

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

IUCr Newsletter

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Original article text and available illustrations

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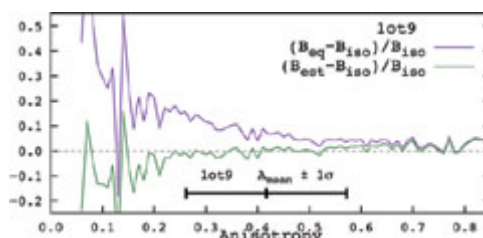
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Some B_{eq} are more equivalent than others

Some B_{eq} are more equivalent than others

Acta Cryst. (2011). A67, 512-516 (<http://doi.org/g3d>)



Mean fractional error in predicting the B_{iso} obtained from 1.0 Å isotropic re-refinement of PDB entry 1ot9. Atoms are sorted on anisotropy. Most atoms in the original structure have anisotropy in the range indicated by the bar.

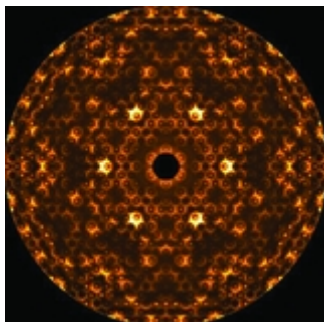
Macromolecular crystal structures are typically refined with isotropic B factors, even though their atoms are substantially anisotropic. To evaluate whether a high-level model for the anisotropy, e.g. from TLS or Normal Mode analysis, adequately describes the structure, we must predict what value of B will in practice be refined for an atom with hidden parameters U^{ij} . Until now the approximation $B_{eq} = 1/3\text{trace}(U^{ij})$ has been used. This paper derives a more accurate predictor, B_{est} , which will allow construction of better TLS models from isotropic input.

E. A. Merritt

IUCR JOURNALS NEWS

Diffuse scattering resulting from macromolecular frustration

***Acta Cryst.* (2011). B67, 516-524 (<http://doi.org/g3f>)**



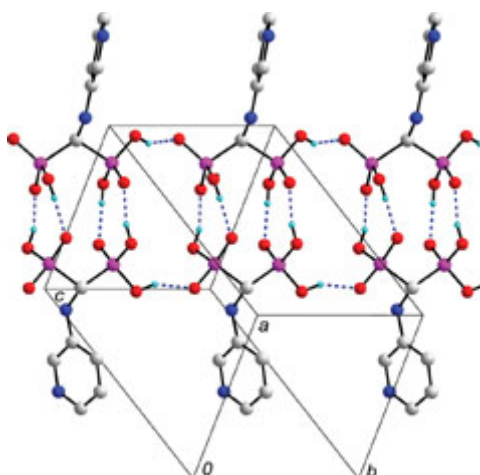
Diffuse X-ray scattering in the $hk1$ section of the diffraction pattern from a crystal of the *N*-terminal fragment of the Gag protein from Feline Foamy Virus.

Strong and very distinctive diffuse scattering has been observed in the diffraction patterns of a crystal of the *N*-terminal fragment of the Gag protein from Feline Foamy Virus. The paper shows that the effects are caused by geometric frustration as the protein molecules try to pack on the triangular b - c mesh of the space group $P6_122$. Since the disorder has so far prevented structure solution of the protein by conventional techniques the possibility of using the diffuse scattering for solving the structure is discussed

T. R. Welberry, A. P. Heerdegen, D. C. Goldstone and I. A. Taylor

Conformations and resulting hydrogen-bonded networks of hydrogen {phosphono[(pyridin-1-ium-3-yl)amino]methyl}phosphonate and related 2-chloro and 6-chloro derivatives

Acta Cryst. (2011). C67, o450-o456 (<http://doi.org/g3g>)



The arrangement of the zwitterions in hydrogen {phosphono[(pyridin-1-ium-3-yl)amino]methyl}phosphonate monohydrate (*pro-E*) within the ribbons along the *b* axis.

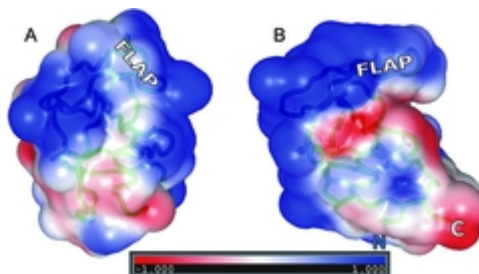
The crystal structures of the two conformational isomers of the title compound, *pro-E* as the monohydrate and *pro-Z* in an anhydrous form, and the related 2-chloro (*pro-E*) and 6-chloro (*pro-Z*) derivatives are described. Chain-chain interactions involving phosphono ($-\text{PO}_3\text{H}_2$) and phosphonate ($-\text{PO}_3\text{H}-$) groups are dominant in determining the crystal packing in all four compounds.

E. Matczak-Jon and K. Slepokura

IUCR JOURNALS NEWS

High-resolution structure of a retroviral protease folded as a monomer

***Acta Cryst.* (2011). D67, 907-914 (<http://doi.org/g3h>)**



Comparison of electrostatic potential surfaces of retroviral protease monomer (left) and a subunit extracted from a dimeric molecule (right).

Although retroviral protease, which is a homodimeric enzyme, has been the subject of numerous studies, the structure of its protomeric subunit has defied crystallographers for a long time. Finally, a suitable molecular replacement model has been created by players of the online protein folding game, *Foldit*. The crystal structure of monomeric protease from an HIV-like monkey virus shows a molecule with a canonical core but with novel conformation of some key elements, *e.g.* the 'flap'. This new information can be used to design novel antiretroviral drugs.

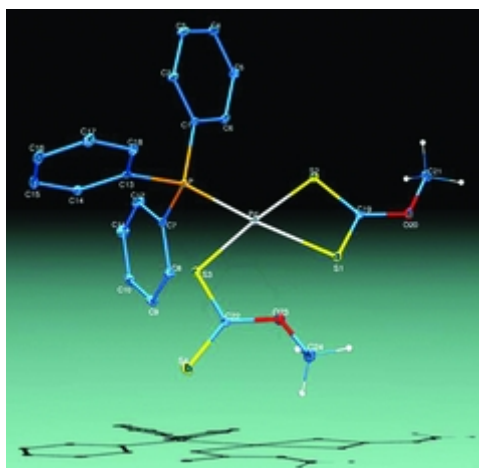
M. Gilski, M. Kazmierczyk, S. Krzywda, H. Záborská, S. Cooper, Z. Popovic, F. Khatib, F. DiMaio, J. Thompson, D. Baker, I. Pichová and M. Jaskolski

IUCR JOURNALS NEWS

Bis(methyl xanthato)- $\kappa S;\kappa^2 S:S'$ -(triphenylphosphane- κP)palladium(II)

Bis(methyl xanthato)- $\kappa S;\kappa^2 S:S'$ -(triphenylphosphane- κP)palladium(II)

Acta Cryst. (2011). E67, m1518 (<http://doi.org/g3j>)



Crystal structure of the title compound with the numbering scheme. Displacement ellipsoids are shown at the 40% probability level. H atoms have been omitted for clarity.

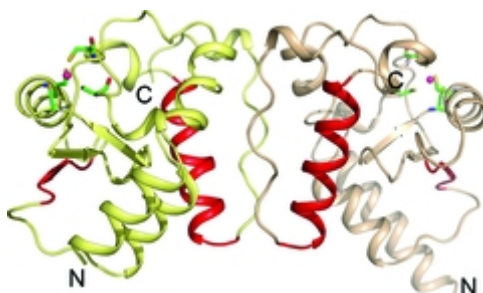
Xanthate ligands are a kind of compound that can be coordinated to metal centers in different fashions, being found in coordination as monodentate, bidentate or even as a bridge. The title compound, $[\text{Pd}(\text{C}_2\text{H}_3\text{OS}_2)_2(\text{C}_{18}\text{H}_{15}\text{P})]$, features a palladium complex with a triphenylphosphane ligand and two xanthate ligands, one of which coordinates in a bidentate manner while the other is attached to the palladium only by one sulfur atom in a monodentate way. The Pd—S bond distances in the bidentate ligand of 2.3386 (6) Å for Pd—S2 and 2.3581 (6) Å for Pd—S1 are longer than Pd—S3 in the monodentate ligand. As a consequence of the differences in distances, C22—S4 has a double-bond character [1.649 (2) Å] and thus is shorter than C22—S3 [1.723 (2) Å], which shows a single-bond character.

R. Reyes-Martínez, S. Hernández-Ortega and D. Morales-Morales

IUCR JOURNALS NEWS

Structure of the catalytic domain of *Plasmodium falciparum* ARF GTPase-activating protein (ARFGAP)

Acta Cryst. (2011). F67, 1339-1344 (<http://doi.org/g3k>)



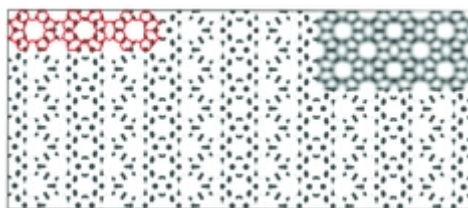
Two molecules of ARFGAP related by the noncrystallographic twofold axis form a dimer in the asymmetric unit. A number of residues on this interface are distinct in the *P. falciparum* ARFGAP. ADP ribosylation factor GTPase-activating proteins (ARFGAPs) play multiple roles in cellular signal transduction and protein trafficking, which are necessary for the survival and growth of the *Plasmodium falciparum* parasite. A strategy for interrupting the protein-trafficking machinery within plasmodium-infected erythrocytes may be effective in arresting the life cycle of the parasite and thereby preventing disease progression. The structure of the catalytic domain of the *Plasmodium* ARFGAP shows several notable differences from human ARFGAP; these unique properties may offer new targets for therapeutic intervention.

W. J. Cook, O. Senkovich and D. Chattopadhyay

IUCR JOURNALS NEWS

Using phases retrieved from two-dimensional projections to facilitate structure solution from X-ray powder diffraction data

J. Appl. Cryst. (2011). 44, 1023-1032 (<http://doi.org/g3m>)



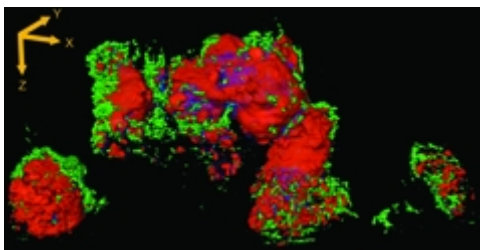
The electron-density map at the right was produced from a two-dimensional subset of reflections extracted from a powder diffraction pattern ($d_{\min}=1.5\text{ \AA}$). For comparison, an HRTEM image of the projection has been overlaid (upper right), and the projected unit cell of the zeolite framework structure (IM-5) superimposed (upper left). It has been found that by applying the charge-flipping structure solution algorithm to such low-resolution two-dimensional subsets of reflections, more correct phases are obtained than when the full dataset is used. By combining a few such subsets, a set of starting phases can be generated, allowing previously inaccessible structures to be solved from the powder diffraction data alone.

D. Xie, Ch. Baerlocher and L. B. McCusker

IUCR JOURNALS NEWS

Three-dimensional imaging of chemical phase transformations at the nanoscale with full-field transmission X-ray microscopy

J. Synchrotron Rad. (2011). 18, 773-781 (<http://doi.org/g3n>)



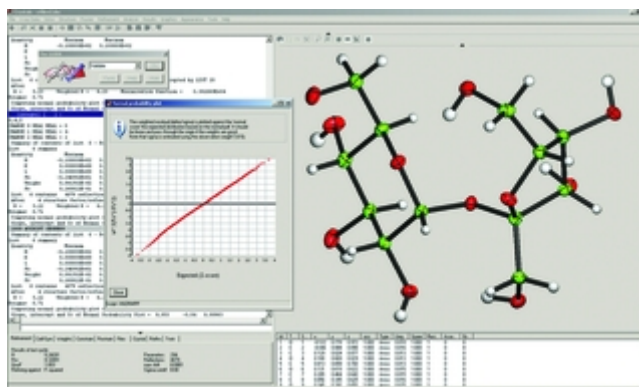
3D chemical map (~50 nm resolution) of partially discharged Li-ion NiO battery electrode showing NiO (red) and Ni (green) components; blue voxels contain both species. Tomography data collected with SSRL full-field transmission X-ray microscope at multiple energies along the Ni *K*-edge.

An X-ray imaging set-up developed at SSRL to correlate 3D morphological and chemical changes at high resolution (tens of nm) has been used to investigate battery electrodes. Using hard X-rays penetrating tens of microns, at large fields of view (30 × 30 square microns or more), this is an ideal tool for probing nanoscale phenomena in hierarchical materials such as batteries, fuel cells and catalysts. This technique can provide new perspectives on factors crucial to performance, directing design strategies for next-generation energy materials.

F. Meirer, J. Cabana, Y. Liu, A. Mehta, J. C. Andrews and P. Pianetta

NOTICE

The Future of CRYSTALS



The *CRYSTALS* program is widely used by Chemical Crystallographers involved with running analytical services, research and teaching. It has been under continuous development since the first FORTRAN versions were created by John Rollett and Bob Carruthers during the 1970's. A large number of people have contributed code or concepts for dealing with specific crystallographic problems, leading to a richness of procedures. A small number of people, in particular Paul Betteridge, Lisa Pearce and Richard Cooper have made substantial changes to the infra-structure to ensure that the program remains suitable for modern users. As well as the monolithic code in *CRYSTALS*, the program also acts as a convenient interface to programs dealing with cifs and several diffractometer data files. It also links smoothly with *checkCIF*, *PLATON*, *SIR92*, *SIR2011*, *Superflip*, *SHELXS*, *Mercury*, *Mogul*, and *MCE* (an electron density visualiser). My own role has been to generally look after the code, to respond to users requests and comments and run an e-mail help desk. Following my retirement in September 2011, I hope to continue to be involved with *CRYSTALS*.

After a period working with Oxford Diffraction, oXray and carrying out research into small-molecule docking with macromolecules at InhibOx, Richard Cooper (richard.cooper@chem.ox.ac.uk) has returned to Oxford to be my successor as head of the Chemical Crystallography Laboratory. In addition to all his other responsibilities, he plans to continue to look after *CRYSTALS*, and when time permits re-develop and extend it. Existing *CRYSTALS* users can be confident that it will be maintained into the foreseeable future, and non-users looking for a single integrated work environment might like to try the program. Oxford University has made the installation kit available to commercial and non-commercial uses without cost from our website: www.xtl.ox.ac.uk. Contact Richard for more details.

David Watkin

MEETING REPORT

IUCr Congress and General Assembly



Madrid, Spain, August 22-30, 2011

KN07 Eva Nogales

Hybrid methods: elucidating molecular mechanisms using electrons and X-rays



Eva Nogales and Michael Rossmann

Hybrid structural methodologies were illustrated with two examples concerning microtubule-kinetochore interactions and the adaptive bacterial immune system.

When eukaryotic cells divide, the genetic material has to be accurately divided among the daughter cells. This process involves the interaction of the microtubule mitotic spindle with kinetochores on special regions of the chromosomes. 3-D cryo electron microscopy (cryo-EM) of microtubules complexed with the kinetochore Ndc80 complex produced a structure at sub nanometer resolution where crystal structures of the component parts were docked. The complexes self-assemble along protofilaments suggesting a mechanism for how the kinetochore employs microtubule depolymerization for chromosome movement during cell division.

Bacteria acquire resistance to phages by integrating short fragments of foreign DNA into Clustered Regularly Interspaced Short Palindromic Repeats (CRISPRs). CRISPRs are transcribed and processed into short crRNAs. In *E. coli*, crRNAs are incorporated into a surveillance complex called Cascade. Cryo-EM analysis of Cascade before and after binding to a target nucleic acid sequence shows that the crRNA is displayed along a helical arrangement of protein subunits that protect it from degradation, while maintaining availability for base pairing. Cascade engages invading nucleic acids through base pairing along the crRNA, resulting in short helical segments that trigger a conformational change likely to serve as a signal for destruction of the invading nucleic acid.

Michael Rossmann

KN 12 Alessia Bacchi**Crystal engineering of flexible metallorganic supramolecular networks: from local to functional**

Alessia Bacchi and Guy Orpen

Alessia described the challenge of designing responsive metallo-organic materials with flexible frameworks able to create voids to accommodate small guest molecules. She discussed how to proceed from local design to the control of collective behaviour by tailoring ligands to give metallo-organic complexes with appropriate shapes. Her focus was on wheel-and-axle systems that have two bulky groups (wheels) connected by a rigid linear spacer (axle). Such species possess the structural motifs required to give host-guest properties, and reversibly take up solvent molecules on exposure to the vapour without loss of crystallinity. A number of related materials exhibiting a range of inclusion behaviour were reviewed, from stiff networks that do not include any guest to extremely dynamic materials that easily transform in the solid state to exchange guests by solid/vapour and solid/liquid processes.

Guy Orpen

KN25 Christiane Schaffitzel***E. coli* co-translational targeting complexes studied by cryo-EM**

Christiane Schaffitzel and Daniela Stock

Christiane Schaffitzel gave a beautiful presentation of her work that uses cryo electron microscopy to visualise snapshots during the translation of membrane proteins by the ribosome and their subsequent insertion into the membrane mediated by the signal recognition particle and the FtsY translocation machinery. All three components are exceptionally large and dynamic complexes that bind to each other to form a bacterial factory producing membrane proteins. Christiane and her team have worked out conditions to purify and assemble this factory and how to trap it in specific conformations amenable for 3D reconstruction. It will be exciting to keep watching this space as it will reveal more details of the movie at increasing resolution, which seems to be only a matter of patiently picking more and more particles.

Daniela Stock

Reports to be continued in Volume 20, Number 1.

SPECIAL REPORT

Crystallography in South-Eastern Europe



Part 3 (see also [Part 1](#) and [Part 2](#))

Crystallography in Moldova



Tadeusz Malinowski (1921-1996).

Crystallographic research began in the Republic of Moldova just after World War II when T. I. Malinowski and A. V. Ablov recognized the value of using physical methods in the field of coordination chemistry. After military service, Malinowski graduated from the Dept. of Physics and Math of the Pedagogical Inst. (Chisinau) and worked as a school teacher. Together with Ablov, he developed single crystal X-ray analysis of coordination compounds. Malinowski began with studies of isomerism in compounds of the MX_2A type, where $M = Co, Ni, Cd$, $X = Cl, Br$, and A are neutral ligands. He received his PhD in 1956 from the Inst. of Cryst. of the Academy of Sciences of USSR (Moscow). His supervisor, N. V. Belov, was the President of the IUCr between 1966 and 1969. Russian crystallographers helped foster crystallographic education and research in Moldova and Malinowski's young co-workers gained experience in Moscow. Weissenberg, precession and other cameras and X-ray generators were set up for experimental work. Structural electronography was begun in Moldova at the same time, by I. Diacon, who studied in Moscow with B. K. Vainshtein.



Members of LPMSSI: Marina Fonari, Paulina Bourosh, Galina Volodina, Peter Petrenko, Natalia Kostriukova, Sergei Shova, Victor Kravtsov, Yurii Simonov, and representative of Oxford Diffraction Mike Barclay.

In 1958, on the base of the Laboratory of Physical Methods of Solid State Investigation (LPMSSI) created by T. I. Malinowski, Dept. of Physics and Math of the Moldavian branch of the Academy of Sciences of the USSR was established. In 1961 the Academy of Sciences of Moldova was founded, and in 1964 the Dept. was reorganized into the Inst. of Applied Physics of the Academy of Sciences of Moldova, where T. I. Malinowski remained as the Head of the Laboratory. In the 1970s, new computers were purchased, and young scientists expanded the scope and productivity of the laboratory. In 1975, the first computer-controlled three-circle diffractometer DAR-UMB was installed, and later a four-circle RED-4 (made at the Inst. of Crystallography in Moscow) was installed together with diffractometers for XRPD. Physicists and chemists who were alumni of Moscow State U. and Moldavian State U. joined the Laboratory. The scientific activity generated dozens of PhD and Doctor habilitate theses in crystallography and crystal physics. After academician Malinowski's death in 1996 the Laboratory of Physical Methods of Solid-State Investigations, renamed after him, was led by Y. A. Simonov (1996-2010).



Two young crystallographers, Lilia Croitor and Elena Melnic, at the entrance of Institute of Applied Physics.

In the 1990s, the Laboratory participated in a number of international cooperative grant programs: INTAS, ISF, SCOPES, CRDF/MRDA. Members of the Laboratory were awarded grants from the International Science Foundation, American Crystallographic Association, Mianowski Foundation and others. International cooperation opened up a wide spectrum of research topics involving cooperation with scientific centers in Russia, Ukraine, European countries and the United States. Collaboration with Polish scientific centers established by T. Malinowski and Y. Simonov was especially important. Many Moldavian crystallographers gained access to modern X-ray diffractometers at the Inst. of Physical Chemistry of the Polish Academy of Sciences in Warsaw, the Faculty of Chem. of the Adam Mickiewicz U. in Poznan, and the Gdansk U. of Technology. In return, Polish scientists often visited Moldova to participate in conferences, to discuss joint scientific results and to plan future projects.

Moldavian crystallographers reported their results at international meetings in Europe and the USA, Schools on Supramolecular Chemistry (Ustron, Poland) and Crystallography of Supramolecular Compounds (Erice, Italy). They organized similar meetings in Moldova, including a series of International Meetings on Physical Methods in Coordination and Supramolecular Chemistry, held in Chisinau, Moldova. In 2002 the IUCr President, W. L. Duax, attended the meeting.

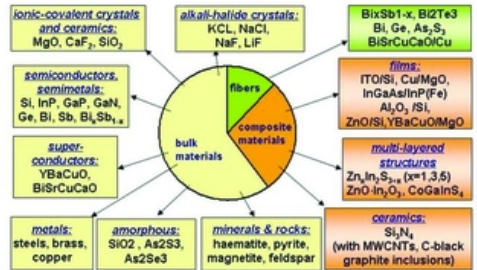
The interests of the members of the Laboratory range from simple inorganic compounds (semiconductors, oxides, ceramics), to multiple component supramolecular systems. Principal milestones are outlined here:

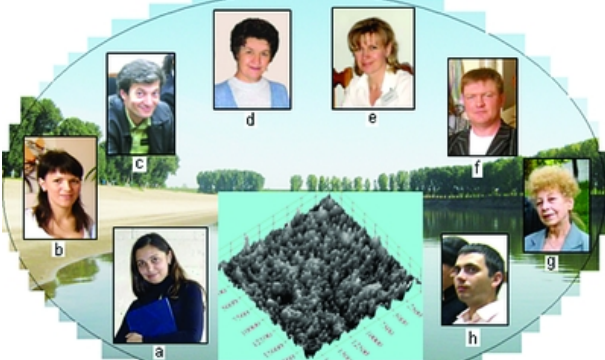
- Algorithms and software for automatic analysis of Patterson function and theoretical development of 3D cross-sections of double Patterson functions and their use;
- Single crystal diffraction of coordination compounds including carboxylates, oxycarboxylates, dioximes, amino alcohols, thiosemicarbazones, and S-alkylisothiosemicarbazides;

- Electron diffraction analysis of the biological activity and polymorphic forms of complexes of aminoacids with copper(II) and other transition metals;
- X-ray, quantum-chemical, and molecular mechanics studies of compounds with antitumor, antiviral, and psychoactive properties (thiosemicarbazones, benzotephum derivatives, benzodiazepines) to establish structure-activity correlations;
- Host-guest interactions and inclusion phenomena in supramolecular systems (macrocycles, crown ethers, cryptands, and novel fluorenone-containing catenanes). Of special interest were intramolecular and weak intermolecular interactions;
- Complexes of strontium, mercury, rare metals and lead with isomers of dicyclohexano-18-crown-6 were investigated to determine macrocycle-metal interactions. Azo and azoxy-crown ethers and calix[4]arenes and their complexes were investigated to understand complexing processes in ion-selective PVC membrane electrodes;
- Study of heterocalixarene inclusion complexes revealed that an almost perfectly closed cavity may selectively encapsulate guest molecules;
- Single-crystal and powder diffraction characterization of semiconductors, semimetals, films, twins, phase transitions, photocatalysts, and bentonite adsorbents.

Currently the LPMSSI (T. I. Malinowski) is focused on crystal engineering of multicomponent pharmaceutical compounds, metal-organic frameworks, nanoporous zeolite-like materials, nanosized polynuclear systems, cluster-based polymers and new magnetic materials. Structural investigations are conducted in cooperation with the U. of South Florida (M. Zaworotko), the Chemistry Dept. of Bucharest U. (M. Andruh), and Brown U. (B. Moulton). A single-crystal CCD Oxford Xcalibur E X-ray diffractometer installed in 2010 will foster the further development of the chemical crystallography in Moldova.

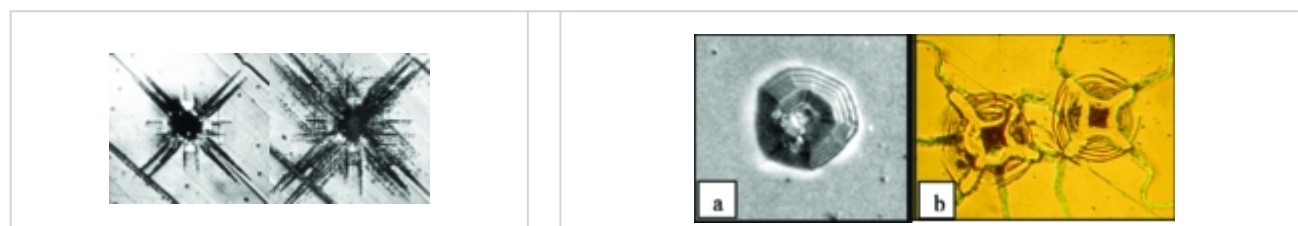






Left: Yulia S. Boyarskaya (1928-1996). Middle: Materials studied in LPM. Right: Members of LPM: Elena Chiriac (a), Zinaida Danitsa (b), Constantin Pyrtsac (c), Daria Grabco (d), Olga Shikimaka (e), Evghenii Harea (f), Raisa Jitaru (g), Adrian Prisacaru (h).

The effects of structural defects on the mechanical properties of crystals (strength, plasticity, brittleness) are investigated in the Laboratory of Mechanical Properties of Materials (LPM) of the Inst. of Applied Physics. Y. S. Boyarskaya founded the lab (in 1961) and for 35 years directed studies of bulk crystals with ionic, covalent and mixed types of bonds, of metals, crystalline and amorphous semiconductors, thin semimetals and semiconductor wires, materials for biomedical applications, coated systems, high-temperature superconductors, construction materials, minerals and rocks.



Slip lines and dislocation structures near indentations on the (001) plane of MgO crystals produced by indenter under load (left) and after unloading (right). $P = 5.0$ N.

Specific character of plastic deformation under indentation in composite materials as coatings/substrates. a - SnO_2/Si , an image on the surface of the composite structure; b - image on the Si substrate after removal of the ITO coating ($\text{In}_2\text{O}_3 \cdot \text{SnO}_2$).

The research in the LMPM has focused on deformation of materials by concentrated (local) load action (microindentation, nanoindentation). New physical phenomena characterized in the LMPM include elastic recovery of indentations after unloading, polarity of plastic deformations of materials with different chemical bonds, reverse plastic deformation, mobility of dislocations in the field of non-homogenous stresses and interstitial mechanism of plastic deformation. The influence of impurities on the mechanical properties of crystals has been studied, and the effects of X-ray and γ -irradiation on the plastic and brittle behavior of crystals have been determined.

Models of material plastic flow for ionic, ionic-covalent and covalent crystals, semiconductors, and semimetals have been proposed. The phenomenon of reversible and prolonged plastic deformation under microindentation was characterized. The dislocation-disclination-interstitial deformation mechanism was formulated and confirmed based on experimental data. A quasi-structured zone near the indentation, which contributes to mass transport during deformation, has been detected. Specific plastic deformation was detected on coating/substrate composites such as SnO_2/Si , ITO/Si , Cu/MgO . A corrugated shape is characteristic not only for the delaminated area of coating, but also for the substrate around the indentations. The Laboratory collaborates with scientific centers in Moldova, Greece, Germany, Hungary, Russia, Ukraine, Romania, Latvia and other countries.



Alexander Zamorzaev (1927-1997).

A. M. Zamorzaev (1927-1997) established a School of Geometrical Crystallography and Discrete Geometry at the State U. of Moldova. He developed the general theory of antisymmetry in his PhD thesis Generalization of Fedorov groups and is the author of theories of geometry and mathematical crystallography: multiple antisymmetry, similarity, conformal and P-symmetry, and generalizations of Shubnikov's antisymmetry and Belov's color symmetry. His students applied the theory of P-symmetry to the study of multidimensional crystallography and the discrete symmetry groups of Lobachevski and Minkowski spaces. In the last decade, generalized groups of different categories for five-seven dimensional Euclidean space have been described and new theories of 'physical' generalization of classical symmetry and geometrical generalizations of pseudoeuclidean and noneuclidean space have been explored.

Victor Ch. Kravtsov (kravtsov@phys.asm.md)

Crystallography in Bulgaria

The Beginnings

Crystallography began in Sofia U., Bulgaria, in 1893 with the establishment of the Dept. of Natural History by G. Bonchev. Bonchev, the first PhD student in crystallography in Zagreb, Croatia, taught geology, introduced a course in crystallography and published the first books on crystallography in Bulgaria in the 1890s. In 1905 he was appointed Chair of the Dept. of Mineralogy and Petrography.



New minerals found in Bulgaria: Manganilvaite, $\text{CaFe}^{2+}\text{Fe}^{3+}(\text{Mn}, \text{Fe}^{2+})(\text{Si}_2\text{O}_7)\text{O}(\text{OH})$ (approved by IMA-CNMMN 16-2002; I. Bonev *et al.*, 2005) from the Madan region, Central Rhodopes, Bulgaria.



Academician Prof. Ivan Kostov.

I. Kostov graduated from the Natural Sciences Dept. of Sofia U. 'St. Kliment Ohridski' in 1936. After studying at the Imperial College of Science and Technology in London (1940-1945), he returned to Sofia U. In 1953, as the first Head of the Dept. of Mineralogy and Crystallography, he taught crystallography, organized mineral collections, published Bulgarian, Russian and English editions of his textbooks on Mineralogy and Crystallography, and supervised doctoral studies. In 1967, Kostov was elected to Membership in the Bulgarian Academy of Sciences (BAS), where he served as Head of the Geological Institute, Head of the Sector Mineralogy and Geochemistry, and Director of the National Museum of Natural History. He was a member of the German and Russian Academies of Sciences and an Honorary member of the Bulgarian, Russian and Ukrainian Mineralogical Societies. His successor at the Dept. of Mineralogy and Crystallography V. Breskovska, conducted crystallographic activities with G. Kirov, M. Maleev and S. Petrov.



Mikhail Maleev and Kostadin Petrov discussing in front of a giant quartz crystal during the 2nd National Crystallographic Symposium.

Equipment currently available for crystallographic studies in the Geological Inst. of BAS includes a modern digital image foil Guinier camera (Huber GmbH), older Weissenberg and precession cameras, and the last functional optical (double-circle) goniometer for crystal morphology studies in the country.

The Institute of General and Inorganic Chemistry of the BAS was founded in 1960 by G. Bliznakov whose studies of the effects of impurities on the nucleation, growth and shape of crystals received international recognition. Crystallographic research was initiated in the 1960s with an electron microscope and Debye-Scherrer camera. In 1974, a DRON-1 diffractometer equipped with high- and low-temperature chambers was installed. In 2006, the Institute obtained Bruker D8 equipment, which was successfully upgraded in 2010 with a linear LynxEye detector.



(right) Associate Prof. Daniela Kovacheva with her staff and (left) the new XRD diffractometer (2008) in the Laboratory of Solid State Chemistry and XRD analysis.

Between 1982 and 1985, K. Petrov was Head of the Methodical X-Ray Diffraction Lab at the Center of Chemical Sciences, which consists of 10 institutes. His research activities were in the fields of preparative and applied inorganic solid state chemistry, structural perfection and texture of materials for electronics, superconductors, catalysts, refractory compounds, thin films, diffusion layers and galvanic coatings. He applied X-ray and neutron powder diffraction and Rietveld methods to materials identification, phase analysis and determination of crystallite sizes and microdeformations. His PhD thesis was concerned with polycrystalline inorganic catalysts, and microstructure and topotactic synthesis of materials (K. Petrov, N. Zotov and D. Kovacheva).

Crystallography in the 1980s

In the 1980s, researchers from the BAS and Sofia U. held four meetings to discuss X-ray diffraction methods. The meetings evolved into National symposia held in 1983, 1985, 1987 and 1991. These symposia were attended by over 80 scientists from 30 universities, research institutes and industrial laboratories in Bulgaria who gathered to share experiences and plan future studies. The interest in applying XRD-based methods for study of materials grew among physicists, chemists, geologists, mineralogists and soil researchers. Resulting publications concerned small angle diffraction, X-ray topography, micro-deformations of metal structures, thin layers, fiber composites, textures, and high- and low-temperature experiments.

Institute of Applied Mineralogy



The new X-ray single crystal diffractometer Supernova A (Oxford Diffraction) in the Laboratory of X-ray diffraction analysis, IAM (2010).



The new X-ray powder diffractometer D2 Phaser (Bruker AXS) in the Laboratory of X-ray diffraction analysis, IAM (2009).



The recent staff of the Laboratory of X-Ray Diffraction Analysis (IAM). From left to right: Boris Shivachev, Rositsa Petrova, Luiza Dimova, Yana Tsvetanova, Ognyan Petrov, Vladislav Kostov-Kytin.

The Institute of Applied Mineralogy of the BAS was established in 1984 for research on minerals and their applications in industry and ecology. The Institute housed an XRD laboratory with an Enraf-Nonius CAD-4 single-crystal diffractometer and two powder diffractometers, and Electron Microscopy and Crystal Growth laboratories. More than 100 structures of new crystalline materials were published under the leadership of J. Macicek who also supervised the PhD studies of O. Angelova, T. Todorov, R. Petrova and others. In 1988, the research group obtained a grant from the International Centre for Diffraction Data (ICDD) for production of PDF patterns of new crystalline phases. More than 200 new diffraction patterns were added to the ICDD (simple and double selenates, selenites, hydroselenites, adducts of inorganic salts with organic molecules, and perhenates with nicotinic and isonicotinic hydrazides). The research included synthesis and determination of structures and corundum numbers (RIRs). Computer programs were developed for calculating RIRs of powder patterns from known structures and characterization of the data according to IUCr guidelines.

Institute of Mineralogy and Crystallography

The Central Laboratory of Mineralogy and Crystallography (CLMC) of the BAS was established in March 1995 to conduct fundamental and applied investigations, provide consultation on and application of analytical methods and training of specialists in mineralogy and crystallography. At the 5th General Assembly of the BAS, the Laboratory was renamed Inst. of Mineralogy and Crystallography 'Acad. Ivan Kostov' (IMC-BAS). Today, IMC consists of well-equipped laboratories, offices and a library, it is supplied with an optical cable and Internet as well as PC for every research associate and specialist.

Achievements are presented through Annual Reports (www.clmc.bas.bg), at scientific conferences and exhibitions, in periodicals, and *via* the mass media.

The laboratories of CLMC and IAM have produced hundreds of scientific papers, conducted dozens of national and international projects, awarded PhD degrees and acquired a new scanning electron microscope (ZEISS EVO LS25), powder diffractometer (D2 Phaser Bruker AXS), single-crystal diffractometer (Oxford Supernova A with temperature control from 80 to 400 K), a micro-FTIR Spectrometer (TENSOR 37 Bruker, MIR and NIR with ATR accessories), and SETSYS Evolution TGA-DTA/DSC/MS up to 2400 K (Setaram).



Bulgarian crystallographers during the 2nd National Crystallographic Symposium.

The Bulgarian National Committee for Crystallography (BNCC) was founded in 1992 as an adhering body of the BAS. The members of the BNCC are specialists in the fields of structural crystallography, crystal chemistry, crystal physics, mineralogy and materials sciences. BNCC coordinates the activities of the Bulgarian crystallographic community and maintains relations with the IUCr and the European Crystallographic Association (ECA). Former Chairmen of BNCC were A. Apostolov (Sofia U., 1992-2000), K. Petrov (Inst. of General and Inorganic Chem., BAS, 2000-2008), and O. Petrov (Central Lab. of Min. and Cryst., BAS, 2009-2010).

The 1st Bulgarian National Crystallographic Symposium organized by the BNCC in Oct. 2009 was attended by 98 participants presenting 68 oral and poster reports. Full papers were published in the Proceedings volume 1st National Crystallographic Symposium (ISSN 1313-9991, Academic Publishing House. M. Drinov, editor; online at http://clmc.bas.bg/symp09/docs/First_Cryst_Symp.pdf).

An assembly to establish the Bulgarian Crystallographic Society (BCS) was held on February 27, 2010, at the Inst. of Min. and Cryst. of the BAS. 47 crystallographers from institutions throughout the country attended the assembly. The Bulgarian Crystallographic Society was officially registered in Bulgaria in April, 2010 with a Board of seven Managers, O. Petrov, President of the Board, and R. Nikolova, Vice-President. They planned to apply for membership of the IUCr at the XXII General Assembly and Congress in Madrid, 2011.

The 2nd Bulgarian National Crystallographic Symposium (www.bgcryst.com/symp10) was organized by the Faculty of Chemistry, Sofia U., chaired by T. Spassov and featured international speakers B. Krebs (U. of Münster, Germany), M. Aroyo (U. of the Basque Country, Spain), B. Mihailova (U. of Hamburg, Germany), and S. Ferdov (U. of Minho, Portugal). The symposium, attended by 78 participants and more than 20 students, covered crystal growth, inorganic and mineral structures, organic and organometallic compounds, nano materials, macromolecules, structure-properties relationships, defects, microstructures and textures, experimental techniques and equipment. There were round-table discussions on state-of-the-art equipment and modern laboratories in Bulgaria, and planning of further activities of the BCS. Outstanding presentations by three young scientists were awarded prizes. The symposium allowed young crystallographers to present their research, exchange ideas and participate in the open discussions.

In the last two years Bulgarian crystallographers have advanced scientifically and organizationally. The crystallographic community in Bulgaria is fully aware of achievements of scientists and specialists in

crystallography, crystal chemistry, mineralogy, and materials science and recognize that crystallography is crucial to modern materials sciences and the study of mineral systems, natural resources, biomaterials and nanomaterials. Crystallographic research contributes to technological progress and the quality of life, critically needed at times of economic crisis. The BCS hopes to foster investment of the business community in technologically advanced materials.

Ognyan Petrov (*opetrov@dir.bg*)

Crystallography in Albania

The Republic of Albania, in South-Eastern Europe, is poor by Western European standards. After 1990, resources devoted to sciences and technology were drastically decreased and approximately 40% of those with scientific training have emigrated. Expenditure for scientific Research and Development (R&D) is 0.2% of the GDP, few goods are exported and technological development is limited.



Faculty of Natural Sciences, Tirana, Albania.

In 2009 the Government initiated 'National Strategy for Science, Technology and Innovation in Albania', coordinated by a Dept. of the Prime Minister's Cabinet, and the Ministry of Education and Science with assistance from UNESCO. The goals of the plan are: to triple public spending on R&D; to create and equip four or five Albanian centers of excellence in science; to double the number of researchers through 'brain gain' incentives and training of new researchers via new doctoral programmes in Albanian universities; and to stimulate innovation in 100 companies via consortia with academic research institutes or foreign partners. The Strategy is to be implemented in synergy with the planned development of energy, agriculture, natural resources, public health services and communication technologies (ICTs).



'Mineralism Gallery' by Enkeleida Beqiraj Goga, Faculty of Geology and Mining, Dept. of Earth Sciences, Tirana, Albania (May, 2009).



Presentation of the monograph 'Cryst-Art' by Enkeleida Beqiraj Goga, Faculty of Geology and Mining, Dept. of Earth Sciences, Tirana, Albania (May, 2007).

Crystallography is taught at the U. of Tirana (UT, www.unitir.edu.al) and the Polytechnic U. of Tirana (UPT, www.upt.al), but the only crystallographic research is theoretical work in the Chemistry and Physics departments.

In Albania, Crystallography is primarily part of the Geology Faculty. A. Sinojmeri heads the Crystallography - Mineralogy and Petrography Research Group and is engaged in 'Mineralism Gallery' and 'Cryst-Art' projects, funded by Albanian Mobile Communication (AMC).

A project on zeolite effects on soil properties and fertility is financed by the Polytechnic U. of Tirana, and one on analysis of water quality in rural Albania is financed by the Academy of Sciences of Albania.

In the Chemistry Dept., E. Andoni (eduard.andoni@unitir.edu.al) conducts powder diffractometry on organometallic compounds and chalcogenide halides with layered and spinel structures.

In the Physics Dept., T. Dilo (teuta.dilo@unitir.edu.al) offers an MA programme in 'The Physical and Chemical Structure of Materials' including a module on X-ray diffraction.



Kastriot Spahiu (left) with Dritan Siliqi. The set-up of the Seifert Diffractometer at X-ray Laboratory (June 1990), Dept. of Chemistry, Fac. of Natural Sciences, Tirana, Albania.

In partnership with Inst. für Werkstoffwissenschaft, Technische U. Bergakademie Freiberg, efforts are underway to expand research in crystallography. At present there are no neutron, electron or functioning X-ray facilities in Albania. During the 1990s, the Laboratory of X-ray Diffraction sponsored by UNESCO in the Chemistry Dept. of the U. of Tirana was equipped with a Seifert X-ray powder diffractometer. Due to inadequate maintenance the measurements are not always reliable.

W. Depmeier of the Executive Committee of the European Crystallographic Association and D. Siliqi (Bari, Italy) are engaged in efforts to create a National Crystallography Association in Albania, to strengthen the scientific infrastructure in the country, foster collaborations with crystallographers outside Albania and help Albanian scientists to gain access to neutron/electron and X-ray facilities elsewhere.

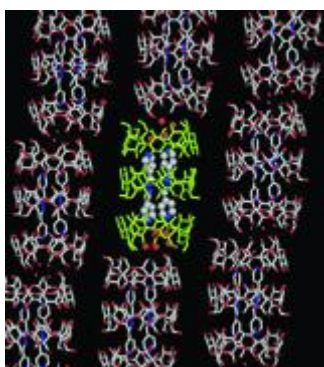
Organizations critical to the development of crystallography and science in Albania include: Albania Acad. of Science, Sheshi 'Fan Noli' 7, Tirane, Albania (G. Beqiraj and S. Bushati), Ministry of Education and Science, Rr: 'Rruga e Durrësit' 23, Tirane, Albania, (M. Tafaj, A. Gjonaj, H. Shamata), Tirana U., Sheshi 'Nënë Tereza', Tirane, Albania (D. Kule, E. Demo), Faculty of Natural Science, Bulevardi 'Dëshmorët E Kombit', Tirane, Albania (X. Teliti, E. Andoni, M. Koni, A. Mema), Polytechnic U. of Tirana, Sheshi 'Nënë Tereza' 4, Tirane, Albania (J. Kacani, F. Premti), Geology and Mining Faculty (P. Hoxha, E. B. Goga), Inst. of Geosciences (I. Milushi).

Dritan Siliqi (dritan.siliqi@ic.cnr.it)

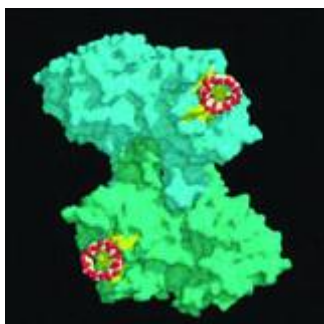
Crystallography in Greece

Molecular structure determination started in the late 60's in Greece, but crystallography related to mineralogy and powder diffraction was practiced long ago. I. Mitsopoulos was the first professor of Mineralogy and Petrology at U. of Athens in 1845 when Greece was established as a free state. A Mineralogy and Petrology Museum, established at the Natural History Society in Athens in 1835, was

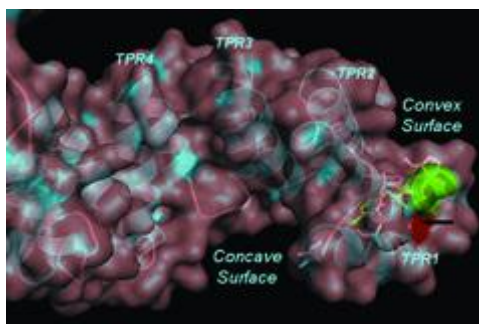
acquired by the U. in 1837. In 1940, a Mineralogy and Crystallography professorship was established (P. Kokoros) at the U. of Thessaloniki, and in 1968 P. Rentzeperis created a molecular structure determination laboratory and installed the first four-circle diffractometer in the Dept of Physics, the only one in Greece. In the late 70s, when I returned from Michigan State U. and started molecular structure studies in NCSR Demokritos, Athens, I had to collect data abroad. NCSR Demokritos acquired a single-crystal diffractometer in 1979 and the first facility for macromolecular crystallography in 1997. The same year a similar facility was established in the Foundation of Research and Technology (FORTH) in Crete. Today most universities and research institutions in Greece have groups pursuing molecular structure determination by crystallography. The European synchrotron facilities have advanced capabilities of Greece's crystallographic community. The Hellenic Crystallographic Association (HeCrA, www.hecra.gr) was established in 2001 to promote crystallography, raise scientific, public and political awareness, and train young researchers. Through HeCrA, Greece has joined IUCr and ECA. HeCrA organizes interdisciplinary conferences and workshops with international participation every two years.



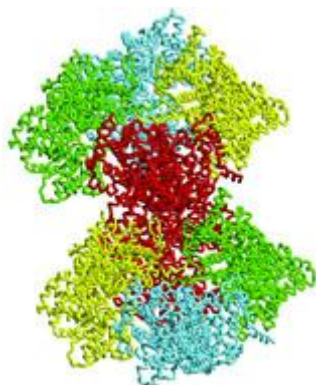
Channels of novel β CD trimers enclosing a cluster of a 4-pyridinealdazine dimer and several water molecules.



Gamma-cyclodextrin bound to the glycogen storage site of the glycogen phosphorylase *b* dimer.

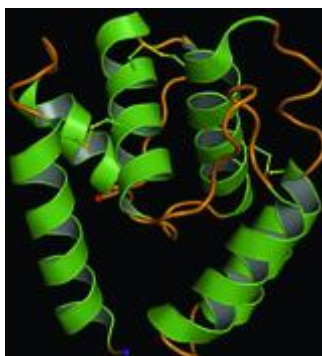


The TPR domain of Ssn6: the concave surface is responsible for the formation of the Ssn6-Tup1 transcriptional repressor.



The octamer of glycogen phosphorylase *b* in the R (active) conformation.

Crystallographic research started in NCSR Demokritos, Athens (www.demokritos.gr) in the Inst. of Materials Science, where S. E. Filippakis, A. Hountas and M. Calamiotou were studying dynamical X-ray diffraction. Presently, the team of A. Terzis, C. P. Raptopoulou and V. P. Psycharis focuses on small molecule crystallography and structure determination by the Rietveld Method. In the Inst. of Physical Chemistry, Irene M. Mavridis (Moustakali-Mavridis), although trained in macromolecular crystallography, has worked on the structures of Schiff bases with photochromic and thermochromic properties, crystal engineering aspects of guest influence on the packing of cyclodextrin inclusion complexes and chemical modifications of these cyclic carbohydrates in collaboration with K. Yannakopoulou (<http://lssc.chem.demokritos.gr/>). There was a resurgence of protein crystallography after the macromolecular data collection facility was installed in Demokritos (with participation of graduate students N. Pinotsis, P. Giastas and S. D. Chatziefthymiou). Collaborations were developed with the late N. Oikonomakos (glycogen phosphorylase *b* - cyclodextrins complexes, 2003), M. Willmans (giant muscle protein titin, 2006) and J.-M. Moulis and P. Kyritsis (structures of ferredoxins containing two 4Fe-4S clusters, 2006 and 2009). The appointment of E. Saridakis and collaboration with N. Chayen's group at Imperial College, London, has fostered the development of methodologies for macromolecular crystallization. In the Inst. of Biology (<http://bio.demokritos.gr/>), M. Vlassi is combining molecular modeling with biophysical and biochemical methods to the study of repeat containing proteins, *i.e.* the TPR-containing Ssn6 and the BRCT-containing BRCA1 to unravel the role of the structural stability of these modules as parts of multiprotein complexes. Techniques such as homology modeling, threading, molecular docking and molecular dynamics (MD) simulations are being applied to enzymes of medical importance and structure-based drug design. The group has recently developed a bioinformatics tool (program package *Gromita*, a GUI to *Gromacs 4*, [D. Sellis *et al.*, *Bioinformatics and Biology Insights*, **3**, 99, 2009]) for MD simulations of proteins and their complexes in water.

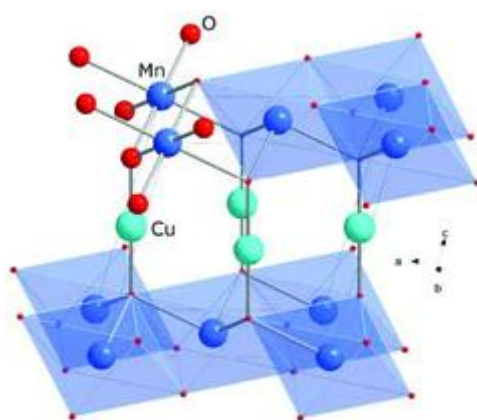


The TPR domain of Ssn6: the concave surface is responsible for the formation of the Ssn6-Tup1 transcriptional repressor.

Crystallography at the National Hellenic Research Foundation, Athens (NHRF, www.eie.gr/index-en.html) started when in 1983 the late N. G. Oikonomakos established a collaboration with L. Johnson (U. of Oxford) to study glycogen phosphorylase *b*, a target for structure-based drug design that attracted funding from pharmaceutical companies. The NHRF laboratory is equipped for protein expression,

purification, crystallization, biochemical characterization and structural studies of mechanisms of catalysis, inhibition, regulation and molecular recognition of enzymes. A third X-ray macromolecular data collection facility has been installed now and serves researchers in the group of S. E. Zographos and E. D. Chrysina, who pursue independent research at NHRF and elsewhere in Greece. Zographos investigates the mosquito's Olfactory Binding Proteins to design antimalarials, and enzymes that control glucose and nucleotide homeostasis in mammals. Chrysina works on glycogen phosphorylase isoenzymes related to type 2 diabetes and hydrolases (xylanases, feruloyl acid and other esterases) that play key roles in degradation of plant biomass and neurodegenerative disorders.

Protein crystallography at the Hellenic Pasteur Institute, Athens (www.pasteur.gr/205/2387.aspx) is focused on monoclonal antibodies to nicotinic acetylcholine receptors (nAChR). The structure of Fab192 and Fab198 against the main immunogenic region of the nACh, determined by S. Tzartos in collaboration with E. Eliopoulos, D. Leonidas and the late N. Oikonomakos, has therapeutic potential. Structural studies of extracellular domains of human muscle and neuronal nAChR subunits (P. Giastas and K. Poulas) are being combined with NMR and bioinformatics investigations of the Dept. of Pharmacy of the U. of Patras (K. Poulas and G. Spyroulias).

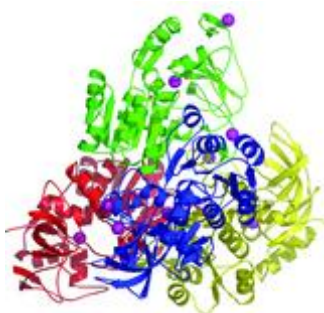


Symmetry breaking in frustrated antiferromagnets $[\text{Cu}(\text{Na})\text{MnO}_2]$ lifts the ground-state degeneracy [*Phys. Rev. Lett.*, **99**, 247211, 2007].

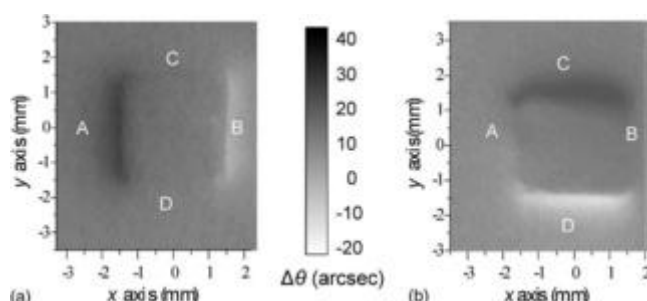
In the Solid State Physics Dept of the U. of Athens (www.phys.uoa.gr), M. Calamiotou organized the X-Ray Diffraction Laboratory which is equipped with single-crystal and powder diffractometers. Crystal defects and lattice strain in semiconductor heterostructures (GaAs/Si, LTGaAs/GaAs, AlGaIn/GaN, ZnSe/GaAs) are studied in collaboration with the MBE group of the U. Crete as well as strain effects in piezoelectric-photorefractive materials and phase separation in high- T_c superconducting materials induced by doping. Part of the research employs the ESRF synchrotron facilities for area diffractometry, high-resolution powder diffraction and powder diffraction at non-ambient conditions. At the Faculty of Biology, U. of Athens, S. Hamodrakas (<http://biophysics.biol.uoa.gr>) leads the Biophysics and Bioinformatics Laboratory and studies insect and fish chorion (eggshell), arthropod cuticle, membrane and globular protein structures, self-assembly of amyloids, prediction of protein structure, function and interactions, and development of relational protein databases.

Since 1978, D. Mentzafos of the Science Dept. at the Agricultural U. of Athens (www.aua.gr/index.php) is investigating cyclodextrin inclusion complexes with plant-growth regulators, non-hormonal weed killers and antioxidant oils as guests molecules. A. Hountas and K. Bethanis collaborate with G. Tsoucaris (CNRS, France) developing algorithms (Twin Variables and Determinants) for solving the phase problem using the Schrödinger equation in momentum space. In the Biotechnology Dept., E. Eliopoulos (www.aua.gr/tmhmata/biologia/eliop/index.htm/) develops computational methods for the analysis of protein folding and interactions, *ab initio* and homology protein modeling for medical applications (*i.e.* Mediterranean fever, rheumatoid arthritis), analysis of Fabs and restriction enzymes (with the U. of Crete) and ligand design of odorants, insect repellents and enzyme inhibitors.

In the Laboratory of Applied Physics of the U. of Thessaloniki, founded in 1968 by P. Rentzeperis (www.physics.auth.gr/en/section/index/5), D. Kavounis, G. Stergioudis, G. Voutsas and A. Mpozopoulos work on: (a) the structures and properties of inorganic (semiconductors of Tl and Sb, metal alloys of Ti, alloys of Wo, and Copper-genides and Copper-alogenides of As) organic and organometallic compounds of pharmaceutical importance; (b) the effect of composition and manufacturing conditions on industrial materials (rechargeable batteries, catalysts, plastics and thin film semiconductors); (c) electronic density in crystals; and (d) the effect of preferred orientation on diffraction from powder.

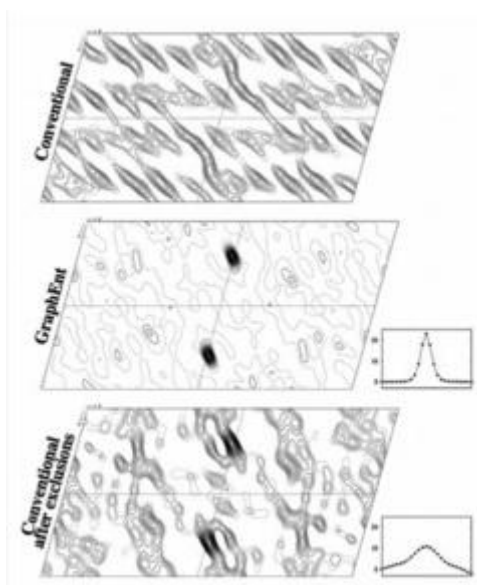


Tetramer of alcohol dehydrogenase from the antarctic psychrophile *Moraxella* TAE 123.



Light-induced distortions in Fe:LiNbO₃ studied with synchrotron area diffractometry [*JAP*, **102**, 083527, 2007].

In the late 80s, M. Kokkinidis and K. Petratos started a crystallographic laboratory in the U. of Crete and the Inst. of Molecular Biology and Biotechnology in Crete (www.imbb.forth.gr/protein_structure-function.html). Kokkinidis' laboratory elucidates structure-function relationships of proteins and protein complexes for specific biotechnology biomedical applications. Petratos is engaged in studies of: (a) the catalytic mechanism for chitinase A based on complexes with substrate analogues and inhibitors; (b) the motor ATPase component of a pre-protein Sec translocase complex; and (c) a ribosome-inactivating protein from the Mediterranean plant *Charybdis maritima*. The most recent projects involve antibiotic resistance, disulfide bond formation at the inter-membrane space of mitochondria and naturally occurring antibiotic peptides. In the Inst. of Electronic Structure and Lasers (FORTH), A. Lappas (Materials Physics Laboratory, <http://fun.iesl.forth.gr>) examines solid-state materials which display strong electronic correlations between spin, charge and lattice. They synthesize model compounds (from oxides and their nanocrystals to molecular solids) and study their electronic and magnetic behaviour. They uncover relationships between the microscopic structure and macroscopic properties that exploit novel quantum mechanical phenomena for the development of magnets, superconductors, multiferroics, electronics or photonics. In-house experimental methods (e.g. SQUID magnetometry and powder XRD) are complemented with data from large-scale neutron, synchrotron and muon facilities to advance understanding of structure-reactivity of solids at the atomic scale.



Maximum entropy versus conventional Harker sections of an anomalous Patterson function of a myoglobin crystal.

N. M. Glykos' group (www.mbg.duth.gr/~glykos/) at the Democritus U. of Thrace focuses on crystallographic computing methods including: (a) the multidimensional molecular replacement program *Queen of Spades* which led to the structure determination of a small protein using a 23-dimensional search (the highest dimensionality molecular replacement search reported to date); (b) maximum entropy methods for calculation of crystallographic maps with the program *GraphEnt*; and (c) a teaching tool illustrating the properties of the Fourier transform. The group is interfacing molecular dynamics simulations with macromolecular crystallography, using TLS groups for refinement. The group is also involved in protein structure determinations including two topology-switching mutants of ROP and the HrcQb and BcZBP proteins.

The Structural and Functional Biochemistry Laboratory (SFBL) in the U. of Thessaly in Larissa (www.bio.uth.gr/index.php?option=com_content&view=article&id=193%3Alab-bio-7&catid=52%3Areslabs&Itemid=72&lang=en) headed by D. D. Leonidas focuses on structure-based drug design with a current emphasis on type 2 diabetes, cancer, inflammation, thrombosis, glycogen metabolism, ribonucleases, deadenylases, mitochondrial steroid hormone receptors, and gene expression and homeostasis factors.

This survey of crystallography in Greece is by no means complete. V. Nastopoulos is doing crystal engineering, small-molecule and protein crystallography at the U. of Patras (www.chem.upatras.gr/index.php?lang=en), the team of A. Michailidis and S. Skoulika at the U. of Ioannina (www.uoi.gr/en/sciences3.php) studies supramolecular systems, V. Perdikarsis in the Technical U. of Crete (www.mred.tuc.gr/p013201_UK.htm) focuses on geochemistry. Moreover, many groups in the fields of mineralogy (*i.e.* Inst. of Geology and Mineral Exploration) and materials (in the academic and industrial sector) are extensively using diffraction methods in their research. New groups are being created recently by scientists who returned to Greece from abroad: I. Margiolaki at the U. of Patras, Bogos Agianian at the Democritus U. of Thrace, G. Kontopidis at the U. of Thessaly and M. Karpousas at the Agricultural U. of Athens. The crystallographic community endeavours to enhance its potential in human resources and in infrastructure via National and International collaborative research and the Hellenic Crystallographic Association's participation in ECA, IUCr and INSTRUCT activities help towards this end.

Irene M. Mavridis (mavridi@chem.demokritos.gr)

MEETING REPORT

Crystallographic Society of Japan



Osaka, Japan, December 2010

<http://crsj2010.bio.sci.osaka-u.ac.jp/index.html>

The 2010 Annual Meeting and General Assembly of CrSJ featured 231 oral and poster presentations covering all aspects of crystallography, an industrial exhibition and a special event marking the 60th anniversary of the CrSJ. Over 360 crystallographers attended.



Award winners of the 2010 Annual Meeting and President of CrSJ: Y. Kai (President), Y. Fujii, T. Tsukihara, T. Ozeki, K. Tsuda and N. Numoto.

The 60th anniversary session included two plenary lectures and a symposium. The first plenary lecture was given by T. Tsukihara (Hyogo U.) with a title of 'Structure and Function of Macromolecular Super Complexes'. The second plenary lecture was given by A. Yonath (Weizmann Inst.) with a title of 'The amazing ribosome, its tiny enemies and hints about its origin'. Prof. Yonath ended her talk with a message encouraging all young (especially woman) scientists. These two plenary lectures were open to the general public. In the symposium, leading scientists in four fields presented lectures on 'Structural change and chemical reaction by time-resolved X-ray analysis' (M. Kawano, POSTECH), 'Studies of lithium ion batteries with pulsed neutron diffraction' (T. Kouyama, KEK), 'Local structure analysis using convergent-beam electron diffraction' (T. Tsuda, Tohoku U.) and 'Atomic structure of a bacterial multi-drug efflux transporter' (S. Murakami, Tokyo Inst. Tech.).



Poster Awardees with CrSJ President: H.Narita (Osaka U.), Y. Abe (Tokyo U. Science), M. Saito(Tokyo Inst.Tech.), Y. Kai (President), M. Kataoka (Kwansei Gakuin U.), K. Hirabayashi (Osaka U.), H. Tanaka (Yonago Nat. Coll. Tech) and T. Nakamura (Osaka U.).

At the annual CrSJ Awards Ceremony, the S. Nishikawa Award was presented to T. Tsukihara (Hyogo U.), Research Awards were given to T. Ozeki (Tokyo Inst. Tech,) and K. Tsuda (Tohoku U.), the Young Crystallographer Award went to N. Numoto (Kyoto U.) and the Poster Awards went to H. Narita (Osaka U.), Y. Abe (Tokyo U.Sci.), M. Saito (Tokyo Inst. Tech.), M. Kataoka (Kwansei Gakuin U.), K.Hirabayashi (Osaka U.), H.Tanaka (Yonago Nat. Coll. Tech) and T. Nakamura (Osaka U.).

A full program of the meeting can be viewed at the CrSJ website <http://crsj2010.bio.sci.osaka-u.ac.jp/index.html>. The Local Chair was K. Fukuyama (Osaka U.) and the Program Chair A. Nakagawa (Osaka U.).

Yusuke Yamada

MEETING REPORT

The ECA Executive Committee's 'Winter Meeting' 2011



Budapest Hungary, February 2011

www.ecanews.org

ECA President, Santiago García-Granda, opened the meeting by summarising the numerous matters arising from the minutes of the ECA Executive Committee (EC) Meetings in Darmstadt 2010. The adhering body 'Chemists and Technologists of Macedonia, Division of Crystallography' joined ECA at the end of 2010. It is the 33rd National Member of the Association. Individual Members currently have three representatives on the ECA Council. By the request of the corporate affiliate members (CAM), with the agreement of the EC in Darmstadt, a CAM Councillor and deputy were elected to represent the approximately thirty CAMs of ECA. The CAMs will bring valuable expertise to the EC as they have widespread contacts with crystallographers and attend conferences throughout the World. It is also hoped that they will recruit new CAMs since the CAM Councillors have voting rights on the EC. It is important for the ECA to increase the number of individual members. Individual members can check their information and make any necessary updates on the publicly available webpage: www.ecanews.org/membership.php.



The Participants of the 'Winter Meeting'. From left to right: Alessia Bacchi (Officer, SIGs), Carl Henrik Görbitz (ECM27), Wulf Depmeier (Officer, ECA links), Andreas Roodt (Vice-President), Enrique Gutierrez-Puebla (XXII IUCr Congress, Chairman), Santiago García-Granda (President), Radomír Kužel (Treasurer), Petra Bombicz (Secretary), Luc van Meervelt (Officer, Schools), Massimo Nespolo (Education Coordinator and Webmaster), John R. Helliwell (Past-President), Elena Boldyreva (IUCr representative), and Alexander Blake (ECM28).

The activities of the Special Interest Groups (SIGs) are reviewed every year. In summary: the number of individual members registered with SIGs has increased significantly; the web form for online submission of the annual reports has been created and refined; online abstract submission will be available in 2012; and two thirds of SIG/GIGs now have web sites. A new system of networking groups has been introduced in the ECA. These are named 'General Interest Groups' (GIGs) and follow the same rules as the SIGs. The

GIG - Young Crystallographers has already started to operate enthusiastically *ad interim* since 2010. The ECA is pleased to support the activities of the younger generation of crystallographers such as their organisation of scientific meetings, sessions and exchange of information. SIG13 and GIG1 cooperated to organize a IUCr22 satellite workshop for young crystallographers in Madrid. By request, the parallel establishment of a General Interest Group for Senior Scientists is also proceeding. The GIG for 'Teaching' and others may be established in the future.

Education of future generations of crystallographers at all levels is extremely important. A collaboration of several universities (U. Henri Poincaré Nancy, Charles University Prague and U. degli Studi di Padova, with contributions from the universities of Antwerp, Liège, Pays Vasco, Aveiro, Oviedo and ESRF, Grenoble) has submitted a proposal to establish a European Graduate School of Crystallography (Masters and PhD). The ECA supported eight conferences, workshops, and schools in 2011. The ECA is preparing to commemorate the centenary of the discovery of X-rays and the Friedrich, Kipping and Max von Laue celebration. The ECA also supports the initiative of the International Year of Crystallography 2014.

Hartmut Fuess, Chair of ECM26, gave a final report on the greatly successful event that took place in Darmstadt 2010 jointly with EPDIC12. The Chairs of ECM27 (Bergen 2012) and ECM28 (Warwick 2013) presented their organisation progress. Two documents, 'How to prepare and submit a bid to host a future ECM' and 'Guidance for ECM Organisers' have been placed on ECANews.

For information on the European Crystallographic Association please visit the ECANews website: www.ecanews.org.

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