, as an essential start towards a writing of the History of the ECA; Past-President Hartmut Fuess, with his long standing and strong involvements with the ECA will be our Archivist. This also is our first step towards establishing a base for an ECA office; in the long term we would like to have our own employees, like the ACA for example have at Buffalo.

Taking ECA forwards also means making stronger efforts in offering our members more diverse benefits. Firstly, the ease of joining; we now have a credit card possibility to join as an Individual Member (IM). Besides the IM category there are the national association derived members and the industrial ie corporate members. In terms of benefits to members much of course revolves around the ECM. At ECM24 we will have a training workshop, before the main conference on "Computational methods and use of synchrotron facilities for crystallography", where this is an example of a training opportunity for 'Continued Professional Development'. There are two other ECM24 Satellites that I must mention: "Science meets industry" and "The enchanting crystallography of Moroccan ornaments". Most recently, in terms of ECA Individual Members benefits, we are pleased to now be able to announce, here, that we have entered into an agreement with the publisher Taylor and Francis for a reduced personal subscription to Crystallography Reviews; the practical details will be announced at the ECA website.

John R Helliwell, President of the ECA

Since the ECA was created from the European Crystallographic Committee (ECC), around 1997, the Special Interest Groups have been key for the development of ECA. The statutes define the SIGs in Statute 12 as “Special Interest Groups in any area of crystallography may be proposed by four (4) or more Councillors or twenty (20) or more Affiliate or Individual Members. The establishment of any Special Interest Group requires the approval of the Council. Rules about the establishment, dissolution and procedures of Special Interest Groups shall be specified in the By-Laws.”

The current structure of the SIGs within the ECA includes thirteen SIGs covering most aspects of Crystallography, each is devoted to a particular yet wide crystallographic topic: SIG 1 is Macromolecular Crystallography, SIG 2 is for Charge, Spin & Momentum Density, SIG 3 deals with Aperiodic Crystals, SIG 4 is oriented to Electron Crystallography, SIG 5 covers Mineralogical Crystallography, SIG 6 deals with Instrumentation and Experimental Techniques, SIG 7 gathers the Molecular Interaction and Recognition community, SIG 8 groups the Powder Diffraction (EPDIC) community, SIG 9 promotes Crystallographic Computing, SIG 10 is interested in Diffraction Physics and Optics, SIG 11 is dedicated to Crystallography under Extreme Conditions, SIG 12 covers Materials Science and SIG 13 promotes activities within the Molecular Structure and Chemical Properties field.

In the 10 years of the ECA, the role of the SIGs was generally recognized as the driving force of the ECA. In order to maintain the leading role of the SIGs in the ECA's development, especial attention is to be paid to all developments related to their activities. Whilst allowing for the internal activities and self organization of each particular SIG to have a ‘personality’ this should be combined with a more formal common organization. Basically, considering the number of existing SIGs, it is essential to follow some common guidelines in the number and type of SIG Officers and the minimum information to be shown for every SIG on the ECA website. One point of discussion is the adoption of a common reporting style. The SIG Officers' structure should comprise:- Chair, Vice-Chair (Co-Chair) and Secretary. Exceptionally there may be, for instance, two Co-chairs for the most populated SIGs. Each SIG manages its membership, maintaining a website and link to the ECA website. The ECA maintains obviously a distribution list, including all the SIG officers and the SIG's Executive Committee Members, in order to facilitate a quick communication among all. The SIGs' memberships, although not yet known as precisely as we would like, can be measured via the number of abstracts around the ECM Microsymposia.

The activity, based on the five last years activity reports, of the existing SIGs and their impact on the ECA activities has been analysed producing some interesting conclusions:-:

Most SIGs develop their activities in the ECM (IUCr in some cases) meetings, including Satellite Symposia and Workshops. In addition other activities were reported by some SIGs, such as involvement in schools and teaching activities, which are likely, hopefully, to be important in their impact in the longer term in sustaining the health and growth of our field. In general the compiled Activity Reports follow quite different styles, and are a mixture of projects and reports. The suggestions for the future are to standardize the annual Activity Reports, promote more joint activities between the SIGs and give an increased priority to support the activities promoted by more than one SIG and/or a number of IMs. Other possible improvements will be to support the web hosting costs of each SIG by the ECA. An especially interesting idea is that there should be one hour reserved for SIG meetings during ECMs when no other simultaneous meeting would be held. One member of the Executive Committee will be appointed to coordinate and supervise the SIG's activities and particularly their ECMs' activities. In particular the ECA will try to further the aims of achieving adequate Geographical, Nationality and Gender distributions. Another important issue to develop concerns the possibility of ECM ‘focus areas’, harnessed in the Durban ECM meeting, to increase the level of overlap and harmonisation among the SIGs. This possibility is to be put into discussion with the SIG leaders, ahead of the ECM25 Program Committee meeting.

With the aim of clarifying the SIGs' membership, and to persuade and promote Individual Membership in

ECA, the following guidelines have been agreed by the ECA Executive Committee to be recommended to the ECA Council in August 2007 at the ECM24 in Marrakech:

- Becoming a SIG officer - Chair, Co-Chair or Secretary - is restricted to Individual Members (IM), with the caveat that the Individual Membership is not a priori required for a person to be a candidate but must be effective after election.
- National Associate Members (NAM) may be 'registered' SIG members. Some SIG's, however, may require that you are an Individual Member for being listed as a 'Founding Member' (thus showing the interest towards European cooperation in crystallography)
- Colleagues from non-ECA countries may be IM's and therefore SIG members and SIG officers.
- Colleagues from non-ECA countries who are neither IM's nor NAM's of course are very welcome as 'Guest Members' of a SIG General Meeting, but the ECA Executive Committee would hope they would join the ECA as IMs as soon as possible. This would thereby encourage a global participation to the ECA.

Santiago Garcia-Granda, ECA Executive Committee Member, responsible for coordinating the ECA SIGs

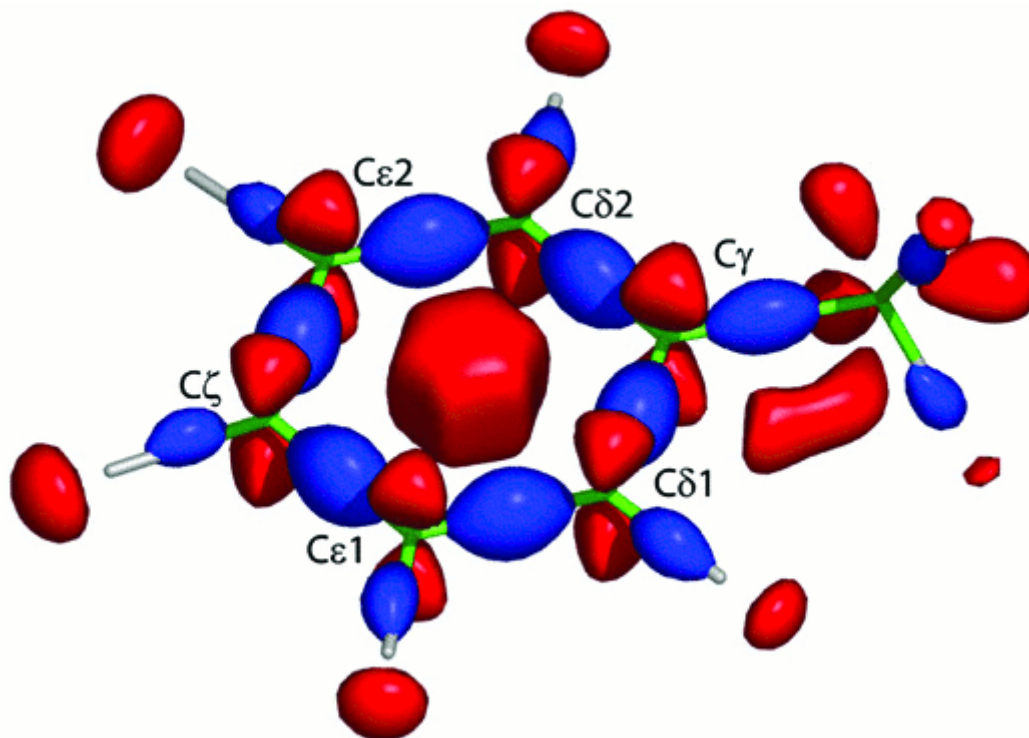
AWARDS AND PRIZES

IUCr poster prizes at AsCA'06

Photo courtesy of Yoshio Matsui, NIMS

Congratulations go to young scientists Yi-Wei Chang (third from right; Institute of Molecular Biology, Academia Sinica, Taipei, Taiwan) and Pance Naumov (third from left; National Institute for Materials Science, Tsukuba, Japan), who won the IUCr poster prizes at the 2006 meeting of the Asian Crystallographic Association in Tsukuba, Japan. The winning posters were “Crystal Structures of the dTDP-4-keto-2,3,6-trideoxy-3-aminohexose Reductase (DnmV) from *Streptomyces peucetius*: Implications for the Inhibition and Catalytic Mechanisms” by Y.-W. Chang, C.-C. Wu, Y.-J. Sun, H.-T. Chiu and C.-D. Hsiao, and “Small imperfection causes a very small molecule to pack in a very large cell: Sodium saccharinate 1.875 hydrate with unit cell of 15.6 nm^3 ” by P. Naumov, G. Jovanovski, O. Grupce, B. Kaitner, D. Rae and S. W. Ng. Judging the competition and awarding the prizes were IUCr Executive Committee members Yuji Ohashi (President, second from right) and (from left) Peter Colman, Gautam Desiraju and Gernot Heger.

On the application of an experimental multipolar pseudo-atom library for accurate refinement of small-molecule and protein crystal structures



Static deformation of the electron density for a phenyl group $C_6H_5-CH_2-$ after library transfer. Blue and red surfaces denote positive $+0.4 \text{ e } \text{\AA}^{-3}$ and negative $-0.1 \text{ e } \text{\AA}^{-3}$ density levels respectively.

***Acta Cryst.* (2007). A63, 108-125 [doi:10.1107/S0108767306053748]**

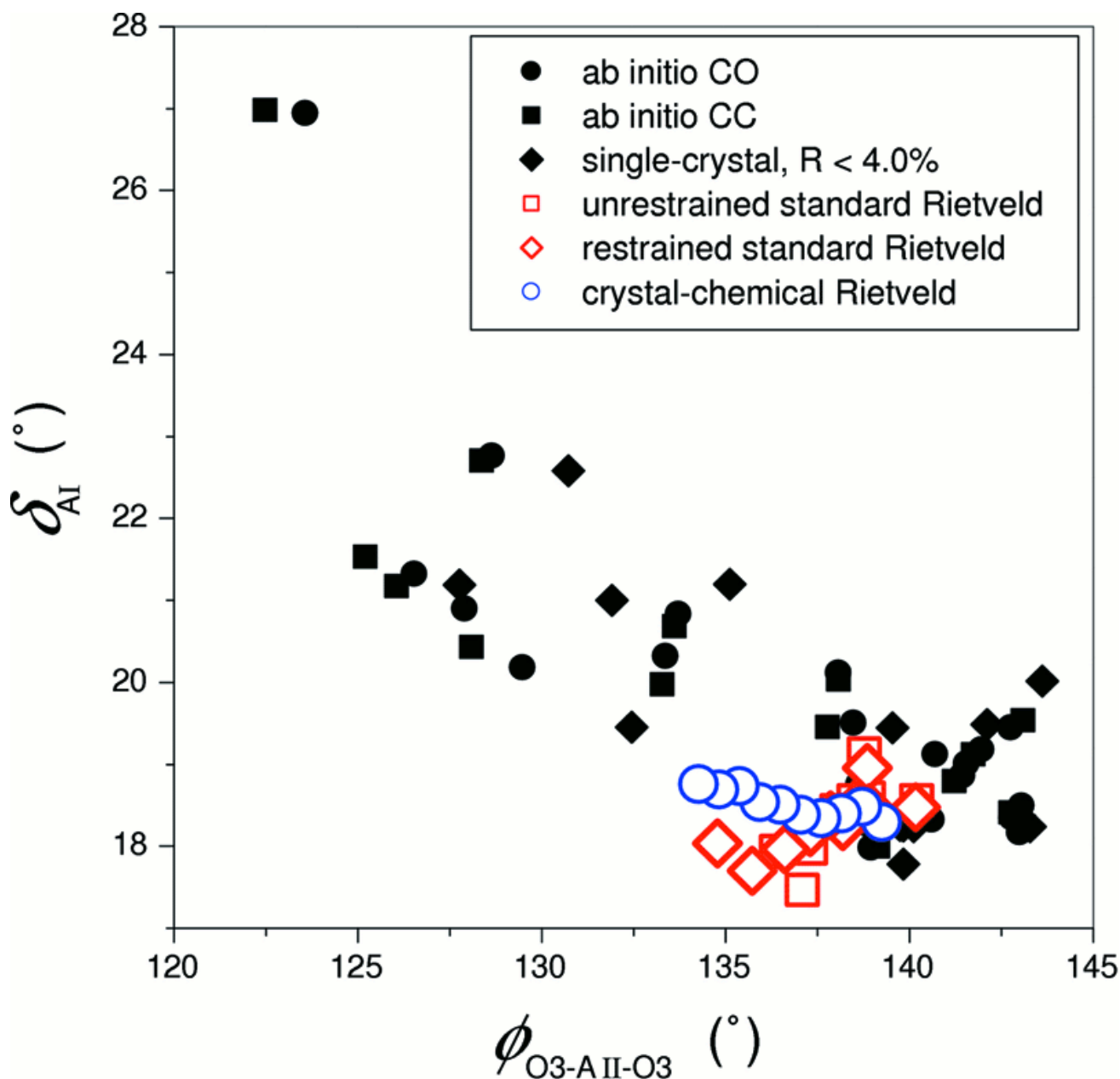
A library describing the precise electron density of all chemical groups present in proteins has been developed. The deformation electron density of atoms is described in terms of multipolar functions. The library is obtained from the crystallographic analysis of several peptide crystals at ultra-high resolution. Library transfer to a crystal structure at atomic resolution results in improved crystallographic indices and electrostatic potential.

B. Zarychta, V. Pichon-Pesme, B. Guillot, C. Lecomte and C. Jelsch

Ab initio constrained crystal-chemical Rietveld refinement of $\text{Ca}_{10}(\text{V}_x\text{P}_{1-x}\text{O}_4)_6\text{F}_2$ apatites

Ab initio constrained crystal-chemical Rietveld refinement of $\text{Ca}_{10}(\text{V}_x\text{P}_{1-x}\text{O}_4)_6\text{F}_2$ apatites

Acta Cryst. (2007). B63, 37–48 [doi:10.1107/S0108768106045538]



Standard (red) and *ab initio* constrained crystal chemical (blue) Rietveld refinement results for $\text{Ca}_{10}(\text{V}_x\text{P}_{1-x}\text{O}_4)_6\text{F}_2$ apatites compared with accurate single-crystal refinements and *ab initio* simulations for known $P6_3/m$ end-member structures (black).

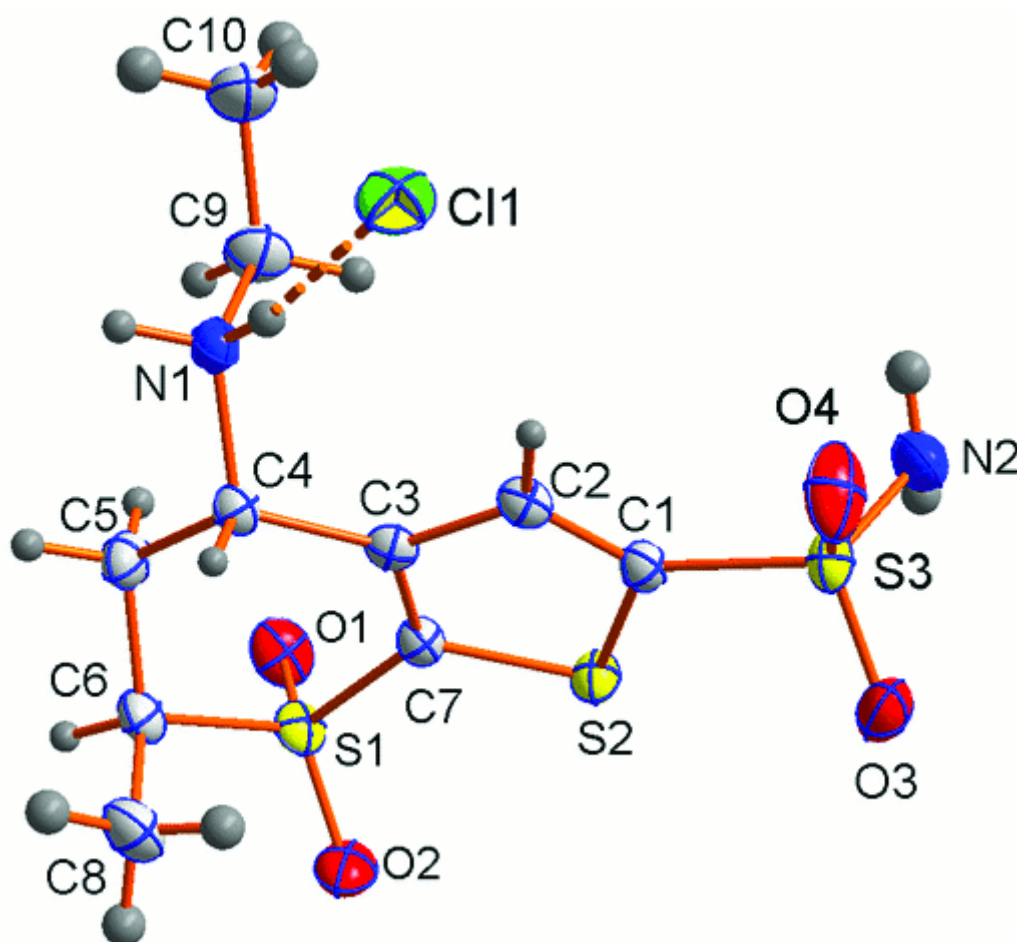
Extraction of reliable distances and angles for $\text{Ca}_{10}(\text{V}_x\text{P}_{1-x}\text{O}_4)_6\text{F}_2$ apatites using standard Rietveld refinement was impaired by large imprecision for O-atom coordinates with X-ray powder data.

Constraining crystal-chemical Rietveld refinements for two oxygen-metal-oxygen angles with results from *ab initio* modeling produced experimental results in agreement with quantum ones and residuals similar to unconstrained standard refinements. *Ab initio* simulations were performed with *VASP* and *Materials Toolkit* (www.tothcanada.com/toolkit). Expansion of BO_4 tetrahedra and rotation of Ca-Ca-Ca triangular units are observed upon replacement of phosphorus by vanadium. The crystal-chemical refinement method provides more accurate bond angles than standard refinement of the same data. Complementarity of quantum methods and problematic least-squares structural analyses of crystal chemistry is discussed.

P.H.J. Mercier, Z. Dong, T. Baikie, Y. Le Page, T.J. White, P.S. Whitfield and L.D. Mitchel

Dorzolamide hydrochloride: an antiglaucoma agent

Acta Cryst. (2007). C63, o108-o110 [doi:10.1107/S0108270106055338]



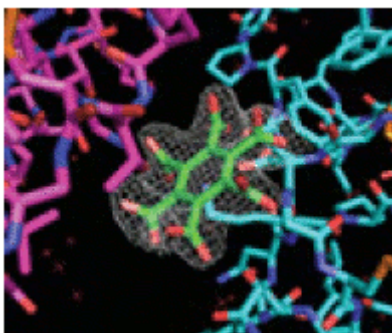
This article describes the crystal structure of the small organic molecule $C_{10}H_{17}N_2O_4S_2^+ \cdot Cl^-$, known as dorzolamide hydrochloride — an antiglaucoma agent. The sulfonamide group plays an anchoring role at the active site through coordination of its nitrogen atom with the zinc atom of HCAII. Given the potential importance of a C3 substituent, the orientation of the ethylamino chain is considered to be significant. Structure–activity distances between the center of the thiophene ring and the two nitrogen atoms (the interaction sites) are N1, 3.625 Å and N2, 3.894 Å and to the methyl carbon occupying the lipophilic groove 4.145 Å. The crystal structure is stabilized by a network of hydrogen bonds largely mediated by the Cl^- anions.

K. Ravikumar and B. Sridhar

IUCR JOURNALS NEWS

A novel strategy for the crystallization of proteins: X-ray diffraction validation

***Acta Cryst.* (2007). D63, 310–318 [doi:10.1107/S0907444906053303]**



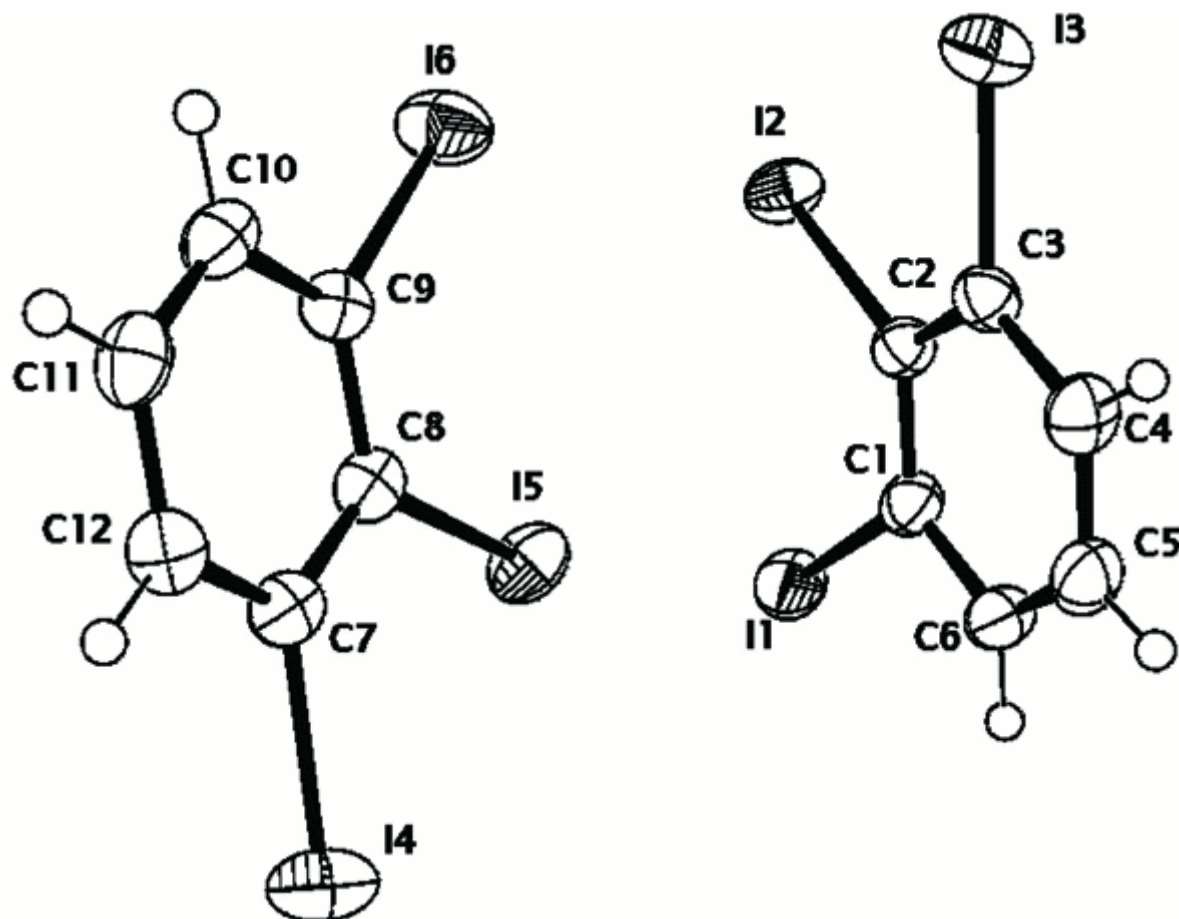
A molecule of mellitic acid serves as the lynchpin of a hydrogen-bonding network between two bovine trypsin molecules in a crystal lattice.

An alternative strategy for the crystallization of macromolecules was recently proposed [McPherson & Cudney (2006). *J. Struct. Biol.* **156**, 387–406] based on the promotion of lattice interactions by conventional, small molecules. This paper presents difference Fourier syntheses of crystals that validate the concept. Proteins, including trypsin, thaumatin, ribonuclease and lysozyme were observed (see figure) interacting in crystals through hydrogen-bonding networks involving such conventional organic molecules as mellitic, trimesic, sulfanilic, oxamic and aminobenzoic acids. The work opens new avenues for biological macromolecule crystallization.

S.B. Larson, J.S. Day, R. Cudney and A. McPherson

1,2,3-Triiodobenzene

Acta Cryst. (2007). E63, o438–o439 [doi:10.1107/S1600536806054535]



Structure of 1,2,3-triiodobenzene, which relieves I–I steric repulsion by splaying.

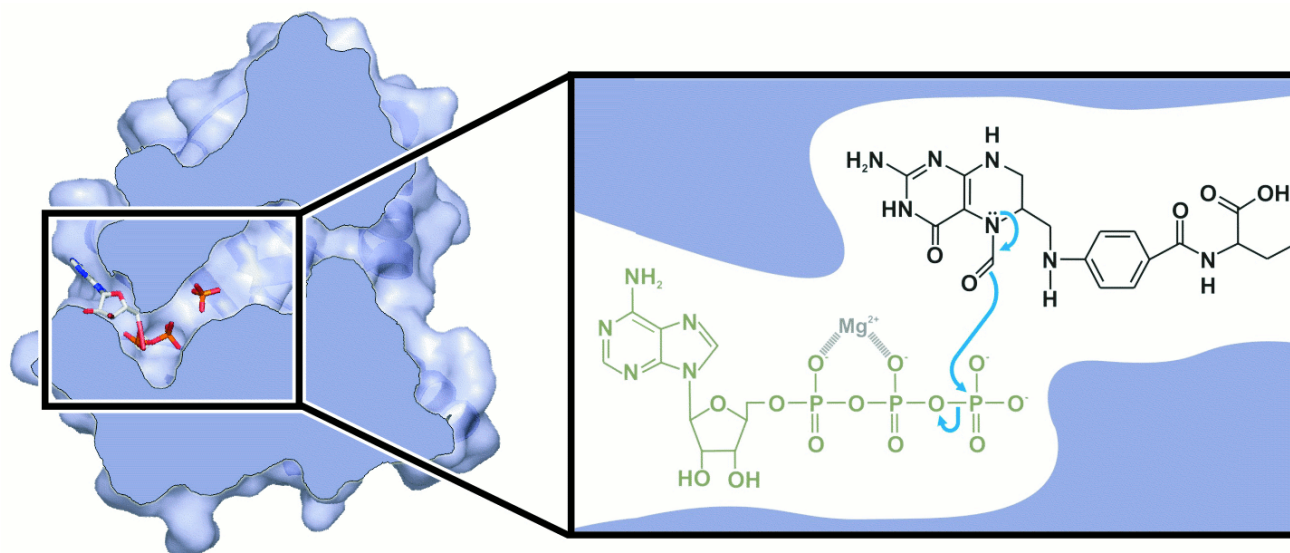
Steric repulsion between bulky substituents is of considerable interest to structural chemists. We reported the crystal and molecular structure of 1,2,3-triiodobenzene, which shows evidence of splaying, i.e. the outer iodines are pushed away from the middle iodine by non-bonding repulsions. This is evidenced by the ICC angles, which increase from 118.8° in 1,3,5-triiodobenzene to 123° in 1,2,3-triiodobenzene. The endocyclic CCC angle (at the carbon carrying the middle iodine) decreases from 121.5 to 118.7° , respectively. Interestingly, the I–I distances ($3.60 \text{ \AA}$) are much smaller than the sum of the van der Waals radii ($4.3 \text{ \AA}$).

I. Novak and D. Li

IUCR JOURNALS NEWS

Structure of 5-formyltetrahydrofolate cyclo-ligase from *Bacillus anthracis* (BA4489)

Acta Cryst. (2007). F63, 168–172 [doi:10.1107/S1744309107007221]



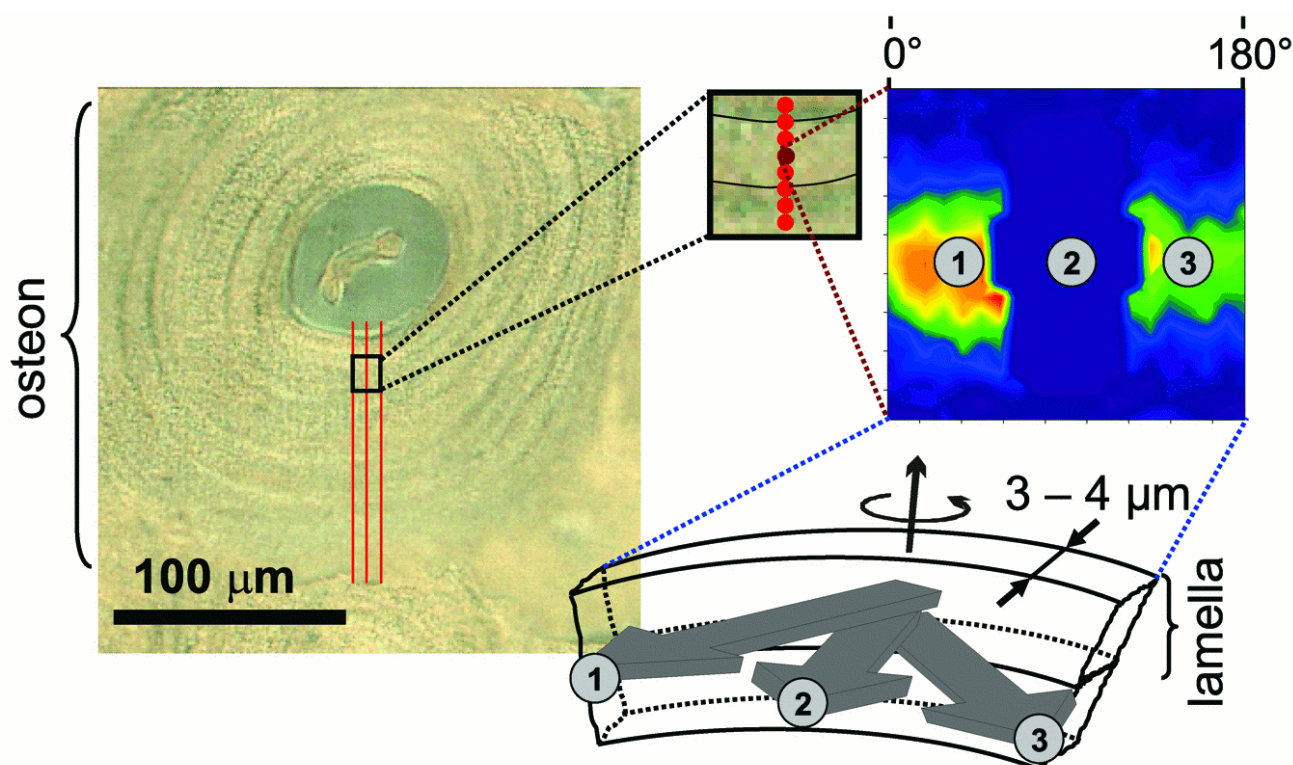
The cyclo-ligase enzyme from *Bacillus anthracis* catalyzes the chemical conversion of 5-formyltetrahydrofolate (vitamin B₉). A cut-through of the structure reveals an internal pocket, where the catalytic process occurs.

Bacillus anthracis, responsible for the life-threatening disease anthrax, has been used as an agent of bioterrorism. To provide information to underpin the discovery of new drugs against anthrax, we have analyzed the structure of a number of *anthracis* proteins as part of the Structural Proteomics in Europe initiative. We report the crystal structure of 5-formyltetrahydrofolate cyclo-ligase, an enzyme involved in regulating bacterial cell growth. The atomic-resolution structure gives a detailed picture of its catalytic mechanism and suggests how inhibitors of the enzyme might be designed.

C. Meier, L.G. Carter, G. Winter, R.J. Owens, D.I. Stuart and R.M. Esnouf

Scanning texture analysis of lamellar bone using microbeam synchrotron X-ray radiation

J. Appl. Cryst. (2007). 40, 115-120 [doi:10.1107/S0021889806044888]



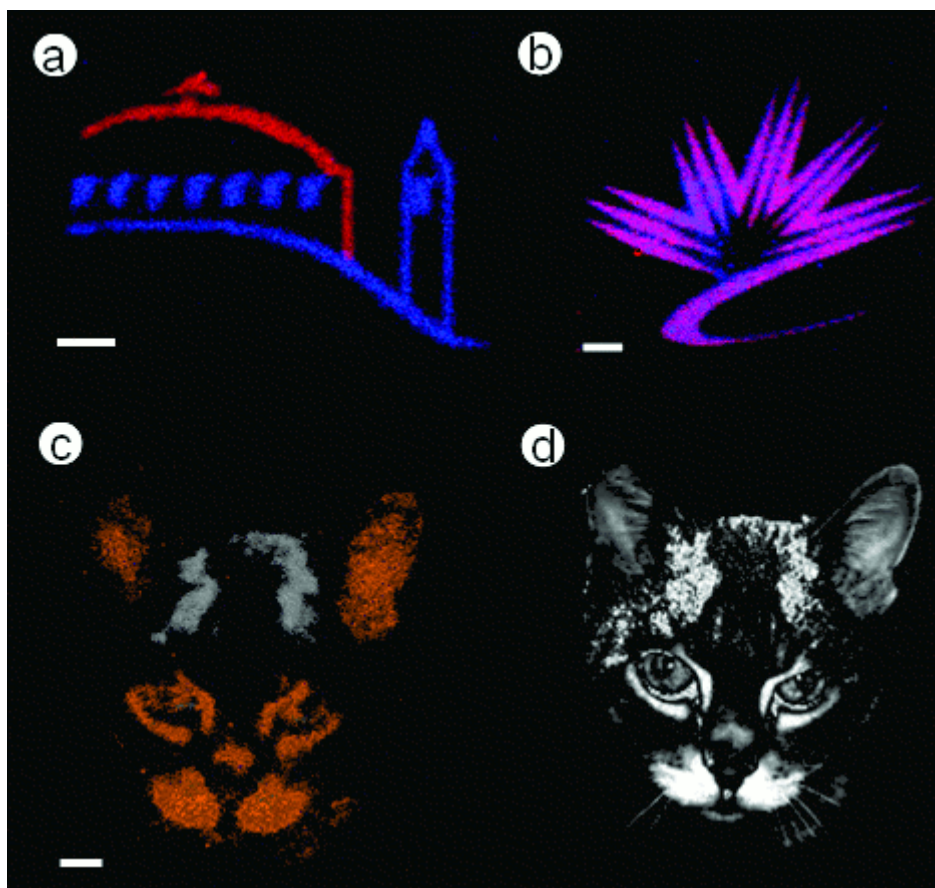
Scanning microbeam texture measurements in bone osteons (left) reveal 3D fiber orientations, with 1 μm resolution, inside single bone lamellae (right).

The fiber texture of compact bone tissue is adapted to its biomechanical function, but the precise architecture at the micron level is controversial. A synchrotron microbeam with 1 μm diameter was used for scanning texture measurements on thin bone sections. The spatial variation of 3D fibril orientation within single bone lamellar units revealed a chiral spiraling architecture of the tissue. The method can be applied to study fiber architectures in a variety of inhomogeneous tissues ranging from arthropod chitin to trabecular bone or artificial composites.

W. Wagermaier, H.S. Gupta, A. Gourrier, O. Paris, P. Roschger, M. Burghammer, C. Riekkel and P. Fratzl

Chemically selective soft X-ray patterning of polymers

J. Synchrotron Rad. (2007). **14**, 181-190 [doi:10.1107/S0909049506053829]



Using monochromated soft X-rays and a two-layer polymer structure, Wang *et al.* have demonstrated chemically selective patterning using the high brightness, fine focused, 50 nm beam of the polymer scanning transmission X-ray microscope (STXM) at the Advanced Light Source. Writing and reading at strong absorption lines was used to make and image patterns independently in polymethylmethacrylate (288.4 eV) and polyacrylonitrile (286.8 eV) layers using STXM. Examples include (a) the logo of Lawrence Berkeley National Lab, (b) the logo of the Canadian Light Source (PMMA = red, PAN = blue) and (c) 'Smokie' (PMMA = brown, PAN = grey); (d) input. Scale bar = 1 micron.

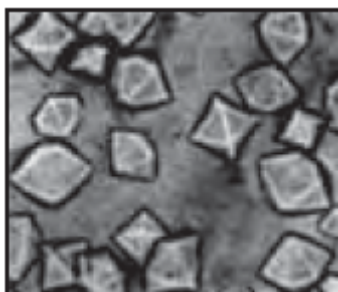
J. Wang, H.D.H. Stöver, A.P. Hitchcock and T. Tyliszczak

SPECIAL REPORT

Crystallography in Poland



The first description of crystalline minerals written in the Polish language was published in 1692 by Wojciech Tylkowski. Polish textbooks of mineralogy containing elements of crystallography were published in the universities of Krakow and Lwow in the second half of the 19th century. Between the World Wars, crystallography operated at the Krakow, Lwow, Poznan, Warsaw and Wilno universities. At the Jagiellonian U. in Krakow in 1933, S. Kreutz, an author of books on theoretical crystallography, supervised the Ph.D. thesis of S. Janik on the X-ray structure of $\text{ZnCl}_2 \cdot 2\text{NH}_3$. At the Lwow U., L. Chrobak studied inorganic crystals by X-ray methods, T. Baranowski grew protein single crystals of muscle myogen and Z. Wayberg, studied crystal symmetry and morphology. Other early crystallographic studies included analysis of metal alloys by powder methods (W. Trzebiatowski, Technical U. of Lwow), iron hydroxides using Debye Scherrer methods (A. Krauze, Poznań U.) and geological samples (A. Rychlewski and E. Passendorfer, Wilno U.). At Warsaw U., S. Pienkowski studied polymers and single crystals by X-ray and electron diffraction and in 1935 A. Laszkiewicz, published a paper on the structure of hexamethyltetramine salicylate. J. Czochralski (Technical U. Warsaw) studied growth and properties of single crystals of metals.



Hexagonal crystals of myogen.

After World War II, the borders of Poland were changed and people from Lwow (Lviv) were transferred to Wroclaw, people from Wilno (Vilnius) were moved to Gdansk and Torun and intellectual refugees from a demolished Warsaw, settled in Lodz. The Polish scientific infrastructure was rebuilt at new academic centers in these cities and young people began to study crystallography. W. Trzebiatowski began the first

X-ray crystallographic laboratory at the Technical U. of Wroclaw, in 1946. In 1953, crystallography was introduced as an obligatory subject in university chemistry curricula producing new crystallographic laboratories, and separating crystallography from mineralogy. In 1958 powder neutron diffraction studies were initiated in Swierk.



Jan Czocharlski

In 1956 W. Trzebiatowski initiated annual “X-ray Crystallographic Meetings” at the Wroclaw Tech. U. which became the “Crystallographic Meetings” of the Polish Academy of Sciences (PAN). In the years 1967-1987, nine international schools on solving crystal structure were organized. Also, conferences on applied crystallography (Z. Bojarski, U. Silesia), solid crystals and liquid crystals (J. Zmija, Military U. of Tech.), defects in crystals (J. Auleytner and M. Lefeld-Sosnowska), and organic Crystal Chemistry (A. Mickiewicz, U. of Poznan). In 1966, Poland became a member of the IUCr and the 11th Int’l Congress of Crystallography was held in Warsaw in 1978 under the leadership of J. Auleytner. European Crystallographic Meetings (ECM) were held in Wroclaw (1986) organized by K. Lukaszewicz, and in Krakow (2001) organized by S. Hodorowicz. In the 1980’s, two young crystallographers in Wroclaw, D. Kucharczyk and S. Malinowski, constructed a single-crystal four-circle kappa diffractometer, known as the KUMA KM-4, which was later equipped with a CCD detector. This successful Polish firm merged with “Oxford Instruments” to become “Oxford Diffraction”.

Organizations of Polish crystallographers include The Committee of Crystallography of PAN (chair, A. Pietraszko), The Polish Society of Crystal Growth (chair, S. Krukowski), The Polish Society of Synchrotron Radiation, (chair, B. Orlowski), The Polish Society of Neutron Scattering, (chair, A. Szytula.), and the Polish Crystallographic Association (PCA), (chair, S. Hodorowicz). Universities and Institutes of PAN are the main centers of crystallographic research in Poland and there are X-ray powder diffraction laboratories in industrial institutions. In this report five areas of crystallographic study in Poland are summarized: I) chemical crystallography, II) physical crystallography, III) applied crystallography, IV) crystal growth and liquid crystals and V) protein crystallography. An additional section (VI), written by Z. Dauter (editor of *Acta Cryst.* Section D) discusses Polish crystallographers working outside of Poland.

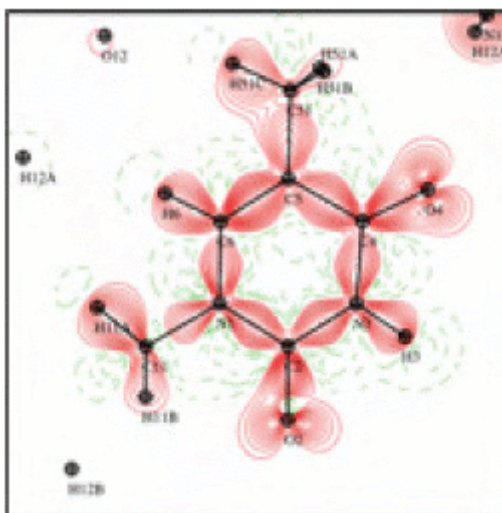
Chemical crystallography

The largest groups investigating chemical crystal structures are at the Universities of Krakow, Lodz, Poznan, Warsaw and Wroclaw and the Institutes of the PAN in Warsaw and Wroclaw. Crystallographic research is also pursued in laboratories in Gdansk, Katowice, Lodz, Lublin, Opole, Torun, Czestochowa and Siedlce.

The Crystal Chemistry and Crystal Physics Dept., Jagiellonian U., Krakow (K. Stadnicka, stadnick@chemia.uj.edu.pl.) was founded in 1963 by J. Chojnacki, who studied fibrous isopolymolybdates and published the structure of cadmium oxycyanomolybdate(IV)dihydrazine tetrahydrate, in 1969. His followers lead five independent research groups. B. Oleksyn concentrates on biologically important

compounds including antimalarials, flavonoids and sweeteners, potential drugs containing Se and Te, and inhibitors of urokinase-type plasminogen activators and HIV-1 integrase. K. Stadnicka's research interests include molybdate complexes, anti-hypertensive hydrazinephthalazines, anti-arrhythmic hydantoin derivatives, optical properties of crystals, structures of molecular magnets, engineering of crystalline phases with NLO properties, and experimental electron density distribution in crystals. S. Hodorowicz's interests include isopolymolybdates, high-temperature superconductors, the history of crystallography, the kinetics of crystallization, and phase transitions in crystalline state. W. Lasocha pursues powder diffraction analysis with *ab initio* and Rietveld refinement procedures. K. Lewinski's protein studies are described in section V. Together with the staff of the Dept., S. Hodorowicz organized ECM 20 in Krakow in 2001 and promoted the Jagiellonian U. *doctors honoris causa* degree to Isabella and Jerome Karle in 2002. S. Hodorowicz was recently elected president of PCA.

In 1954 Z. Galdecki determined the crystal structure of KAs₄O₆, the first structure determination at the **Crystallography Lab., Lodz U. of Technology** (M. Glowka, mareklo@p.lodz.pl). Galdecki headed the Crystallography and Crystal Chemistry Group for almost 50 years. At present the 20 member staff of professors, senior scientists, PhD students, and technicians use crystallography to explore structure - activity relationships, drug-receptor interactions, crystal engineering, weak interactions in molecular crystals, stereospecific reaction mechanisms, polymorphism, electron density and solid catalysts. Current targets for analysis include anticonvulsants and adenosine receptor ligands (J. Karolak-Wojciechowska), antibacterial quinolones (M. Glowka), herbicides and structurally constrained endomorphine analogs (R. Kruszynski), Cu(II) complexes (L. Sieron), stereoelectronic control of molecular conformation and crystal packing (W. Wolf), nitroaryl complexes of Re (T. Bartczak), and charge density studies of biological phosphates (W. Maniukiewicz). In 1990 Lodz U. of Technology became the National Affiliated Center of the Cambridge Crystallographic Data Center in Poland. The Crystallography Group has wide international collaborations, and awarded the degrees of *doctors honoris causa* to H. Hauptman and W. Duax.



Charge density in (1 - thyminyl) acetamide (by M. Kubicki)

After post-doctoral study with A. I. Kitaigorodskii, in the sixties, Z. Kaluski, Z. Kosturkiewicz and T. Borowiak began X-ray structural investigations in Poznan of ferrocen, and hydrogen bonding in crystals, heterocyclic compounds and natural products. Presently, five groups in the **Dept. of Crystallography, A. Mickiewicz, U. Poznan** (M. Gdaniec, magdan@amu.edu.pl) are active in organic crystal chemistry and one group pursues protein crystallography. T. Borowiak and M. Kubicki analyze charge density distribution, phase transitions, metallo-organic compounds, supramolecular structures, heterocyclic, macrocyclic complexes and the hierarchy of intermolecular interactions (weak and strong hydrogen bonds, halogen bonds, dipole-dipole interactions, π - π stacking, etc). The main topics of interest to M. Gdaniec (a co-editor of *Acta Cryst.* Section E) include crystalline inclusion compounds, achiral compounds, and supramolecular synthesis of organic and metallo-organic materials with predictable

architecture. The research group of A. Katrusiak studies materials science, thermodynamics and phase transitions, temperature- and pressure-controlled crystallization, pharmaceutical polymorphs, meteorites, environmental pollution, equipment design, diffractometry and new methods of data-analysis and visualization. Z. Kosturkiewicz investigates intra- and intermolecular hydrogen bonds in crystals of organic compounds and problems of polymorphism. U. Rychlewska (co-editor of the *Acta Cryst.* Section B) and her group are engaged in studies of inclusion properties of supramolecular aggregates with chiral building blocks, multidentate ligands, crystal engineering and the role of weak interactions in the stabilization of crystal structures. Although the main focus of M. Jaskolski (a member of EMBO and editor of the *Journal of Molecular Biology*) is the structures of proteins (described in section V) he also investigates hydrogen bonds and weak interactions in small molecule systems. The researchers in the crystallography dept have also organized eleven international symposia on organic crystal chemistry. In the 1970's powder diffraction studies of zeolites were initiated in the **Crystallography Dept., M. Curie-Skłodowska, U. Lublin** (M. Koziol, akoziol@hermes.umcs.lublin.pl) under the leadership of T. Penkala. Since 1976 the A. Koziol group has pursued single crystal studies and polymorphism of biologically active compounds and the S. Pikus group has used powder diffraction and SAXS methods to analyze amorphous and microporous materials.



The staff of the Crystallography Laboratory at Warsaw U.

Crystallography Lab., Warsaw U. (K. Wozniak, kwozniak@chem.uw.edu.pl). A. Laszkiewicz, led the crystallographic group after WWII. Next, L. Chrobak, developed powder methods to investigate minerals, and synthetic crystals (1951-1970) and A. Wiewiora applied powder methods to study phase transitions. (1970-1977). Since 1977 the crystallographic unit has focused on analysis and molecular models of aromaticity, hydrogen bonding, weak interactions and long distance effects in organic crystalline compounds under the leadership of T. M. Krygowski. Today one of his former students K. Wozniak combines X-ray and neutron diffraction and NMR charge density studies to explain weak interactions in supramolecular organic, inorganic and hybrid systems.



Tadeusz Glowiak

T. Glowiak initiated crystallographic research in the **Chemical Crystallography Dept., Wroclaw U.** (T. Lis, tlis@wch.uwr.chem.uni.wroc.pl) in 1959 with studies of oxocomplexes of metals. Amino acid cation complexes were studied by photographic methods in the 1970's and, since 1973, with the first automatic four-circle diffractometer in Poland. The first molecular magnet ($\text{Mn}_{12}\text{O}_{12}$) was synthesized and described in this laboratory. Current fields of interest include the role of weak, directional interactions in molecular recognition, low temperature resolution of racemates, and studies of biochemical intermediates, organic sulphates and phosphonate esters. More than 1000 new compounds have been structurally characterized and described in over 700 research papers.

In the **Dept. of Physical Chemistry and Crystallography, Jan Dlugosz, U. Czestochowa** (M. Wieczorek, wandaB@autograf.pl) that was founded in 1990 by B. Marciniak, three professors (M. Krzesinska, M. Wieczorek and W. Pawliuk), study the growth, structure, morphology, perfection and properties of crystals formed by organic and intermetallic compounds.

In the 1970s' Z. Dauter, A. Hempel and A. Konitz investigated crystal structures of biologically active compounds in the **Crystallography Lab., Dept. of Chemistry, U. of Technology, Gdansk** (J. Chojnacki, jarekch@chem.pg.gda.pl). In 1995 W. Wojnowski established a laboratory for X-ray single crystal structure studies of inorganic and metallorganic compounds. Currently, X-ray crystal structures of metal complexes with ligands including low valent PP compounds and silicon-sulfur compounds are determined by J. Chojnacki and K. Baranowska and A. Konitz continues structure investigations of organic and metallorganic compounds.

In 1954, the Dept. of Solid State Chemistry was organized by W. Trzebiatowski at the **Inst. of Theoretical and Physical Chemistry, Wroclaw U. Technology** (I. Turowska-Tyrk, ilona.turowska-tyrk@pwr.wroc.pl) and a single crystal study of BaO_4TiO_2 was completed by K. Lukaszewicz. Presently, T. Luty with his research group studies the dynamics of crystal lattices. I. Turowska-Tyrk studies structural changes in organic crystals during photochemical reactions and phase transitions and V. Videnova-Adrabska (Dept. of Inorg. and Struc. Chem.) investigates inclusion compounds of molecular recognition, and organic crystal engineering.

The **Lab. of X-ray Structural Analysis, Inst. of Physical Chemistry (PAN), Warsaw** (J. Lipkowski, klatrat@ichf.edu.pl) was founded by W. Wolfram in 1964 and has been led by J. Lipkowski since 1978. Research is focused on the study of heteromolecular complexes in which one of the components (the host) binds a variety of molecular species (the guests) in a selective and reversible manner. The ultimate goals of the research are the design of systems that selectively separate mixtures, activate chemical reactions, self assemble and transport specific molecules. Host systems with internal cavities of molecular dimensions (organic, zeolites, cyclodextrins, and calixarenes) involving H-bonds and other non-covalent bonding are under analysis. The physicochemistry and phase transitions structure dynamics of supramolecular complexes are studied over a temperature range of 80 to 400 K. The Laboratory head, J. Lipkowski, is presently the Vice President of the PAN and a member of Editorial Advisory Board of *Central European J. of Chem.* K. Suwinska manages the distribution of the *IUCr Newsletter* in Poland.

In 1969, after post-doctoral study with J.D. Dunitz, T. Krajewski produced the first Polish integrated computer system for structure solution and refinement in the **Crystallography Lab., Inst. of Organic Chemistry, PAN, Warsaw** (Z. Urbanczyk-Lipkowska, ocryst@icho.edu.pl). The research team (P. Gluzinski, J. Krajewski, Z. Urbanczyk-Lipkowska) was engaged in conformational studies of mono- and disaccharides, structure - activity relationships of small biomolecules and application of molecular recognition in chemistry.

Chemical crystallography has also been studied in other Polish universities. In the early years

crystallographic research in this area centered on organic compounds including acridine derivatives (**Lab. of Crystallography, U. of Gdansk**, A. Sikorski, art@chem. u.gda.pl), metal complexes and small organic molecules (**Dept. of Crystallography, Copernicus U., Torun**, A. Wojtczak, awojt.@chem.uni.torun.pl), crystal structures and quantum chemistry studies of organic compounds (**U. of Lodz**, S. Grabowski, slagra@uni.lodz.pl). since 1987, organometallic compounds and neutron spectroscopic studies of hydrogen bonds in amino acids (**Inst. of Nuclear Chemistry and Technology, Warsaw**, J. Leciejewicz, jlec@orange.ichtj.waw.pl).

Since 1997 projects have focused on organic crystals, high-pressure studies, phase transitions, electron charge density, chemical reactivity, ferroelectrical, piezoelectrical and ferroelastic materials (**U. of Opole**, J. Zaleski, zaleski@uni.opole.pl), magnetic properties of metal alloys (**U. of Silesia, Katowice**, I. Okonska, okonska@uranos.cto.us.edu.pl), organic compounds with pharmaceutical activity including Cinchona alkaloids, and glucocorticosteroids, and polymorphism of new liquid crystal materials including cholesterol-containing dimers in collaboration with Wageningen U. in Holland (**U. of Podlasie, Siedlce**, Z. Karczmarzyk, kar@ap.siedlce.pl.).

Physical crystallography and crystal defects



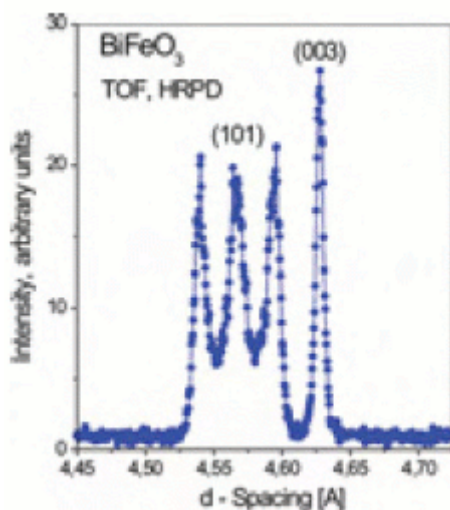
The staff of the Dept. of Structural Research, Warsaw U.

The main centers of physical crystallography in Poland are at the Universities in Warsaw, Krakow and Katowice as well as the Institutes of the PAN in Warsaw and Wroclaw. X-ray research was initiated in the 1920's in the **Dept. of Structural Research, Warsaw U.** (M. Lefeld-Sosnowska, maria.lefeldsosnowska@fuw.edu.pl) by S. Pienkowski. In the 1960s, X-ray diffraction topography was developed by J Auleytner and next by M. Lefeld-Sosnowska to study defects in single crystals. Since the 1990s high-resolution X-ray diffractometry has been used to study diffuse scattering from point defects in gallium arsenide (GaAs) crystals, semi-insulating low-temperature GaAs containing defects, low temperature GaAs doped with beryllium and mismatched layers of nitrides grown on sapphire. Recently, synchrotron topography has been used to analyze defects in gadolinium-calcium oxyborates and, to detect, for the first time, dislocations in nonlinear optical crystals used to generate second and higher harmonics of light, using neutron diffraction and inelastic scattering. Investigations of semimagnetic semiconductors ($\text{Cd}_{1-x}\text{Mn}_x\text{Te}$) have revealed antiferromagnetic ordering of manganese spins. In an EuS and superlattice strong antiferromagnetic coupling of the EuS layers across the nonmagnetic PbS layers was revealed, whereas much weaker coupling was observed across the YbSe layers in a EuS/YbSe superlattice. Reflectometric measurements using polarized neutrons proved that magnetic ordering detected in GaMnAs had a long-range character. The exchange interactions between pairs of Mn-Mn atoms in diluted magnetic semiconductors have been studied using neutron inelastic scattering.



Bronislaw Buras

Structure and lattice dynamics studies of condensed matter by neutron scattering and Mossbauer spectroscopy are the main activities of the **Div. of Structural and Lattice Dynamics, Warsaw U.** (I. Sosnowska, izabela@fuw.edu.pl) The Time-of-Flight (TOF) neutron diffraction technique was developed by B. Buras in the 1960s. The pulsed neutron source in Dubna (USSR) was used for the first time for crystal structure determination and phonon dispersion determinations by Sosnowska. Due to the extremely high resolution of the TOF method, a long period magnetic cycloid (620 Å) was detectable in BiFeO_3 . Since the 1970's members of the division staff have studied the anisotropy of hydrogen diffusion in crystals (R. Kutner, I. Sosnowska, K. Kehr), hydrogen behavior in ferroelectrics, the mobility of water in opal (with a Research Center in Julich), magnetic moments in spin glass systems (with ETH, Zurich), neutron diffraction studies of phase transition in polycrystalline materials, and inelastic neutron scattering studies of rare earth metals in hard magnetic materials (with M. Loewen, Julich). Recently it was found (with Bonn U.) that the modulation of the cycloid in BiFeO_3 changed drastically when iron ions are replaced by manganese ions. High resolution synchrotron radiation studies have shown phase separation and charge modulation in $\text{CaMn}_7\text{O}_{12}$. Neutron diffraction studies have shown that the Yoshimori model cannot be used to describe long range magnetic ordering of Mn^{4+} ions in $\beta\text{-MnO}_2$ (M. Regulski) and that nanocrystalline Cr has spin density-wave modulated magnetic ordering characteristic of Cr single crystals. Small angle neutron scattering studies of the microstructures of electrodeposited nano-Ni, Co and Cr revealed a fractal-like density autocorrelation function (R. Przenioslo with R. Hempelmann, Saarbrücken, and A. Hewat, Grenoble).



Magnetic satellites in BiFeO_3

Research in the **Dept. of Phase Transition Kinetics, Jagiellonian U.** (R. Kozubski, rafal.kozubski@uj.edu.pl) concerns Monte-Carlo and molecular dynamics simulations of structural transformations in intermetallics, elementary atomic-migration processes, and structural relaxation in superalloys. Recent discoveries include detection of different ordering and diffusion mechanisms in FePt intermetallics, self diffusion of iron in ordered FePt films and stability of superstructure variants in FePt nanolayers. The research is performed in cooperation with scientists from U. of Wien, the CNRS Inst. in Strasbourg, the Inst. of Theor. and Gen. Phys. in Stuttgart, and Network of Excellence of E. U.



M. Shiojiri and his wife visiting I. Sosnowska's Laboratory.

In the **Solid State Physics Dept., Jagiellonian U. Krakow** (A. Szytula, szytula@if.uj.edu.pl) crystal and magnetic structures of binary intermetallic rare earth compounds with varying stoichiometries are investigated by powder and neutron diffraction methods. Neutron diffraction data are used to analyze and correlate atomic and molecular structure with classical magnetic measurements. The majority of these compounds show a change in the magnetic structure from the collinear form commensurate with the crystal structure at low temperature to a modulated incommensurate form near the Neel temperature. The structures of over 200 intermetallic compounds have been determined and published in *The Handbook of Crystal Structures and Magnetic Properties of Rare Earth Intermetallics*, (1994), and *Crystal Structures and Magnetic Properties of RTX Rare Earth Intermetallics*, (1998) by A. Szytula and J. Leciejewicz. Neutron diffraction experiments are carried out in collaboration with the Berlin Neutron Scattering Center, the Hahn-Meitner Inst., Germany, and the Paul Scherrer Institute, Villingen, Switzerland.

In 1963, A. Oles began neutron diffraction investigations of crystal and magnetic structures, and phase transitions in crystals at the **Stanislaw Staszic U. of Science and Technology, Krakow** (J. Wolny, wolny@novell.ftj.agh.edu.pl).

A neutron diffractometer was constructed and mounted at the reactor in Swierk. The method of texture determination by neutron diffraction was worked out, and in 1976 A. Oles published the book *Magnetic Structures Determined by Neutron Diffraction*. Recent research areas include: solid state electronic structures (St. Kasprzyk), group theory analysis of crystal symmetry (W. Sikora), aperiodic systems (J. Wolny), and investigations of the mechanisms of plastic deformation (K. Wierzbowski).

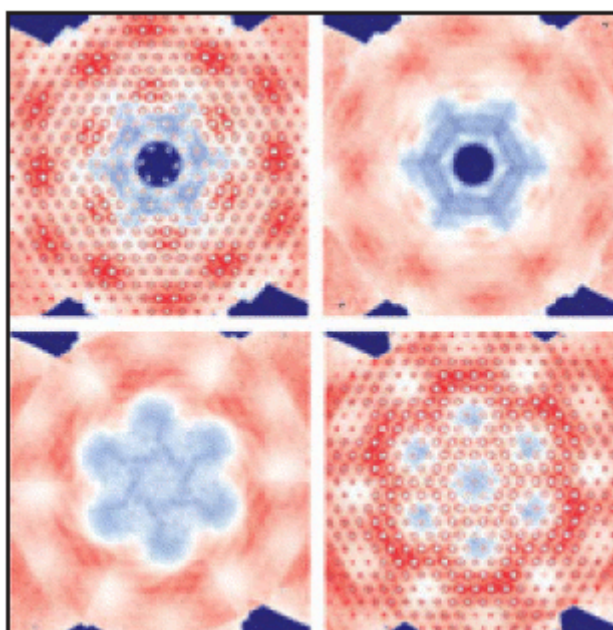
Research in the **Dept. of Crystal Physics, U. of Silesia, Katowice** (J. Warczewski, warcz@us.edu.pl) concerns crystalline and magnetic periodic and aperiodic structures, modulated and electronic structures, quasicrystals, and the magnetic properties, transport phenomena, mathematical analysis and theory of the condensed phase including chromium containing magnetic crystals having commensurate and incommensurate modulation.

Since 1968, magnetic, electric and transport properties of ionic perovskite, spinel crystals, metals and alloys have been investigated at low and high temperatures in the **Dept. of Solid State Physics, U. of Silesia, Katowice** (A. Ratuszna, ratuszna@us.edu.pl).



Staff of the Central Lab. of X-ray and Electron Microscopy of the Inst. of Physics, PAN, Warsaw.

The **Central Lab. of X-ray and Electron Microscopy of the Inst. of Physics, PAN, Warsaw** (K. Ludwiczak-Jablonska, jablo@ifpan.edu.pl) led by J. Auleytner since 1967 focuses on interdisciplinary characterization of matter using microanalysis spectroscopy, X-ray optics, applied crystallography and electron microscopy. Studies include investigations of the mechanisms of the solid surface damage induced by ultra short VUV pulses from free electron lasers and simulations of the propagation of strong EM pulsed beams within the XUV and SXR wavelength. Chemical bonds, ionic strength, phase and dipole analysis are studied with X-ray absorption and emission spectroscopy, using conventional and synchrotron radiation. The shape of the spectra is a fingerprint of the chemical compound, useful for solving a variety of scientific problems including determination of the composition of disordered composites. Electron microscopists are engaged in the characterization of semiconductors, metal oxides, superconductors and fullerene nano-objects. Computational analysis, simulation of diffraction patterns and transmission electron microscopy images are used to determine the structure of new materials. EXAFS oscillations provide information on short-range order in low-dimensional structures and dopants in semiconductors.



X-ray diffuse scattering in $(\text{CH}_3)_4\text{NCdCl}_3$ a: hk0, b: hk 0.5, c: hk 1.5, d: hk 2 reciprocal layer. (A. Pietraszko)

Crystallographic studies initiated at the **Dept. of Crystallography, Inst. of Low Temperature and Structural Research, PAN, Wroclaw** (A. Pietraszko, APietraszko@int.pan.wroc.pl) by W. Trzebiatowski

in 1966 and expanded by K. Lukaszewicz and A. Pietraszko currently focus on temperature and pressure dependent phase transitions in ferroelectric, ferroelastic and magnetic crystals, superconductors, superionic conductors, intermetallic and organometallic compounds. Modulated phases of a number of crystals have been determined using computer programs developed by K. Lukaszewicz, A. Pietraszko and W. Paciorek. Precise measurement of lattice parameters of single crystals in a broad range of temperatures are obtained using the Bond-type diffractometers constructed for this purpose. X-ray diffuse scattering is studied using 2-dimensional detectors. Other studies in the department include electron crystallography of mono- and multi-component oxides (M. Wolcyrz) and analysis of lattice defects, impurities and dielectric relaxation in silica glasses after ionic exchange processes (M. Suszynska). The Department collaborates with institutes in Stockholm, Copenhagen, Darmstadt, Padova, Bello Horizonte, Lviv, Luts'k, Vilnius and Moscow. Two crystallographers from the Department, (D. Kucharczyk and M. Malinowski), designed and produced an automatic four-circle X-ray diffractometer KM-4. Now, the Oxford Diffraction Company, through a joint venture of KUMA Diffraction and Oxford Instruments produces Xcalibur and Gemini systems in its production facility located in Wroclaw. The Inst. of Low Temperature and Structural Research houses the Committee of Crystallography, PAN, chaired successively by W. Trzebiatowski, K. Lukaszewicz and A. Pietraszko. The Committee, which represents Poland in the IUCr, organizes the annual Polish Crystallographic Meetings (48th in 2006).



Participants of the conference in Bialowieza in 2000.

In 1958, a group of scientists and engineers at the **Inst. of Nuclear Research, Swierk** (J. Leciejewicz) headed by B. Buras constructed a neutron spectrometer, at the EWA reactor and large single monochromators of copper, zinc, lead and aluminium were grown by A. Modrzejewski. Early studies included powder neutron diffraction of lead oxides and tungsten carbides (J. Leciejewicz) and magnetic studies of intermetallic uranium compounds (A. Murasik and J. Leciejewicz). Some neutron diffractometers built in Swierk from 1960 to 1970 under the supervision of K. Blinowski, were sold abroad. In 1963 B. Buras adopted time-of-flight techniques for neutron powder diffraction and experiments using a Fermi chopper and silicon powder samples were performed with J. Leciejewicz. In 1983 The Inst. of Nuclear Research was subdivided into three Institutes. Activities at the Inst. of Nuclear Chemistry are described, in section I and the others are described below.

The main topics of study at X-ray Lab. of the **Inst. of Atomic Energy, Swierk** (K. Wieteska, k.wieteska@cyf.gov.pl), a successor of the Inst. of Nuclear Research, are crystal lattice defects using X-ray topography, phase transitions in ceramics using powder diffraction, phase transitions in polycrystalline materials using electron microscopy and organic X-ray crystal structures. Magnetic and spectroscopic properties of crystals and electronic charge density in crystals are studied in the **Inst. of Experimental Physics, U. of Bialystok**, (L. Dobrzynski, ludwik@ipj.gov.pl). International conferences on polarized neutron scattering, high resolution Compton scattering as a probe of Fermiology and charge, spin and momentum density were organized by L. Dobrzynski.

Lattice defects in the single crystals applied in optoelectronics are investigated by J. Pajaczkowska and colleagues at the Inst. of **Technology of Electronic Material** (J. Pajaczkowska, pajacz.a.@itme.edu.pl).

Applied crystallography



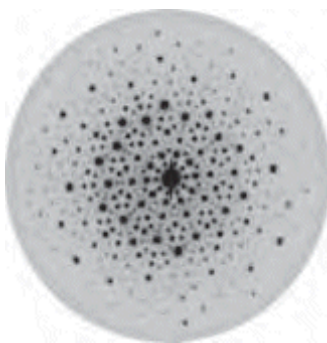
Participants of the 18th Conference on Applied Crystallography

Since 1974 the **Inst. of Material Science, U. of Silesia, Katowice** (E. Lagiewka, lagiewka@us.edu.pl) has been led by Z. Bojarski. X-ray and electron diffraction, topography, small angle scattering and spectroscopic methods are used to study metallic, ceramic and polymeric materials and alloys having crystalline, amorphous, nanocrystalline and quasicrystalline structures. Targets of study include phase transitions, mosaicity, textures, chemisorption, whiskers growth and electrochemical processes. Techniques applied include the Bond method for lattice parameter analysis, Rietveld and *ab initio* methods of refinement and structure solution and Auger spectroscopy for the investigation of alloy surfaces. Instruments have been designed and constructed at the Inst. and crystallographic textbooks have been edited by Z. Bojarski and co-authors. Research groups are headed by Z. Bojarski, J. Barcik, J. Frackowiak, H. Morawiec, L. Pajak, J. Rasek, M. Surowiec, K. Wokulska and Z. Wokulski. The 20th Conference of Applied Crystallography and a School on *ab initio* methods of analysis of polycrystalline materials was held in September 2006.



Whiskers of TiN. (K. Wokulska)

At the **St. Staszic Inst. of Iron Metalurgy, Gliwice** (T. Bold, tbold@imz.gliwice.pl) studies of the structures of minerals and phase transitions of steel products began in 1957 using instruments constructed in the institute. The textures of thin sheets of iron and phase transitions in the range -180°C to $+1200^{\circ}\text{C}$ were investigated. The techniques of replication in electron microscopy and X-ray microanalysis were perfected and inter-laboratory tests of quantitative phase analysis were organized.



Electron diffraction of decagonal quasicrystal (by W. Bogdanowicz)

At the **Inst. of Textile Engineering and Polymer Materials, U. of Bielsko - Biala** (A. Wlochowicz, awlochowicz@aath.bielsko.pl), A. Wlochowicz and colleagues investigate the degree of crystallinity of

polymers and fibrousness of materials using small-angle scattering methods. Nanostructures, thermal properties of homogenous copolymers and phase transitions in fibrous materials are also studied by using synchrotron radiation. The Sixth International Conference on X-ray Investigation of Polymer Structures organized by the Bielsko-Biala U. and the Catholic U. of Leuven (Belgium) was held in 2004. At the **Inst. of Technology and Chemical Engineering, Poznan** (J. Garbarczyk, jozef.garbarczyk@fct.put.poznan.pl), J. Garbarczyk and coworkers determine X-ray crystal structures of organic crystals and are currently analyzing conditions of crystallization and polymorphism of isotactic polypropylene.

At the **Dept. of Macromolecular Physics, Adam Mickiewicz U., Poznan** (M. Kozak, mkozak@amu.edu.pl), M. Kozak investigates structures of fibrous materials using the small-angle X-ray scattering and is currently studying the effect of cationic surfactants on the structure of phospholipidic systems.

The staff of the **Lab. of X-ray Powder Diffraction and Spectrometry, Inst. of Physical Chemistry, PAN, Warsaw** (Z. Kaszukur, zbig.ichf.edu.pl) is engaged in phase determination and Rietveld refinement of high resolution powder diffraction data as well as dynamical and kinetic powder diffraction studies at variable temperature (up to 600°C) and pressure. Quasi-amorphous materials are analyzed using X-ray powder diffraction and radial distribution function methods. Numerical methods for studying highly dispersed solids (transition metals) deposited on supports (SiO_2 , Al_2O_3) are developed including reliable background estimation data, smoothing procedures, and quantitative analysis for *in situ* studies. Recently, analytic tools allowing an insight into the structure and dynamics of nanocrystalline metallic particles in a chemical reaction have been developed. Violations of Bragg's law and subtle changes in the peak intensity and width can be traced to nanocrystalline variations during chemical reactions. A similar approach has been used successfully for the analysis of concentration profiles for bimetallic nanoalloys modified by chemisorption of gasses.

In the **Dept. of Powder Diffraction, Inst. of Low Temperature and Structure Research, PAN, Wroclaw** (R. Kubiak, kubiak@int.pan.wroc.pl) phthalocyaninato complexes with rare earth metals and their salts are synthesized and investigated by X-ray and electron diffraction methods. The synthesis of new cyanic derivatives including new sandwich-type metallodipthalocyaninato complexes, investigation of their transformations and crystal structure determination are the specialty of the research group.

A semiconductor strip detector with a significantly increased rate of acquisition of powder diffraction data was constructed in **Dept. of Physics and Applied Informatics, St. Staszic U. of Science and Technology, Krakow** (A. Zieba) by a group led by A. Dabrowski. The detector was commercialized by Bruker – AXS under the name Lynx Eye.

X-ray powder methods are used by A. Mazurek and coworkers at the **Central Forensic Lab. of Polish Police, Warsaw** (A. Mazurek, mazurek-al@wp.pl) for the identification of drugs, explosives, and unknown substances. The most effort is focused on analysis of trace samples found in clandestine amphetamine laboratories and amphetamine samples from the illegal drug market.

Powder X-ray diffraction methods are also used in the investigation of inorganic and organic materials in five other laboratories in Poland (Inst. of Material Engineering, Poznan U. of Technology; Dept. of Engineering & Polymer Technology, Wroclaw U.; Inst. of Material Engineering, Technical U. of Czestochowa; Dept. of Magnetochemistry, Fac. of Chemistry, A. Mickiewicz U.; Inst. of Electronics, Wroclaw; Condensed Phase Physics Group, AGH U. of Science & Technology).

Crystal growth and liquid crystals



Single crystals grown in the MUT Lab

The main center of crystal growth and research on liquid crystals in Poland is at the **Div. of Physics and Crystal Growth, Military U. of Technology, Warsaw** (J. Zmija, jzmija@wat.edu.pl). In 1958, J. Zmija began investigating the growth of intermetallic compounds, metallic single crystals, and diffusion effects in crystals. In 1965 studies were begun on new materials for lasers and microwave acoustics. The self-diffusion of dopants in crystals of semiconducting compounds (ie AlIIB^{V} , AlIB^{VI}) were studied using radioisotopic methods and small-angle scattering. Structures of single crystals doped with Al, Cd, Se, In, and Mn were investigated and a theory of diffraction from polytype crystals was developed. Studies of epitaxy on GaAs led to the production of a semiconductor laser. In 1974, under the direction of J. Zmija chemists, physicists and materials engineers began work on liquid crystals. They created new mixtures and phases for displays and other electro and thermo-optical elements including smectic- and thermo-ferroelectrics. New methods for liquid crystal study were developed. Research using single crystal technology of boron, bismuth, lead and other oxide materials was begun. Due to their acoustic properties single crystals of BGeO and BeSO₄ were used in construction of transducers of surface waves and a filter model for medium frequencies of color television were designed. The photochromic effect was detected in the BGeO single crystals.



The participants of the International Conference on Single Crystals and Liquid Crystals in Zakopane. Presently, the group prepares single crystals of $\text{KGd}(\text{WO}_4)_2$ (KGW), pure and doped by rare earth ions to enable construction of diode pumped lasers, doubled frequency lasers and Raman shifters. Single crystals of LiB_4O_7 , $\text{CsLiB}_6\text{O}_{10}$, and BiB_3O_6 having large nonlinear optical properties are used in the generation of higher harmonics of laser radiation with the ultimate goal of obtaining lasers with doubled frequencies. Acousto-optical single crystals of TeO_2 are used as light modulators and tuning filters and to steer laser beams. Other studies include structures of semiconductors in the group of E. Igras and small-angle X-ray scattering by J. Frydrychowicz and R. Swilla. The 16 scientists engaged in liquid crystal research make this the largest group in Poland and one of the largest in Europe working in the liquid crystal field. 43 scientists from the Division received PhDs and ScDs degrees. The Military U. of Tech. has been organizing international conferences on single crystals and liquid crystals since 1972.

Other institutions engaged in studies of single crystal growth and epitaxial film technology include groups investigating the dependence of liquid crystalline properties on molecular mass at the **Inst. of Physics, Lodz U. of Technology, Lodz** (G. Derfel, gderfel@p.lodz.pl), defects in single crystals of pseudoperovskite at the **Inst. of Electronic Materials Technology, Warsaw** (A. Pajaczowska, pajacz_a@itme.edu.pl), the influence of impurities on the kinetics of crystal growth and structural and

electrical properties of amorphous alloys at the **Inst. of Chemistry & Environmental Protection**, Jan Dlugosz U., Czestochowa (M. Wieczorek), cubic nanocrystalline La_2O_3 in transmission electron microscopy at the **Inst. of Low Temperature and Structural Research, PAN, Wroclaw** (M. Malecka, M.Malecka@int.pan.wroc.pl), crystal growth from water solutions in a magnetic field at the **Technical U. of Rzeszow** (W. Proszak, wproszak@prz.edu.pl) low-temperature synthesis of garnet – powder luminofors of submicron dimensions at the **Faculty of Chemistry, Wroclaw U.** (E. Zych, zych@wchuwr.pl), crystal seeding, the kinetics of crystal growth, and influence of dopants on inorganic crystal growth at the **Inst. of Physics, Lublin U. of Technology** (K. Sangwal, sangwal@antenor.pol.lublin.pl), and the modeling of the process of single crystal growth from solutions at the **Dept. of Physics, Lodz U. of Technology** (G. Derfel, gderfel@p.lodz.pl). Other research on liquid crystals, is being conducted at Lodz U. of Technology (P. Adamski, G. Derfel), Poznan U. of Technology (D. Bauman), Inst. of Molecular Physics, PAN (J. Jazdzyn, W. Kuczynski), U. of Podlasie (Z. Karczmarzyk), Warsaw U. (J. Przedmojski), and Jagiellonian U. (S. Urban).

Protein crystallography



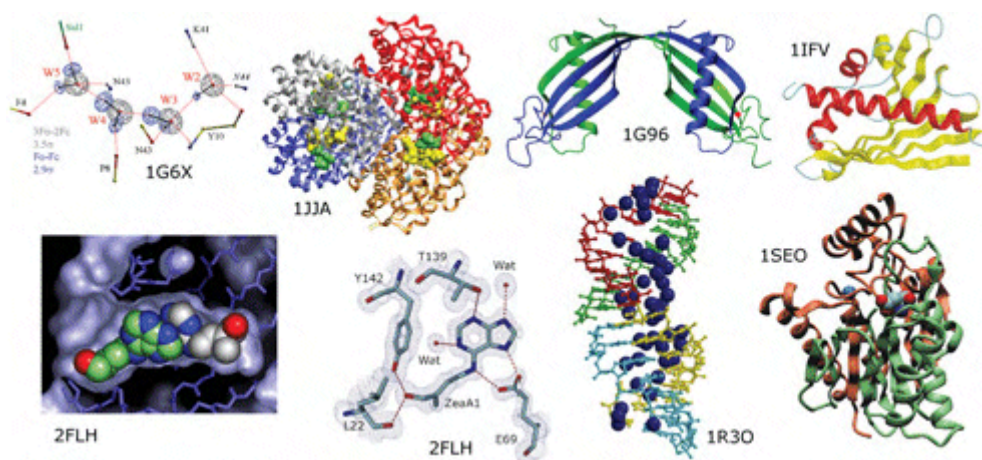
People working at the CBB, left to right, H. Fernandes, M. Sikorski, G. Bujacz, O. Pasternak, M. Gilski, O. Cakici, A. Hernandez-Santoyo, E. Bartoszak-Adamska, E. Tykarska, K. Michalska, K. Brzezinski, A. Wojtkowiak, Sz. Krzywda, M. Jaskolski, K. Banaszak, W. Rypniewski, J. Raczynska.

The **Center for Biocrystallographic Research, Inst. of Bioorganic Chemistry, PAN, Poznan** (CBB) (M. Jaskolski, mariuszj@amu.edu.pl) was created in 1994 with financial support from the Foundation for Polish Science as a joint initiative of the Dept. of Crystallography, A. Mickiewicz U. and the Inst. of Bioorganic Chemistry, PAN. It was the first macromolecular crystallography laboratory in Poland, and the second in Central and Eastern Europe. From its inception, the Center had three main goals: to conduct competitive biostructural research, to breed a new generation of protein crystallographers, and to become a site for integration and collaboration around structural biological problems on a national and regional scale. The CBB has always been an open laboratory, making its infrastructure, in particular the protein crystallization and data collection facilities, freely available to colleagues who had interesting projects but no equipment to study them.

Throughout the years, we've had visitors from Warsaw, Cracow, Gdansk, Torun, Wroclaw and Lodz in Poland, and from Prague, Halle, Lund, Vilnius, and Lviv. Several of those visits have resulted in lasting and fruitful collaborations. A regular visitor, C. Sansom (Birkbeck College, London) worked on our asparaginase project and was instrumental in the development of our teaching program. Specifically, there were very close connections between our institutions when Birkbeck was introducing their innovative internet courses on protein structure and crystallography. A number of our students graduated with Advanced Certificates, some with MSc from the U. of London. Two of our Indian postdoctoral fellows (A. Addlagatta and R. Thaimattam) were transmuted from smallmolecule-to macromolecular crystallographers while conducting high-caliber research on protein structure at atomic resolution. Currently, we have two candidates in a European Ph.D. program, H. Fernandes (Portugal) and O. Cakici (Turkey), a postdoctoral associate from Mexico (A. Hernandez-Santoyo) and a host of native students. A number of masters and doctoral degrees have been conferred in CBB. Sz. Krzywda brought a study of myoglobin variants from G. Dodson and A. Wilkinson in York. M. Kozak, now using SAXS for macromolecular studies at the Physics Dept. of the university wrote a thesis about antileukemic bacterial asparaginases. D. Borek, who discovered a new plant enzyme and its cousin in *E. coli*, and initiated a fascinating series of structural studies as a student is now in the Otwinowski Lab in Dallas, TX. R. Janowski who's Ph.D. thesis concerned domain-swapped dimers in amyloidogenic cystatin C. is now

working in the MTB structural genomics project at EMBL in Hamburg. J. Biesiadka determined the structure of proteins responding to pathogens in symbiotic plants. The project is now evolving towards hormone-binding plant proteins, while J. Biesiadka is busy with the structure of a photosystem in W. Saenger's lab. at FU, Berlin.

We also have projects based on collaborations with Polish partners (Universities of Wroclaw, Gdansk) and foreign labs (U. of Lund). A. Wlodawer (another Polish compatriot) at the National Cancer Inst. (USA) has been the initial seed for our scientific growth and an inexhaustible source of support, and scientific inspiration. Our protein crystallographic work started in collaboration with Wlodawer, included studies of retroviral protease, retroviral integrase and an antileukemic amidohydrolase. After nearly 20 years this collaboration is very much alive. The Wlodawer lab has provided training in protein crystallography to a number of postdocs and associates from Poland including G. Bujacz, a Professor at the Tech. U. of Lodz, who also holds a part-time position at the CBB. He is Poland's foremost asset in protein crystallization. During his visits to Poznan he supervises nearly all students' crystallization projects.



Selected macromolecular structures determined at the CBB (with PDB codes). 1G6X, water molecules (with H atoms) in a BPTI map at 0.86 Å; 1JJA, antileukemic asparaginase from *E. coli*. 1G96, 3D domain-swapped dimer of human cystatin C; 1IFV, pathogenesis-related protein from yellow lupine; 2FLH, plant hormone-binding protein in complex with a ligand (1.2 Å); 1R30, left-handed RNA duplex; 1SEO, bacterial isospartyl aminopeptidase.

In 1998, during ECM-18 in Prague, with encouragement from E. and G. Dodson and A. Lewit-Bentley, we organized a Consortium of Central and Eastern European Struc. Biology Groups (CCEESBG) and we were among the initiating groups, who under the leadership of R. Hilgenfeld and M. Weiss began annual meetings of young biocrystallographers in the Heart of Europe (HEC). The 3rd HEC meeting in 2000 took place in Poznan. In 2001, the CBB was one of the sites of a practical workshop "Determination of High-Resolution Structures for the Post-Genomic Age" sponsored by the National Science Foundation (USA), for young researchers from Central and Eastern Europe. The organization of the workshop was coordinated by A. Wlodawer with financial support from the Howard Hughes Medical Inst. The CBB established an EU-supported Training, Implementation and Dissemination (TID) Centre of the European BioXHIT project in 2005. The TID Centre organizes practical training workshops for the future users of synchrotron beamlines.

Our research has been supported by grants from the State Committee for Scientific Research, Howard Hughes Medical Inst., and the International Centre for Genetic Engineering and Biotechnology. Smaller grants have supported bilateral collaborations, like that with G. Desiraju in India. This collaboration is worth emphasizing because it reflects our efforts to treat macro- and small-molecule crystallography as one discipline. Initiated many years ago by the late M. Wiewiorowski - the founder of our Institute and a great advocate of biocrystallographic research in Poland, our studies into the unifying role of hydrogen bonding and other weak intermolecular interactions continue to be an exciting and evolving story.

Recently, the CBB has been reorganized to incorporate two new groups led by highly skilled specialists. In 2002, W. Rypniewski returned to Poland after receiving training in western laboratories at a time when he was entering the most creative period of his scientific career. Few scientists have the courage he has shown in resisting the brain drain to take on the challenge of working in “less privileged” regions. He has started a vigorous research program that includes determination of large macromolecular complexes and atomic resolution structures of proteins and nucleic acids. M. Sikorski heads the other new group doing protein expression and purification.

Other protein crystallography laboratories in Poland

After a post-doc in A. Wlodawer's Lab, G. Bujacz started research in the field of protein crystallography at the **Inst. of Technical Biochemistry, Lodz U. of Technology** (M. Bujacz, gdbujacz@p.lodz.pl) and at CBB in Poznan. His achievements include crystal structure and mutational analysis of the cofactor-binding domain of the Cb1 transcriptional regulator, and an HIV protease complexes with inhibitors. He was an initiator of the **Lodz U. of Technology** award of *doctors honoris causa* to Alex Wlodawer (USA).

K. Lewinski and his research group investigate enzymatic mechanisms and inhibition of proteins in the **Dept. of Crystal Chemistry and Crystal Physics, Jagiellonian U., Krakow** (K. Lewinski, lewinski@chemia.uj.edu.pl). In collaboration with L. Lebioda (U. of South Carolina, USA) they determined the crystal structures of human prostatic acid phosphatase, enolase, glutaminase-asparaginase, arylsulphatase A and formyltetrahydrofolate synthetase. Their field of research also includes crystallographic studies of ribonuclease A and its variants under ambient and high pressure conditions. K. Lewinski is the editor of the Bioorganic Crystal Chemistry section in the *Central European Journal of Chemistry*,

A. Wojtczak with his research group at the **Dept. of Crystallography, Nicolaus Copernicus U., Torun** (A. Wojtczak, awojt.@chem.uni.torun.pl) has solved protein crystal structures of human and rat transthyretin.

The **Int'l Inst. of Molecular and Cell Biology, Max-Planck - PAN Joint Junior Research Group, Warsaw** (M. Bochtler, mbochtler@iimcb.gov.pl) was established in 2001 as a collaborative venture between the Polish Academy of Sciences and the German Max-Planck- Society. Its head, Matthias Bochtler (a former student of Robert Huber) is officially a Junior Group Leader in the Max-Planck-Inst. of Molecular and Cell Biology and Genetics (MPI-CBG) in Dresden, but in practice he is on “loan” to IIMCB in Poland. With funding from the MPI in Dresden, the European Union, and Polish sources, M. Bochtler, has quickly established a dynamic and competitive group, which is almost exclusively Polish. Its short but impressive record of achievement includes discoveries in the area of new peptidases, endonuclease, nucleoside phosphorylases and their inhibitors. The Bochtler lab is advancing protein crystallography in Poland at the international level.

Polish crystallographers outside of Poland or anomalous scattering of multi-poles

(Z. Dauter, zdauter@anl.gov)

It is quite remarkable how many Polish scientists scattered abroad are crystallographers, or especially protein crystallographers. “Scattered” is not a good word as many of us preserve close links, often involving the “old land”.

Already in the 1960's and 70's, several senior crystallographers had a vision to organize excellent schools and workshops where young disciples were taught by such authorities as Nikolay V. Belov, Yuri T. Struchkov, Mikhail A. Porai-Koshits, from Russia, Dorothy Hodgkin, Tom Blundell, Eleanor and Guy Dodson

from the UK, Herbert Hauptman, Jerome and Isabella Karle, and Bill Duax from the USA, John Stezowski and Wolfram Saenger from Germany, Ivar Olovsson from Sweden, and Lodovico Riva di Sanseverino from Italy. We were in Poland a very happy crystallographic family with strong links to our “cousins” all over the world. We could learn good crystallography, but unfortunately in those days in Poland access to advanced computing was almost impossible and good X-ray facilities were scarce. It was virtually impossible to pursue protein crystallography.

The political difficulties of the 1980's created additional problems. As a result, a number of Polish scientists decided to stay abroad and today we find many of them at senior positions in various institutions (Aleksander Roszak, U. of Glasgow, UK; Andrzej Joachimiak, Argonne Natl. Lab., USA; Andrzej M. Brzozowski, U. of York, UK; Boguslaw Stec, USA; Ewa Ciszak, NASA, USA; Ewa Skrzypczak-Jankun, Toledo, USA; Jacek Lubkowski, Zbigniew Dauter, Alex Wlodawer, NCI, USA; Krzysztof Appelt, pharmaceuticals, USA; Lukasz Lebioda, U. of S. Carolina, USA; Mirek Cygler, NRC, Canada; Pawel Dokurno, Ribotargets Ltd., UK; Pawel Grochulski, U. of Saskatchewan, Canada; Tadeusz Skarzynski, Glaxo-Wellcome, UK; Zbyszek Otwinowski, U. of Texas, USA; Zdzislaw Wawrzak, APS, USA; Zygmunt Derewenda, Wladek Minor, Michal Sabat, U. of Virginia, USA). In addition, there is a host of younger postdocs in virtually all places where crystallography is being done.

It is interesting that several of us have direct or indirect links to various synchrotron facilities. Alex Wlodawer participated (with Jim Phillips and Keith Hodgson) in the first ever synchrotron diffraction experiment on protein crystals at Stanford in 1975. Andrzej Joachimiak, who earlier worked at the Universities of Chicago and Yale, is now directing the Structural Biology Center and its synchrotron facility at Sector 19 of APS (Advanced Photon Source) at Argonne and heads the Midwest Center for Structural Genomics. Zbigniew Dauter served for ten years at the EMBL synchrotron outstation at DESY in Hamburg and now for the last eight years heads the Synchrotron Research Section of the National Cancer Inst., located first in Brookhaven and now at the Argonne synchrotron site. Zdzislaw Wawrzak after several years at the Hauptman-Woodward Inst. in Buffalo, since 1998 has been taking care of crystallographic activity at the DND (DuPont, Northwestern, Dow) Sector 5 of the APS synchrotron at Argonne. Pawel Grochulski, after a post at the NRC lab in Montreal, since 2000 is responsible for the construction and activity of the protein crystallography beamlines of the Canadian Light Source at Saskatoon. Last but not least, Zbyszek Otwinowski and Wladek Minor are the authors of the HKL2000 data processing suite, widely used at almost every synchrotron beamline.

As I said before, our younger years bring back very fond memories. But when I really think about it, we are still a very happy and closely knit community. This is why this note belongs in “Crystallography in Poland”.

Article Edited by Zofi a Kosturkiewicz

Editors Note: As we did not have access to a full set of diacritical marks, they were omitted from proper names in the article.

Thank you to the many contributors of Crystallography in Poland:

Grzegorz Bujacz, Jaroslaw Chojnacki, Zbigniew Dauter, Jozef Garbarczyk, Mariusz Jaskolski, Zbigniew Karczmarzyk, Anna Koziol, Tadeusz Marek Krygowski, Janusz Leciejewicz, Maria Lefeld-Sosnowska, Krzysztof Lewinski, Eugeniusz Lagiewka, Barbara Oleksyn, Andrzej Oles, Jerzy Pielaszek, Izabela Sosnowska, Katarzyna Stadnicka, Kinga Suwinska, Katarzyna Slepokura, Ilona Turowska-Tyrk, Zofi a Urbanczyk-Lipkowska, Jerzy Warczewski, Michal Wieczorek, Andrzej Wlochowicz, Janusz Wolny, Marek Wolcyrz, Krzysztof Wozniak, Jacek Zaleski, Andrzej Zieba, Jozef Zmija,

Rare crystallographic phenomenon recorded in Poznan



An extremely rare natural phenomenon has been observed early in the morning on April 1, 2007, from the windows of the Department of Crystallography, Faculty of Chemistry, A. Mickiewicz University in Poznan, Poland. A series of crystallographic two-fold screw axes (2_1) appeared in this unusual sighting on an opposite building wall. The scientific background of this phenomenon is still a mystery but it is widely believed that it heralds good fortune for those who have sighted it.

Mariusz Jaskolski, photographed by. M. Gilski

MEETING REPORT

2006 happenings in Poland

Wisla, Poland, September 10-14, 2006



"Happy Birthday Prof. Massalski...!!!"

The XX International Conference on Applied Crystallography was held in Wisla, Poland, September 10-14, 2006. The conference was organized by the Inst. of Material Science of Silesia in Katowice and was followed by a workshop on Strain Determination and summer schools on Polycrystalline Structure Determination and Strain/Stress Determination by Transmission Electron Microscopy (TEM).



Participants of the XX CAC 2006 on the excursion to Istebna and Koniakow – the Beskid Mountains region

The Committee of Crystallography and the Committee of Material Science of the Polish Acad. of Sciences were co-organizers of the events. The IUCr awarded scholarships to enable attendance by young scientists. The conference was also sponsored by the Rector of the U. of Silesia, Polish Ministry of National Education and the Polish Acad. of Sciences.



Summer School on Strain/Stress Determination by TEM

115 participants from 19 countries engaged in lively discussions throughout the plenary, oral (31) and posters (52) sessions. Plenary lecturers included: Tadeusz Massalski (USA), Jaroslav Fiala (Czech Republic), Carmelo Giacobazzo (Italy), Fujio Izumi (Japan), Gernot Kostorz (Switzerland), Henryk Morawiec (Poland), Wolfgang Neumann (Germany), Jerzy Pielaszek (Poland), Adam Pietraszko (Poland), Paolo Scardi (Italy), Veniamin Sh. Shekhtman (Russia), and Walter Steurer (Switzerland). Topics discussed included: development of methods and techniques of structure determination; crystallography of phase transformations; texture analysis studies of metals, alloys, ceramics, and polymers; thin films; quasicrystals; amorphous materials; nanomaterials; and molecular crystals.



Carmelo Giacobuzzo

Tadeusz Massalski, who will celebrate his 80th birthday this year, presented a lecture at the Conference. His work in the areas of Hume-Rothery phases, phase diagrams and phase stability has been widely recognized. He discovered one of the principal reactions through which metals and alloys transform and is still very active in the field of physical metallurgy and solid state physics. The conference proceedings will be published in the *Solid State Phenomena*, Trans Tech Publications in Switzerland.



Armel le Bail

Social aspects of the conference included an excursion to Istebna and Koniakow in the Beskid Mountains region. At the Workshop on Strain Determination 13 participants from 6 countries listened to the lectures of T. Ungar (Hungary) and R. Pielaszek (Poland).



Summer School on Polycrystalline Structure Determination

The Summer School on Polycrystalline Structure Determination under the direction of Carmelo Giacobuzzo (Italy) and tutorship of A. Le Bail (France), Vincent Favre-Nicolin (France), and W. Lasocha (Poland) included 30 participants from 6 countries while the Summer School on Strain/Stress Determination by TEM Methods - under the direction of W. Neumann (Germany) and tutorship of P. Strunk (Germany), H. Kirmse (Germany), K. Scheerschmidt (Germany), J.P. Mornirolli (France), P. DLuzewski (Poland), and S. Kret (Poland) had 20 participants from 6 countries. Attendees had a chance to practice their skills at the extended computer sessions.

Solving crystal structures from powder data and by TEM analysis is scientifically challenging but the results will be useful for many industrial and technological problems. The main purpose of these schools was to train young scientists in the use and application of methods for determination of crystal structures, strain and stress. The students worked with the following programs: EXPO 2005, FULLPROF, FOX, GRINSP and qHRTEM, CBED, FEM method for strain determination (programs: DALI, OPTIMAS).

Malgorzata Karolus, Secretary of XX CAC 2006

MEETING REPORT

BioCrys2006

Oeiras, Portugal, October 6-13, 2006

A typical tutorial session in the computer room during BioCrys2006

The third BioCrys-Course on 'Fundamentals of Modern Methods in Biocrystallography', organized by Maria Arménia Carrondo (ITQB Oeiras, Portugal) and Thomas Schneider (FIRC Inst. of Molecular Oncology, Milan, Italy) took place in the Inst. de Tecnologia Química e Biológica in Oeiras, Portugal, October 6-13, 2006. The course was supported by EMBO, MAX-INF2 cooperation network, BIOXHIT Integrated project, the IUCr, FEBS, The British Council, FLAD, the Cambridge Crystallographic Data Centre, Oeiras Council, Qiagen and Corning. It brought together 36 students and 19 tutors from 20 and 10 different countries, respectively.

Subtitled 'What you always wanted to know about crystallography but never dared to ask ...', the course aimed at teaching the fundamental concepts of macromolecular crystallography to scientists in the early stage of their crystallographic career. In fact, while learning the efficient use of automated tools in crystallography, it is also critical to understand the underlying concepts for tackling difficult problems of structural biology that are not amenable to the current generation of these tools.

Lectures and tutorials covered topics all the way from the cooling of crystals to the validation of the final structural model. For the computational tutorials, a cluster of 18 Linux-computers was used, especially set up for the course by Pedro Matias and Daniele de Sanctis (both from ITQB). The scientific program of most days was concluded with an evening lecture, in which tutors or invited speakers reported about a current topic in structural biology.

Ed Hough (U. Tromsø, Norway) laid out the basics of crystallography in real and reciprocal space. Sean McSweeney (ESRF, France) gave an overview about the principles of X-ray sources and beamline automation and Elspeth Garman (Oxford U., UK) lectured and demonstrated about the practical side of crystal cooling and data collection. Kevin Cowtan (U. York, UK) guided the students through the world of structure factors and how they relate to electron densities in his web-based tutorial (www.yorvic.york.ac.uk/~cowtan/sfapplet/sfintro.html). The understanding of the basics was complemented by a tour of crystallographic resources on the world wide web by Isabel Bento (ITQB) and Daniele de Sanctis.

Strategic questions of data collection and both theoretical and practical aspects of data processing were addressed by Zbyszek Dauter (Argonne Nat'l. Lab., USA) and Andrew Leslie (MRC, UK). This included practicals on integration and scaling of diffraction data.

Gordon Leonard (ESRF, France) gave an introduction to the use of anomalous scattering in macromolecular crystallography. The substructure solution process and MAD-phasing were covered by Thomas Schneider (IFOM, Italy). Kevin Cowtan discussed the principles of the different density modification techniques used for phase improvement and Zbyszek Dauter explained various aspects of SAD-phasing. Molecular Replacement was introduced and discussed with the help of examples by Pedro Matias. Carlos Frazão (ITQB) described solutions to problems that one encounters with twinned crystals.

Other topics covered includes the MIR-method (Clemens Vonnrhein, GlobalPhasing, UK), maximum likelihood (Kevin Cowtan), symmetry (Zbyszek Dauter), and refinement and model precision (Thomas Schneider).

The central topics of the remaining two days were molecular replacement and both manual and automated model building. Automated model building and refinement was discussed from methodological and practical points of view by Anastassis Perrakis (NKI, The Netherlands). Morten Kjeldgaard (U. of Aarhus, Denmark) taught the principles and practicalities of manual model building. The discussion of model building was complemented by an overview about the tools and concepts for assessing the correctness of a model by different validation criteria by Margarida Archer (ITQB).

The subjects of evening lectures were protein synthesis by Anders Liljas (Lund U., Sweden), RNA degradation by Maria Arménia Carrondo (ITQB Oeiras), and the preparation of protein samples for crystallization by Peter Donner (Schering AG, Germany).

'Burning questions' submitted anonymously were answered by the tutors in a dedicated session.



Photo group of the participants at BioCrys2006

The City Council of Oeiras generously invited all participants to dinner at the restaurant Caravela Douro where they enjoyed local cuisine and had a hands on introduction to regional folk dances. We thank our sponsors for generous support. We are also grateful to the informatics staff of ITQB and Mafalda Mateus for handling administration and logistics of the course very efficiently.

Maria Arménia Carrondo and Thomas R. Schneider, Organizers

OBITUARY

Mario Mammi (1932-2006)

Professor Mario Mammi died on December 20, 2006 in Padova, Italy. He was born in Reggio Emilia in 1932. He began to study Chemistry at the U. of Modena. He graduated with honors from the U. of Padova where, he began his career as a research assistant of Silvio Bezzi, the founder of the Inst. of the Organic Chemistry in the 1950's. Prof. Bezzi, who strongly believed in the potential of X-ray diffraction for solving problems in organic chemistry, established a crystallography group in the Institute under the supervision of Mario Mammi. Initially, the research interest of the group was mainly devoted to the structure determination of organic compounds, to understand their reactivity in general and in polymerization reactions. The most important breakthrough was the determination of the structure of thio-thiophen, which allowed the definition of a new kind of aromatic system. The structure, determined from projections without the use of computers (in those times, most of the calculations were performed manually, by using ingenious devices to speed up calculations), was published in *Nature* in 1958.

When Mario Mammi's scientific interest shifted towards protein crystallography, he spent some time at the Lab of Molecular Biology in Cambridge in 1962 and 1964. His second visit was interrupted by the sudden death of Prof. Bezzi, which forced him to return to Padova to manage the research group. Major scientific contributions of this period were on the diffraction of biological fibers, in particular elastin, a protein that could not be crystallized and for which even a fiber diffraction spectrum was hard to obtain. Work on globular proteins in Padova started with Ribonuclease. This is a bovine enzyme that catalyzes the hydrolysis of the phosphodiester bond of RNA. Its three-dimensional structure had been determined independently by two groups (a first low resolution model appeared in 1967 by Wyckoff and by Kartha and Harker). In Ribonuclease, the bond between residues 20 and 21 can be specifically hydrolyzed, and the two resulting portions mixed together can recombine, giving an active enzyme, despite the lack of a covalent bond. This feature was used in Padova to produce an artificial enzyme putting together the bigger fragment with a synthetic 1-20 peptide in which one or more amino acids had been modified with respect to the wild-type protein. This allowed the production of a sort of point-mutants *ante litteram*, well before molecular biology was established, and to study the relevance of single amino acids on overall protein conformation. The first (and only) structure of one of these artificial "mutants", Orn-10-RNAase S', appeared only some years later.

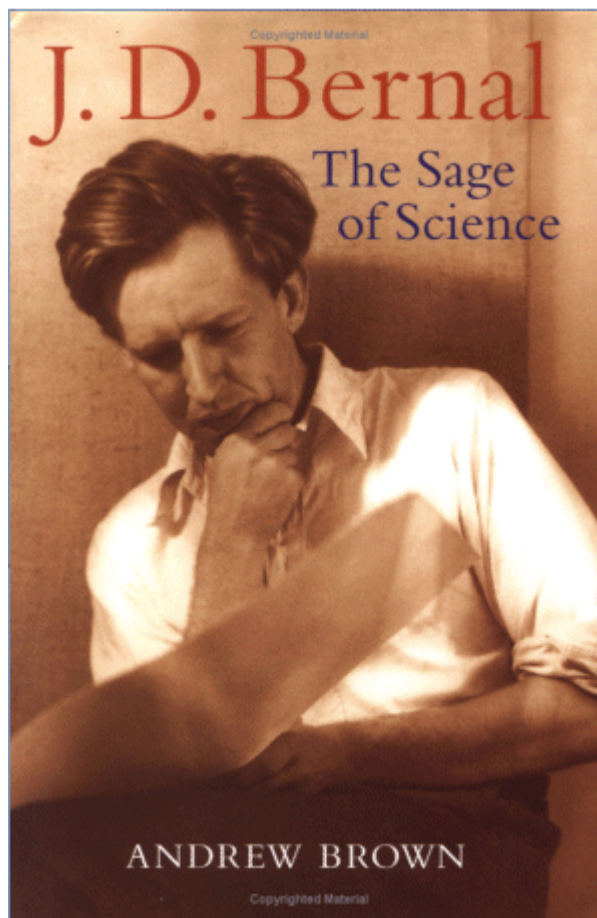
In 1971, Mario was appointed Full Professor and in 1975, he became the Director of the Biopolymer Research Center of the Italian National Research Council (CNR). The Center was hosted in the Inst. of Organic Chemistry of the University and included not only the protein crystallography group, but also peptide and protein chemistry and, later, NMR. With time, he became more and more involved not only in the administration of the Center, but also in other managerial responsibilities, either in Rome with CNR or in Padova, and he applied himself to these commitments with great dedication. Among many other things, he was head of the Dept. of Organic Chemistry (Nov. 1972 - Nov. 1975) and vice-Rector of the University (1993-1996). From 2005, he was in charge of the University budget. He was among the founders of the Italian Association of Crystallography, and served as its President from 1985 to 1987. He was several times the editor of the Italian section of the World Directory of Crystallographers. Mario was

diagnosed with lung cancer in February last year, but he continued to work and tend to university business till summer, when his health prevented him from leaving home. His great wisdom, his proverbial fairness, his unusual sense of the institutions, and his unforgettable smile will be sorely missed.

S. Mammi, P. Spadon and G. Zanotti

BOOK REVIEW

J.D. Bernal: The Sage of Science



Andrew Brown, a medical radiologist and science historian, has compiled an excellent biography, of the brilliant crystallographer, J. Desmond Bernal (1901-1971) (the nickname Sage was acquired at Cambridge, according to Perutz, “because he knew everything, from physics to the history of art”). There have been several biographical accounts of aspects of Bernal’s colorful life, including his own unpublished *Microcosm*, but this is the first attempt to portray the immense range of his scientific and political energies, interwoven with glimpses of his unconventional domestic life. Few novels feature crystallographers but, despite the usual author’s disclaimer, Charles P. Snow clearly used his friend Bernal as a model for the scientist character Constantine who envisaged a multidisciplinary Biological Research Institute in “The Search”. Twenty-five years after the publication of Bernal’s most influential book, *The Social Function of Science* (London, Routledge, 1939), Snow contributed a perceptive personal portrait, emphasizing Bernal’s bravery and imagination, to the multi-author re-assessment volume *The Science of Science* (ed. M. Goldsmith & A. Mackay, Souvenir Press, 1964).

Dorothy Hodgkin composed a beautiful, affectionate, authoritative and detailed appreciation [*Biogr. Mem. Fellows R. Soc.*, **26**, 17-84, 1980] of her friend Bernal’s early life and subsequent career. She included Lord Mountbatten’s admiring memories of Bernal’s pertinent scientific advice for the 1944 Normandy invasion. More recently, Brenda Swann and Francis Aprahamian edited a collection of 15 essays, *J D Bernal* (London: Verso, 1999), predominantly on Sage’s international peace campaigning and other political activities, but including a useful chronology of events in Sage’s life.

Andrew Brown has now produced a comprehensive and scholarly, but very readable biography (Oxford: University Press, 2005) based on five year’s research into Bernal’s papers and war reports and from information derived from many of his family, friends and colleagues. Brown’s approach is broadly

chronological. However, some of the 22 chapters are topic-based. Thus, one chapter on the *Physical Basis of Life* covers the emergence of molecular biology, while another on Peace brokering puts the anti-nuclear-bomb campaigns of the 1950s and 1960s in context.



Bernal was perhaps the most international of crystallographers. At the inaugural UN Educational and Cultural Conference, he was one of the scientists credited with ensuring that the new organization should include an S for Scientific and so be UNESCO. The *Social Function of Science* not only dealt in immense detail with the organization of science education and research in the UK, but also embraced a survey of science across the world. Its proposals as to what science could do were both visionary and controversial at the time. As early as 1930, Bernal was largely involved with Ewald in international crystallographic committees on abstracting and the nomenclature and tabulation of space groups. More generally, early recognition of the problems of dissemination and retrieval amid the information explosion led to far-reaching proposals in 1939, developed further in 1948 for what would ultimately be an international institute for scientific publication (with abolition of full-length papers in conventional journals, a notion revised in 1960) and information abstraction; an international scientific language was even contemplated. The suggestion that new structures should be logged was made in 1948, but it was not until 1970 that Olga Kennard could dedicate the first two volumes of the CCDC's *Molecular Structures and Dimension* to Bernal. His familiarity with post-1945 Schools of Crystallography in Britain and the Commonwealth is shown in Chapter 17 of *Fifty Years of X-ray Diffraction* (ed. P.P. Ewald, Utrecht, IUCr 1962). Having been one of those involved in the 1946 decision to set up the IUCr, he became President in 1963 until incapacitated by his second tragic stroke in 1965.

Several visits to the USSR in the early 1930s made a strong impression on Sage, although his irrevocable position on religion and politics had been established earlier. His first adult visit to the USA (his mother was a bilingual English and French speaking American, but he was educated in Ireland and England) was curtailed by the outbreak of World War II in 1939. Post-1945, many of Sage's visits to the USSR and Eastern Europe (several of whose scientific academies awarded him Membership) and to China and India included both scientific lectures and peace campaigning. He met Khrushchev, Mao Zedong and Nehru, gave a demonstration to Churchill, and participated in committee meetings in the White House, the Kremlin and 10 Downing Street. His experience of less developed countries began with laborious and uncomfortable war-time travel for Mountbatten but thereafter he made many lengthy tours to countries with emerging economies to advise on the development of each nation's science. His expertise across chemistry, physics, mathematics, biology and structural materials made him a valuable and inexpensive science consultant and also enabled him to indulge his wider intellectual interests with visits to historic sites and museums. Throughout this time and amid all his extra-curricular activities, Bernal continued to hold the responsibilities of a university chair in physics at Birkbeck (to which students came to lectures only in the evenings).

X-ray crystallographers of a certain age will be especially conscious that Bernal rejected W.H. Bragg's spectrometer, then in vogue at the Royal Institution in the 1920s, in favor of Polanyi's rotating-crystal photographic method. He made the laborious calculations, first for Bragg and rotation angles and then for reciprocal-lattice co-ordinates, to facilitate the construction of indexing charts. (Incidentally, Polanyi,

another polymath, by this time at Manchester, was in the late 1930s to disagree with Bernal both about his advocacy of the central direction of science and about life in Russia.) Bernal then designed what became the Pye (later Unicam) universal X-ray photogoniometer, widely used from the 1930s to the 1950s.

Perhaps Bernal's greatest scientific contribution was to nurture a clutch of Nobel prizewinners in the development of molecular biology. In his biography, Brown notes that with Bernal's prolific writing, this Renaissance man changed the course of science and initiated much systematic discussion and some action about what we now call science policy and the integration of science with society.

Outstanding intellects often display surprising discrepancies in behavior and judgment. Against much evidence, Bernal remained uncritical of Stalinist Russia (he accepted a Lenin Peace Prize in 1953) and continued to support Lysenko. He also lived what might euphemistically be described as a Bohemian lifestyle. With regard to personal achievement in scientific research, some would feel that he dissipated too much of his, admittedly enormous, energy in committee meetings or, indeed, in just too many activities. Thus, perhaps, was lacking the long-term obsession within a single field (though he returned to liquid structure, for example, quite late in his research career) that might have led to a Nobel Prize, whether in science or for peace. Brown neither ignores nor dwells on these matters unduly. He has produced a fascinating 470-page biography that does justice to the rich life of an inspirational and imaginative scientist and an ebullient, influential and wide-ranging character.

Derry W. Jones, Bradford University, England

AWARDS AND PRIZES

Awards



Artem R. Oganov (ETH Zurich and Moscow State U.) received the University Latsis Prize “for research on crystal structure prediction and for the discovery of several major Earth-forming minerals”.



Colin W. Glass (ETH Zurich) received the ETH Zurich Medal for an outstanding MSc work “USPEX – Evolutionary Crystal Structure Prediction”

AWARDS AND PRIZES

Ada Yonath wins Wolf Prize



Ada Yonath (Dept. of Structural Biology, Weizmann Inst.) was named as one of the winners of the prestigious Wolf Prize in Chemistry. Prof. Yonath will receive the 2006-2007 chemistry prize in May, along with Prof. George Feher, a physicist at the U. of California, San Diego. The two scientists will share the \$100,000 prize granted by the Wolf Foundation in Israel.

In its official announcement, the Wolf Foundation said, “The recent emergence of ribosome structures in the crystallographic community is mainly due to Ada Yonath, who uniquely and single-handedly pioneered ribosomal crystallography over more than two decades ago, when others could not even conceive its possibility. By pushing crystallography to its limits, she demonstrated the feasibility of ribosomal crystallography, thus inspiring prominent groups to repeat her experiments. Throughout, she has been the leading force in all stages of structure determination and has introduced fundamental methodological innovations that have greatly impacted the entire field of structural biology.”

Prof. Yonath received her Ph.D. from the Weizmann Inst. in 1968. After a postdoctoral fellowship at MIT, Prof. Yonath returned to the Weizmann Inst. and began her investigation into the structure of the ribosome. Prof. Yonath is The Martin S. and Helen Kimmel Professor of Structural Biology and Director of The Helen and Milton A. Kimmelman Center for Biomolecular Structure and Assembly at the Weizmann Inst.

The Wolf Prize has been awarded annually since 1978 “to promote science and art for the benefit of mankind.”

The Weizmann Inst., www.weizmann-usa.org

NOTICE

Deposition of structural data redux

It has been almost exactly ten years since the publication of a “revolutionary” suggestion that macromolecular coordinates resulting from crystallographic and NMR studies should be deposited in the Protein Data Bank (PDB) and released immediately upon publication of the relevant papers. IUCr implemented a new policy in 2000 that disallows coordinate holds beyond the date of publication, while allowing a six-month hold on the structure factors. That policy is mandatory for the IUCr journals and provides a template for policies of almost all other journals that publish macromolecular structures, as well as for funding bodies such as NIH or HHMI.

The availability of structure factors is particularly important if there could be any doubts about the correctness of the reported structures. A recent fiasco related to the inverted structure of the proteins MsbA and EmrE provides a very good example. A number of coordinate data sets deposited in the PDB were not accompanied by structure factors, so other scientists could not perform any verification of the models that turned out to be seriously wrong.

Whether enforced or not, the policy of depositing the structure factors (with a possible six-month hold) is already on the books. When a paper is already published, it is unlikely that the availability of structure factors could really hurt the competitiveness of the authors, unless there was a problem that could be detected by others. But that is exactly why these data should be generally available!

I would thus like to make a number of suggestions directed to authors, journals, funding bodies, the IUCr and the PDB. First, I feel that the PDB should not accept deposition of coordinates not accompanied by structure factors. Second, the journals should be much more vigilant in enforcing the rules regarding deposition of structural data. However, I strongly urge the IUCr to reconsider and revise its current policy that allows six-month hold of the structure factors, and instead to treat them exactly in the same way as the coordinates. The PDB should become much more active in assuring the scientific community that the coordinates and structure factors in their repository are accurate, properly annotated and fully cross-referenced to their respective publications. Let us remember that many of the current depositors might be proficient in running crystallographic programs, but have little or no understanding of crystallography as such. Even more important is the fact that major consumers of the coordinates are not structural biologists, but experts in other fields.

To summarize, much has changed during the last ten years and the policies that were adequate then seem no longer to benefit the scientific community in the same way. Thus, time has probably come to take another look at them, and modify them accordingly. The IUCr is the right organization to initiate such a change, but the journals and funding agencies might wish to act even sooner. I hope that my proposal, controversial as it might appear to some (as was the previous one ten years ago), could be a basis of starting a thorough discussion of this important matter.

Alex Wlodawer

An expanded version of this letter with interesting, amusing and provocative details appears in *Acta Cryst.* (2007), **D63**, 421-423.