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Original article text and available illustrations

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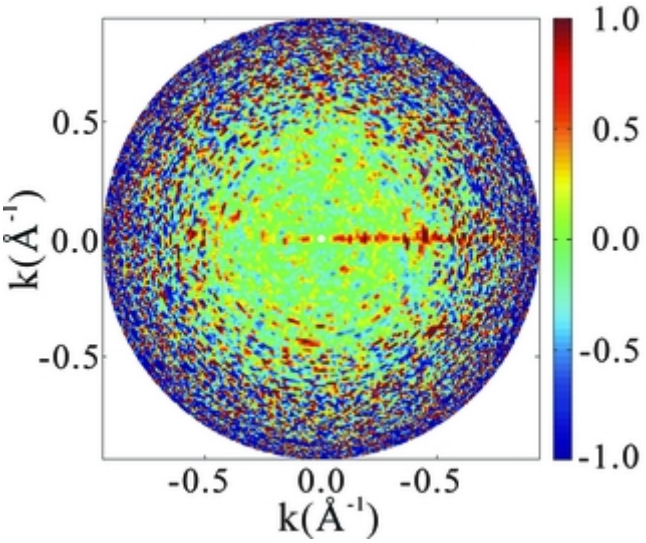
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IUCR JOURNALS NEWS

Classifying and assembling two-dimensional X-ray laser diffraction patterns of a single particle to reconstruct the three-dimensional diffraction intensity function: resolution limit due to the quantum noise

Acta Cryst. **(2012). A68, 366-381 (http://doi.org/hxm)**



Correlation function of a pair of simulated diffraction patterns for a small protein, lysozyme. When a pair is similar, a high correlation line is observed. The highest *k* value, up to which the line can be detected against noise, determines the resolution of structural determination.

New X-ray free-electron laser light sources offer the possibility of high-resolution single-particle imaging from repeated measurements of two-dimensional diffraction intensity patterns, each from a target with an unknown random orientation. An algorithm is developed to assemble these patterns into the three-dimensional diffraction intensity function. A key is the calculation of a newly defined correlation function for a pair of diffraction patterns to detect their similarity. The result indicates that, if the current laser light beam can be further focused, a subnanometer resolution structural determination may be possible.

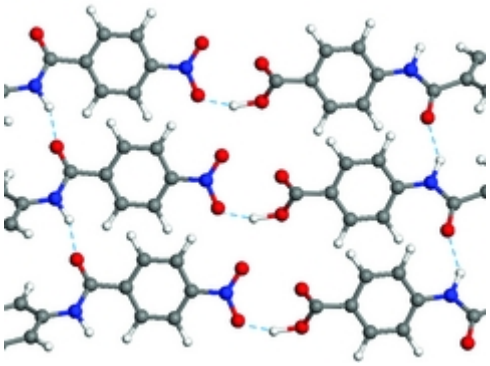
A. Tokuhisa, J. Taka, H. Kono and N. Go

IUCR JOURNALS NEWS

Ab initio crystal structure analysis and refinement approaches of oligo p-benzamides based on electron diffraction data

Ab initio crystal structure analysis and refinement approaches of oligo *p*-benzamides based on electron diffraction data

Acta Cryst. **(2012). B68, 171-181 (http://doi.org/hxn)**



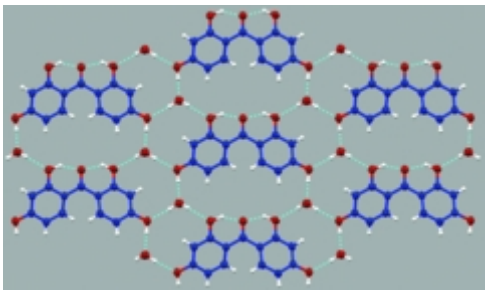
Ab initio crystal structure analysis of organic materials from electron diffraction data, collected using the automated electron diffraction tomography (ADT) technique, is presented. The structure solution and refinement route was first validated for the known crystal structure of tri-*p*-benzamide. The procedure was then applied to the structure analysis of tetra-*p*-benzamide, where an unusual hydrogen-bonding scheme was found, in perfect agreement with solid-state NMR data. The presented procedure can generally be applied for crystal structure analysis of organic nanocrystalline materials.

T. E. Gorelik, J. van de Streek, A. F. M. Kilbinger, G. Brunklaus and U. Kolb

IUCR JOURNALS NEWS

Pseudopolymorphism in hydroxybenzophenones: the dihydrate of 2,2′,4,4′-tetrahydroxybenzophenone

Acta Cryst. **(2012). C68, o156-o159 (http://doi.org/hxp)**



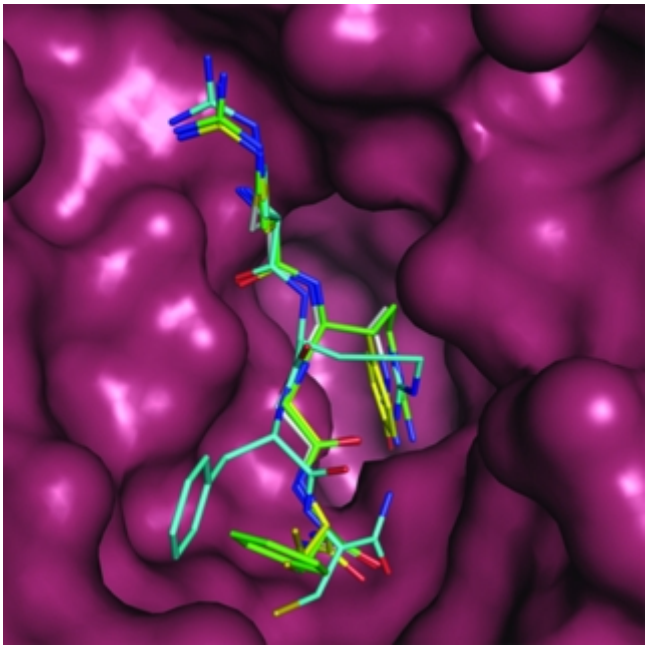
To increase our knowledge of polymorphism in molecular compounds and pharmaceuticals we have committed ourselves to studying hydroxybenzophenone derivatives. The paper describes the structure of a dihydrate pseudopolymorph of 2,2′,4,4′-tetrahydroxybenzophenone or bis(2,4-dihydroxyphenyl)methanone, which was compared with the known anhydrous and hydrated forms of other hydroxybenzophenones. The role of water in the crystal assembly was also studied.

I. M. R. Landre, F. T. Martins, J. A. Ellena, M. H. Dos Santos and A. C. Doriguetto

IUCR JOURNALS NEWS

Peptide inhibitors of botulinum neurotoxin serotype A: design, inhibition, cocrystal structures, structure–activity relationship and pharmacophore modeling

Acta Cryst. **(2012). D68, 511-520 (http://doi.org/hxq)**



Crystal structures of peptide inhibitors with BoNT/A. A close-up view of the BoNT/A active site with peptides is shown.

Botulinum neurotoxin (BoNT) is one of the most poisonous biological substances known to humans, with no drugs available on the market today for post-intoxication treatment. Efforts continue, as illustrated by Kumar *et al.*, to develop inhibitors against the BoNT protease activity that disrupts the SNARE assembly and thus the release of neurotransmitters at neuromuscular junctions. They designed and tested a number of peptide inhibitors against the toxic action. The article illustrates the key pharmacophore features using the high-resolution crystal structures of a few peptide–BoNT complexes.

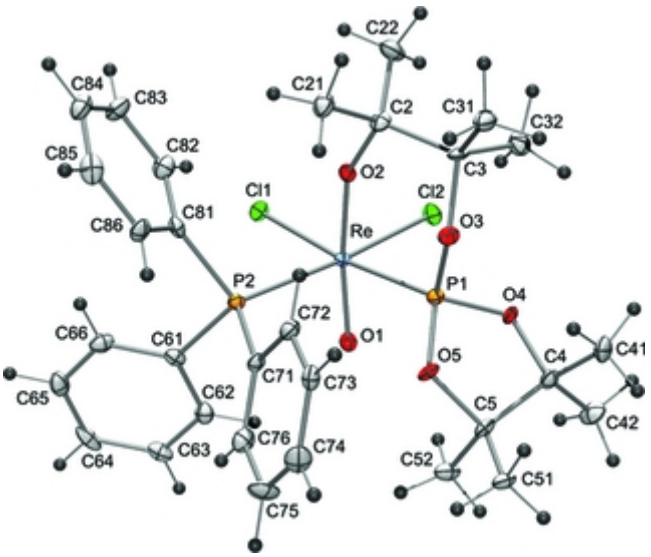
G. Kumar, D. Kumaran, S. A. Ahmed and S. Swaminathan

IUCR JOURNALS NEWS

cis-Dichlorido[2,3-dimethyl-3-(4,4,5,5-tetramethyl-1,3,2l5-dioxaphospholan-2-yloxy)butan-2-olato-κ2O,P]oxido(triphenylphosphane-κP)rhenium(V)

cis-Dichlorido[2,3-dimethyl-3-(4,4,5,5-tetramethyl-1,3,2l5-dioxaphospholan-2-yloxy)butan-2-olato-κ^2*O*,*P*]oxido(triphenylphosphane-κ*P*)rhenium(V)

Acta Cryst. **(2012). E68, m605-m606 (http://doi.org/hxr)**



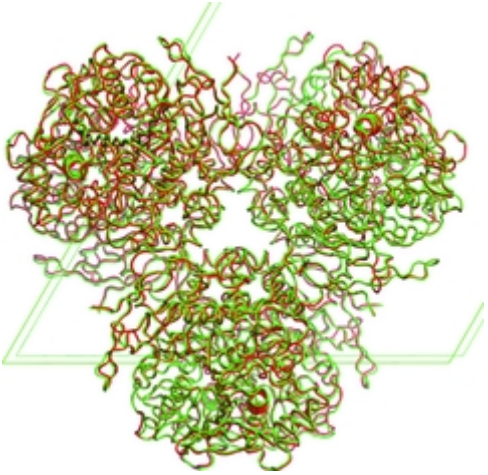
The title compound, *cis*-[Re($C_{12}H_{24}O_4P$)Cl_2O($C_{18}H_{15}P$)], was prepared from the analogous *trans* isomer by a *trans-cis* isomerization reaction. The central Re^V atom adopts a distorted octahedral coordination geometry. The crystal structure was determined as part of a larger study on coordination properties of *H*-spirophosphorane ligands, the design of transition-metal complexes and their application in catalytic reactions. Recent achievements in this area cover the use of oxorhenium complexes as co-catalysts in oxidation of aldehydes involving molecular oxygen as an oxidant and *N*-hydroxyphthalimide (NHPI) as a catalyst.

A. Skarzynska, M. Siczek and A. Gniewek

IUCR JOURNALS NEWS

Structure of recombinant human carboxylesterase 1 isolated from whole cabbage looper larvae

Acta Cryst. **(2012). F68, 269-272 (http://doi.org/hxs)**



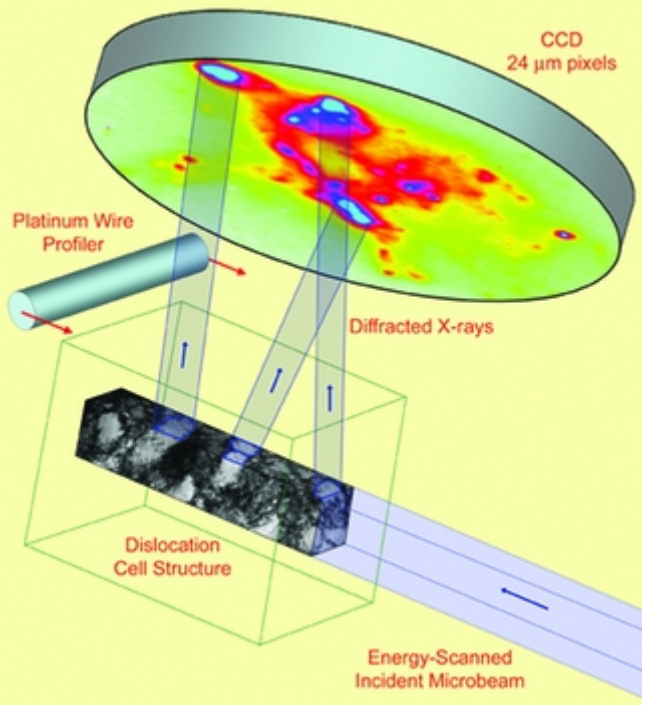
Overlay of the hexameric asymmetric unit of 2h7c (red C^{α} trace) with the hexamer of rhCES1 (green). Human carboxylesterase 1 (rhCES1) has been produced in and isolated from whole cabbage looper (*Trichoplusia ni*) larvae using an orally active baculovirus expression system. The isolated rhCES1 protein was both biochemically active and readily crystallized; its structure was determined at high (2.2 Å) resolution *via* X-ray diffraction. The structure appears to be virtually identical to that previously determined for CES1 from cultured insect cells, validating the use of the whole insect system as a source for recombinant proteins in structure determination studies and other applications.

H. M. Greenblatt, T. C. Otto, M. G. Kirkpatrick, E. Kovaleva, S. Brown, G. Buchman, D. M. Cerasoli and J. L. Sussman

IUCR JOURNALS NEWS

Validating classical line profile analyses using microbeam diffraction from individual dislocation cell walls and cell interiors

J. Appl. Cryst. **(2012). 45, 157-165 (http://doi.org/hxt)**



Synchrotron X-ray system for measuring line profiles from individual dislocation cell walls and individual dislocation cell interiors.

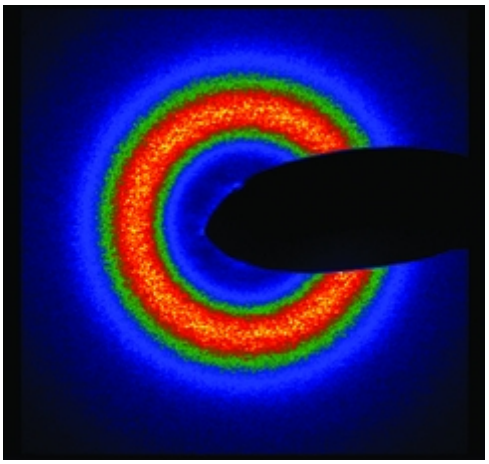
X-ray diffraction is a powerful experimental technique for quantitative analysis of materials microstructure. However, critical assumptions are often required to interpret measurements from sample volumes that significantly exceed the length scales of the microstructural features being studied. We have directly tested long-standing assumptions that are used to analyze volume-averaged X-ray line profiles from deformed metals. Three-dimensional submicrometer-resolution diffraction data were obtained from the dislocation microstructures responsible for the volume-averaged profiles. Our findings show that, without additional constraints, the traditional volume-averaged analyses can produce ambiguous results.

L. E. Levine, P. Geantil, B. C. Larson, J. Z. Tischler, M. E. Kassner and W. Liu

IUCR JOURNALS NEWS

Mapping spatial and field dependence of magnetic domain memory by soft X-ray speckle metrology

J. Synchrotron Rad. **(2012). 19, 293-306 (http://doi.org/hxv)**



In thin ferromagnetic layers, microscopic magnetic domains tend to form. Often, the average size of these domains is well known, but their morphological changes throughout the magnetization loop are unclear. This work concentrates on magnetic domain memory, the ability of the material to retrieve the same domain morphology after field cycling. The memory is here induced in a Co/Pt multilayer *via* exchange coupling with an antiferromagnetic IrMn layer. We probe the memory with coherent X-ray magnetic scattering, a unique technique exploiting the magneto-optical contrast at resonance and the coherence of X-ray synchrotron radiation. The amount of memory is quantified by cross-correlation speckle patterns. The paper shows how to map out the memory at different spatial scales, with field and temperature dependencies.

K. Chesnel, J. Nelson, B. Wilcken and S. D. Kevan

MEETING REPORT

XXII IUCr Congress and General Assembly

Madrid, Spain, August 22-30, 2011
www.iucr2011madrid.es/

Continued from Volume 20, Number 1





Keynote speaker (KN01) Tomitake Tsukihara with chair Yasushi Kai.



Keynote speaker (KN04) Peter D. Kwong with chair David Stuart.



Keynote speaker (KN25) Christiane Schaffitzel with chair Daniela Stock.



Keynote speaker (KN36) Isabelle Mirebeau with chair J. L. García Muñoz.

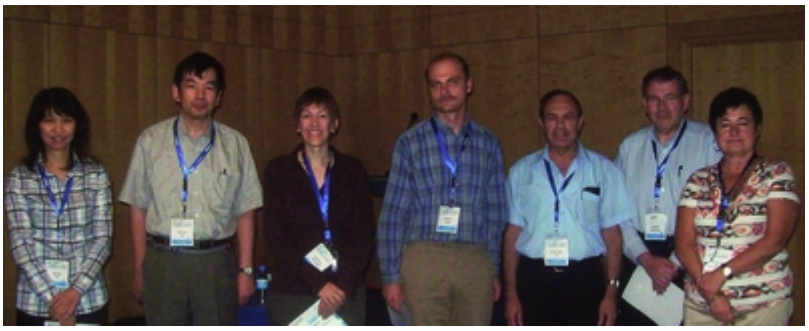
Solid-state reactions, phase transition

Solid-state reactivity (MS60)

The microsymposium highlighted the power and versatility of X-ray diffraction, at non-ambient conditions, in unraveling the interplay between structural features and chemical-physical properties during solid-state transformations. A. Fuertes (ICMAB, Spain) showed how the physical properties of perovskite oxynitrides can be modulated by tuning synthesis conditions, counter-ion nature and anion ordering. *In situ* XRPD experiments allowed K. Chapman (APS, USA) to demonstrate the feasibility of PDF analysis to investigate reactions at the atomic scale, focusing on lithium-ion batteries and catalytically active metal nanoparticles, and L. Barrio (CSIC, Spain) to investigate the behavior of copper/iron spinel catalysts in the presence of reducing gases. Finally, S. Pagola (College of William and Mary, USA) and I. A. Tumanov (Russia) introduced the audience to the world of mechanochemical synthesis: Pagola demonstrated the possibility of isolating and characterizing elusive charge-transfer salts; Tumanov described the potentiality of a home-made device for step-by-step energetic and structural studies of mechanochemical reactions undergone by organic compounds.

Chairs: Simona Galli, John Parise

Solid-state photochemistry (MS80)



MS80 speakers and chairs.

After a short introduction to the subject, P. R. Raithby (U. of Bath, UK) described studies of reversible and irreversible photoactivated reactions of transition metal complexes. He showed the reversible transformation of a metal nitro linkage isomer to the nitrite linkage isomer in a single crystal. When the temperature is raised above 200 K the metasable nitrite isomer changes to the nitro isomer. To illustrate the irreversible reaction he demonstrated how the conversion of a photochromic compound can be increased by connecting the photochromic system to Pt or Au.

M. Scholz (Max-Planck-Inst., Germany) described the real-time dynamics of solid molecular switches investigated by ultrafast pulsed X-ray radiation and discussused averaging, integration methods and intensity corrections. Y. Ozawa (Chuo U., Japan) described the changes observed in the photoexcited state of luminescent hexanuclear d^{10} complexes of Cu and Ag. J. M. Cole (U. of Cambridge, UK) talked about time-resolved photocrystallography of ruthenium sulfur-dioxide complexes and the transformation from Ru-SO_2 to the metastable Ru-OSO isomer, and claimed that the last photoisomer is not metastable at 100 K. A. Sekine (Tokyo Inst. of Tech., Japan) showed a method to control photochromic reactivity by bridging the photochromic compound to cobaloxime.

Chairs: Pilar Gomez-Sal, Menahem Kaftory

Pressure-induced phase transitions (MS40)

Experimental and theoretical investigations described in this microsymposium included solid-solid phase transitions, amorphization and melting. K. Takemura (NIMS, Japan) reported on the pressure-temperature phase diagram of the intermetallic Na-In compounds and its relation to other binary phases. W. Crichton (ESRF, France) showed how the structures of new high-pressure phases that are difficult to solve due to the limited amount of information could be determined using topological features of the known structures. E. Kudrenko (ISSP, Russia) presented amorphization of rare-earth molybdates in which the observed memory glass effect is due to the incomplete amorphization of the samples even at the highest pressures. J. Ruiz-Fuertes (U. de València, Spain) demonstrated that in contrast to the predictions from theoretical models, the Jahn-Teller effect around the Cu^{2+} ions in $CuWO_4$ is not quenched at high pressures, although it is reduced. B. Boates (LLNL, USA) presented a theoretical phase diagram of CO_2. Both the liquid and solid phases were considered and the melting curve was calculated to 150 GPa. A novel method for the calculation of liquid free energies was introduced.

Chairs: Karen Friese, V. Brazhkin

Nanotech

Powder diffraction at the nanoscale (MS18)



MS18 speakers and chairs (l to r): Yuri Andreev, Valeri Petkov, David Keen, Antonio Cervellino, Silvia Milita, Daniel Schaniel and Antonella Guagliardi.

Talks in this session covered a range of different nanosized materials and characterization methods. V. Petkov (Central Michican U., USA) presented the fundamentals of the Pair Distribution Function (PDF) and an overview of its application on gold, CdSe and other semiconductors, highlighting the importance of extracting information from diffuse scattering on high-energy diffraction patterns. D. Keen (Science and Technology Facilities Council, UK) used PDF analysis to describe the *in situ* amorphization of two technologically relevant compounds (zirconium tungstate and ZIF-4), and compared their structural changes when amorphization is pressure- and temperature-induced. A multi-scale characterization of a perylene diimide derivative film was presented by S. Milita (IMM CNR, Italy) to correlate structure and electronic performances. *Ab initio* structure solution from powder data provided the molecular organization in the bulk and grazing incidence X-ray diffraction experiments were used to obtain information on the nanoscale film structure. D. Schaniel (U. de Lorraine, France) combined small- and wide-angle neutron diffraction and Debye function analysis to identify single photo-switchable GuNP molecules embedded in a porous SiO_2 matrix, and to estimate average pore size and filling factor. Finally, treatment of a 2D paracrystallinity effect with the Debye equation was described by A. Cervellino (Paul Scherrer Inst., Switzerland) who used it to model a difficult-to-interpret peak broadening in a polymeric metal-carbonyl sample.

Chairs: Antonella Guagliardi, Yuri Andreev

Atomistic and electronic structures of nanomaterials (MS65)



MS65 speakers and chairs (l to r): Sandra van Aert, Vicky Keast, Quan Li, Cheng-Hsuan Chen, Way-Faung Pong, Marek Malac and Gianluigi Botton.

V. Keast (U. of Newcastle, Australia) discussed theoretical aspects of electron energy loss spectroscopy (EELS), including the effect of gold cluster size on the shape of its valence loss EELS. The overall shape of spectral features obtained from *ab initio* calculations for large clusters approached Mie theory. For clusters below 30 atoms the internal structure of the cluster had the strongest effect on the spectra, whereas for larger clusters the outer shape of the cluster was the most important. C. H. Chen (Nat'l

Taiwan U., Taiwan) presented results on EDX chemical mapping in a JEOL 2100 F with a probe with corrected spherical aberration. The instrument appears to have excellent stability and can produce chemical maps with atomic resolution. Chen also discussed the advantages and setbacks of EDX and EELS. S. van Aert provided a detailed account of a new method for atomic resolution (discrete) electron tomography. She uses statistical methods to 'count' atoms of a given type in projection annular dark-field scanning TEM images. Just two projections are needed to reconstruct the internal structure of a nanoparticle down to individual atoms when using prior knowledge about the particle. G. Botton (McMaster U., Canada) described many examples of EELS at very high spatial and energy resolution. His most impressive example came from the study of carbon nanotubes for which EELS spectra collected from the sides of the nanotube, where the incident beam is perpendicular to the pi* orbitals, differed significantly from the center of the nanotube where the incident beam is parallel to the pi* carbon orbitals. W. F. Pong (Tamkang U., Taiwan) discussed how analysis of the electronic properties of a nanomaterial, (Au nanocrystals in SiO_x), was used to provide insight into photoconductivity.

Marek Malac, Quan Li

Semi-conducting, energy and graphic materials

Energy-related materials (MS39)

The session covered energy-related materials including: solid oxide fuel cells, dyes and solar cells, batteries, nuclear waste, thermoelectrics, and hydrogen storage.

The first lecture was given by M. Bowden (Pacific Northwest Nat'l Lab., USA) on 'The structure and dynamics of hydrogen storage materials based on boron and nitrogen' in which he paid special attention to the structural characterisation of ammonia borane, which is especially attractive from the point of view of hydrogen storage due to its 19.6wt.% H_2.

In 'Synchrotron, X-rays and neutrons as essential tools in Li battery research: new structures and new properties', C. Masquelier (LRCS-UPJV, France) described how fine structural characterisation *in situ* provides understanding of electrochemical mechanisms at the atomic level. Specific examples dealt with lithium iron phosphate and silicate.

L. Suescun (Cryssmat Lab-DETEMA, Uruguay) described 'A new homologous series of oxygen vacancy ordered strontium manganese perovskites' relevant to solid oxide fuel cells. D. Viterbo (Dista-U. Piemonte Orientale, Italy) discussed 'Polyene-diphenylaniline D5 dyes and their role in the efficiency of DSSC solar cells'. He described the crystal structure of D5 (a polyene aniline-based dye), and a very interesting chemometric approach to study the effect of CDCA anti-aggregation studies was presented. C. Stephan (Helmholtz-Zentrum Berlin, Germany) spoke about 'Cation distribution in off-stoichiometric $CuInSe_2$ and $CuGaSe_2$', which are used as absorber layers in thin-film solar cells. Neutron powder diffraction and anomalous X-ray diffraction experiments made possible the determination of the dominant defect types which lead to enhanced understanding of the complex electronic properties of these materials.

In almost all talks, combinations of techniques (*i.e. in situ* diffraction with electrochemistry) that allow structural data acquisition in real time were employed.

Chairs: William I. F. David, M. Rosa Palacín

Graphitic materials (MS52)



MS52 speakers and chairs.

The field of graphitic materials has developed rapidly with the discovery of fullerenes in 1985 and intense research on carbon nanotubes and graphene. The discovery of fullerenes and groundbreaking experiments regarding graphene garnered Nobel prizes, in 1996 and in 2010.

The talks of the MS concerned studies of new members of the fullerenes, carbon nanotubes and graphene family using electron microscopy, X-ray diffraction and inelastic neutron scattering. S. Rols (Inst. Laue-Langevin, France) discussed the rotational and translational dynamics of fullerenes inside carbon nanotubes in terms of confinement and low-dimensionality effects. J. Meyer (U. of Vienna, Austria) reported HRTEM studies of graphene with dopants and defects. A. Parlett (UK) examined the deposition behavior of organometallic complexes with pyrene-synthesized nano-graphene on a graphene substrate. J. Hodeau (CNRS, France) demonstrated that X-ray scattering resolved tomography is a powerful tool to investigate a multi-phased carbon system obtained by pressure-crush of C60; a new carbon phase with an unexpected short inter-layer distance was found. C. Bahtz (ESRF, France) discussed catalyzed carbon nanotube growth observed with *in situ* X-ray diffraction experiments.

Chairs: Pascale Launois, Kazu Suenaga

Wide-band semiconductor and other crystals used in optoelectronics (MS28)



MS28 speakers and chairs (l to r): Krystian Roleder, Wojciech Paszkowicz, Michal Leszczyński, Ewa Talik and Hanna Dąbkowska.

The Microsymposium included five presentations covering (*a*) control of stresses and strains in GaN heteroepitaxy to achieve crack-free device-relevant GaN layers on Si (A. Krost, Germany) (*b*) a method for the determination of the densities of individual defect types in GaN layers, based on diffuse X-ray scattering and reciprocal space mapping (V. Holy, Czech Republic), (*c*) AlGaN and GaN layers grown on misoriented (off-axis) GaN substrates by metalorganic chemical vapour-phase epitaxy (MOVPE) (M. Leszczynski, Poland), (*d*) the dependencies of linear and non-linear electrooptic and photorefractive properties of $LiNbO_3$ crystals doped with Mg, Fe, Zn, or Hf (M. Fontana, France) and (*e*) laser experiments for power scaling carried out with Yb:$KLu(WO_4)_2$ in the thin-disk configuration at high pump powers that showed a significant improvement in thermal management due to the one-dimensional heat flow (M. C. Pujol, Spain).

Chairs: Ewa Talik and Krystian Roleder

Catalysis

Structural implications in catalytic processes (MS31)



MS31 speakers and chairs (l to r): Johan Martens, Claudia Weidenthaler, Jorge Rodríguez-Navarro, Nobuo Kamiya, Clara Gomes, Boguslaw Stec and Maria José Calhorda.

This session addressed the relationship between structure, dynamics and composition of catalysts and the mechanisms of a catalytic process, with emphasis on the trapping of intermediates. Materials discussed were heterogeneous catalysts (zeolites, metal oxides) and homogeneous catalysts from biological (enzymes) and chemical (nickel indenyl derivatives) systems. J. A. Martens (Katholieke U. Leuven, Belgium) discussed the effect of partial exchange of Na^{+} for Ru^{3+} in zeolite Y on cation redistribution and the performance of the resulting material for NO_x trapping from exhaust gases, and proposed a possible catalytic reduction/oxidation mechanism for NO_x scavenging. C. Weidenthaler (Max-Planck-Inst. für Kohlenforschung, Germany) addressed the optimization of iron and molybdenum oxide-based catalysts for ammonia decomposition, a relevant process for dihydrogen production, by means of a specially designed XRPD chamber, which allowed *in situ* insight into the different crystalline phases formed during the catalytic process. C. S. B. Gomes (Inst. Superior Técnico, Portugal) systematically studied the impact of the donor ability of the $X\mathrm{Ph}_3$ ligands on the indenyl ligand distortion of [(indenyl)Ni($X\mathrm{Ph}_3$)Y] (X = P, As, Sb; Y = Cl, Br, I) systems and their eventual effect on the catalytic performance on styrene oligomerisation reactions. B. Stec (Sanford-Burnham Medical Research Inst., USA) discussed the kinetic and thermodynamic difficulties of trapping intermediates in enzyme catalytic reactions and presented different methods for achieving this, by means of blocking a particular conformation using changes in temperature and pH or the addition of an excess of the reaction product. Finally, N. Kamiya (Osaka City U., Japan) described the high-resolution structure of Photosystem II that revealed the details of the $\mathrm{Mn_4CaO_5}$ catalytic active site, in which Ca and Mn belonged to the same cluster. The distortion introduced by the Ca^{2+} ion and its weak coordination to O^{2-} and H_2O appears to facilitate O—O bond formation, giving rise to a new mechanism proposal explaining O_2 evolution.

Chairs: María José Calhorda, Jorge A. Rodríguez-Navarro

Art and forensics

Powder diffraction methods in archaeometry (MS46)



MS46 speakers and chairs (l to r): Petr Bezdička, Carolina Cardell, Claire Gervais, Alicja Rafalska-Łasocha, Pauline Martinetto and Gilberto Artioli.
This session highlighted crystallographic analysis of artworks and ancient materials with powder diffraction and micro-diffraction.

C. Cardell (U. of Granada, Spain) presented a talk entitled 'X-ray diffraction methods as a complementary tool for analyses of historical objects', characterizing various samples of historical objects using different XRD techniques. Among them X-ray thermo-diffraction was found to be a powerful method for studying phase transitions in various materials. Samples originating from Alhambra were analyzed by means of micro-XRD. Finally, the benefits of combining XRD with other analytical techniques (Raman, SEM/EDS) were clearly highlighted.

P. Martinetto (CNRS-UJF, Grenoble, France) described 'Synthetic or manufactured ancient pigments studied by means of synchrotron radiation-based methods' that focused on studying ancient pigments by means of synchrotron radiation. The complex structural features of Maya Blue, an organo-clay compound based on the palygorskite-hosted indigo molecule, was described, as were analogous materials based on zeolite-hosted pigmenting molecules. She descibed chemical and structural investigations of Prussian blue using PDF analysis that demonstrated the relationship between degradation processes and crystal defects.

F. Grazzi (CNR, Sesto Fiorentino Italy), gave a talk entitled 'Quantitative characterization of Japanese ancient swords through time-of-flight neutron diffraction and energy-resolved neutron imaging' that was dedicated to the non-destructive characterization of materials used for manufacturing Japanese swords in different periods. Neutron diffraction was employed for determining the texture and the quantitative distribution of various steel phases in the blades. The data may be used to fingerprint sword-making processes in different periods and regions in ancient Japan.

C. Gervais (Smithsonian Inst., Washington DC, USA), spoke on 'Estimation of iron valences of Prussian blue pigment by anomalous X-ray diffraction'. XANES and XRD analyses led to better understanding of the processes of discoloration of the pigment. A. Rafalska-Łasocha (Jagiellonian U., Poland) presented 'XRPD studies of the objects of cultural heritage made of copper or its alloys' showing the successful application of X-ray powder diffraction and micro-diffraction to the study of copper and bronze artifacts. Several examples demonstrated the origin of the 'bronze disease' and the role of Cl^{-} ions in propagating the degradation reaction.

Chairs: Gilberto Artioli, Petr Bezdicka

X-ray absorption, diffraction and imaging in forensic science and ancient materials (MS91)



Audience view at MS91.



MS91 speakers and chairs (l to r): Francesco d'Acapito, Maria Pia Morigi, Simona Quartieri, Gilberto Artioli, Petr Bezdička, Kia Wallwork and Marek Kotrlý.
This microsymposium was organized jointly by the IUCr Commissions on Crystallography in Art and Cultural Heritage, X-ray Absorption Fine Structure and Powder Diffraction, to review developments in the application of X-ray absorption, diffraction and imaging techniques to the study of historical, archaeological, palaeontogical and forensic materials.

G. Artioli (U. of Padova, Italy) discussed archaeometrical approaches to the study of ancient materials. M. P. Morigi (U. Bologna, Italy) focused on the application of 3D computed tomography to the study of bronze and wooden statues, coffins, fossil skulls, paintings, and remains of forensic interest. She showed the potential for non-destructive investigation of unique artefacts, and medical and forensic applications.

K. Wallwork (Australian Synchrotron, Australia, 'Investigations of ancient Egyptian faience using XAS and powder diffraction') and F. d'Acapito (CNR-IOM-OGG, ESRF, France, 'Evidence of the role of Zn and Fe cations as dopants in lead antimonate yellow by XAS') described application of X-ray absorption fine structure to the study of archaeological glass.

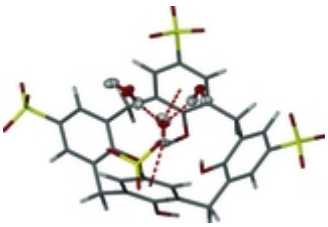
A talk on 'Powder X-ray micro-diffraction in the forensic science', given by M. Kotrlý (Inst. of Criminalistics in Prague, Czech Republic), focused on the application of X-ray micro-diffraction to forensic problems involving materials ranging from drugs and paintings, to bullets and anthropological samples.

Chairs: Simona Quartieri, J. Susini - substituted in Madrid by P. Bezdicka

Topological crystal chemistry

Topological correlations and crystal structure interconnections (MS09)

The advantage of abstracting from pure structure data to make use of a topological view for studying concrete and hypothetical classes of compounds was the main focus of this MS. The contributions showed that neglecting partially or fully information on geometry and symmetry proved to be useful for the systematic description and classification as well as for the prediction of crystal structures.



p-sulfonatocalix[4]arene with hydrogen-bonded water molecules.
M. Schröder (U. of Nottingham, UK) demonstrated in his talk on 'Modulation of structures and gas storage properties in MOF materials' how such a view can be used to study the role of topological factors in the field of metal-organic frameworks, including different forms of interpenetration and possible consequences for the networks of the exchange of extra-framework cations. Results are promising for

the design of new materials with attractive gas-storage properties, such as those with two kinds of cages (or gateways) shown in the figure.

E. Aleksandrov (Russia) reported in his talk 'Underlying nets in three-periodic coordination polymers' the principles of a classification method of coordination polymers performed automatically by the program package *TOPOS*, using topological properties of networks. The results of an exhaustive analysis of existing databases suggested the existence of restrictions to topological types for crystal structures according to the geometrical characteristics of coordination groups.

E. Gobechiya's (U. Leuven, Belgium) talk, 'The role of metal cations as template species in zeolite framework formation', discussed the possibilities of selective orientation of the crystallization reaction pathway, during or after synthesis, to a given zeolite topology.

O. Gagné (U. Manitoba, Canada) proposed in his talk, 'A new approach to crystal-structure prediction', an algorithm based on the application of bond-valence theories in association with information obtained from crystal structure databases to pick out acceptable candidate crystal structures corresponding to a given topology and chemical composition.

If it becomes possible in the long-term to define, *a priori*, ideal synthesis conditions leading to the formation of some crystal structures with a given chemical composition, it is clear that topological considerations will have a place in the solid-state chemist's tool-box.

Hans-Joachim Klein and Jean-Guillaume Eon



MEETING REPORT

Aperiodic Crystals for Beginners

IUCr Satellite Meeting, Alcala de Henarez, Spain, August 2011
http://sig3.ecanews.org/aperbeg2011

Aperiodic crystals (incommensurately modulated phases, incommensurate composite crystals and quasicrystals) are found in many different systems such as minerals, the elements at high pressures, various inorganic compounds, molecular crystals and intermetallics. Their identification is nowadays easier thanks to the steady improvement of instrumentation, modern X-ray and neutron detectors and advanced transmission electron microscopes. The knowledge of the atomic structure of aperiodic crystals is a key point for the understanding of their chemical and physical properties. However, this still remains difficult for the non-specialist. The two-day satellite meeting offered a basic and tutorial introduction to structural analysis of aperiodic crystals. The general concepts of high-dimensional crystallography were introduced step by step and applied to a few organic and inorganic materials. Lectures were given by leaders in the field of aperiodic crystals. The program of the school can be found on the website at http://sig3.ecanews.org/aperbeg2011/aperbeg2011.html#presentation.

Twenty participants, among them 6 young scientists, attended the meeting, which was very fruitful. Lectures were complemented by tutorials where participants practised some of the ideas that had been taught. The feedback from participants was very positive, the school being a very good introduction to this rather difficult field. The broad and interdisciplinary scientific background of the participants (materials science, chemistry, physics …) was a very important key to the success of the school.

The second international school on aperiodic crystals will be organized in spring 2013, following the one organized in 2010 in Carqueiranne France. This five-day school will offer a detailed introduction to this fascinating field.

Marc de Boissieu

REGIONAL NEWS

The ECA Executive Committee's 'Winter Meeting' 2012

Budapest, Hungary, February 2012
www.ecanews.org



The Participants of the 'Winter Meeting' of the Executive Committee of the ECA held in February 2012 in Budapest, Hungary. (From l to r): Front row: Massimo Nespolo (Education Coordinator and Webmaster), Elena Boldyreva (IUCr representative), Santiago García-Granda (President) and Alexander Blake (ECM28). Middle row: Karl Törnroos (ECM27), Marijana Đjaković (ECM29), Alessia Bacchi (Officer, SIGs Coordinator), Petra Bombicz (Secretary) and Wulf Depmeier (Officer, ECA links). Back row: Aleksandar Višnjevac (ECM29), John R. Helliwell (Past-President), Radomír Kužel (Treasurer), Carl Henrik Gørbitz (ECM27), Andreas Roodt (Vice-President) and Luc van Meervelt (Officer, Bursaries for Schools).
The Executive Committee (EC) of the European Crystallographic Association (ECA) met in Budapest, Hungary in February 2012. Elena Boldyreva represented the IUCr. The ECA President, Santiago García-Granda, summarized the Minutes of the ECA meetings held at Madrid 2011. The Irish Crystallographic Association, representing both the Republic of Ireland and Northern Ireland, has applied to become a National Member of the ECA; the EC will recommend approval of the application at ECM27 in Bergen. The ECA EC welcomes applications for membership from countries in Europe, Africa and the Middle East.

The number of Individual Members registered with SIGs has increased significantly in the last year. Two thirds of the SIG/GIGs have websites and one quarter have a mailing list. A new system of social and academic networking groups was introduced at ECM25. A 'Young Crystallographers' GIG1 was formed at IUCr Madrid. A Senior Crystallographers GIG2 will have their first session at ECM27 in Bergen. A 'Teaching' GIG is also being formed.

In the process of establishing a European Graduate School of Crystallography, an improved proposal for an ERASMUS MUNDUS Master Course was submitted to the European Community Offices in Brussels. The ECA will support five Conferences/Workshops/Schools in 2012. While continuing to support local initiatives, ECA intends to promote a high level European Crystallographic School (ECS) for rigorous education in crystallography such as that initiated by the Italian Crystallographic Association. The ECS

will be held annually in different European countries. The schools will have direct involvement of ECA through an *ad interim* Sub-Committee on Education (ECA-SE). Guidelines for potential applicants for these ECS are in preparation.

In Madrid Tony Savill was elected by the Corporate Affiliate Members (CAMs) of the ECA to represent them on the ECA council. Revised guidelines for ECM organizers and corporate exhibitors are now available on line (www.ecanews.org/Guidelines_ECM.php). The ECA is grateful to Tony Savill and Sandy Blake for assisting with the revisions.

The EC has begun a campaign to secure donations to aid those in need of financial assistance to attend the ECMs. These ECA Scholarships will be in addition to the existing ECA Student Bursaries for ECMs. Applicants have to have been an IM for at least 3 years to qualify to apply for an ECA Scholarship to attend an ECM; detailed rules will be made available soon.

The ECA supports the IUCr initiative of the International Year of Crystallography. The Chairs of ECM27 Bergen (2012), ECM28 Warwick (2013) and ECM29 Rovinj (2015), presented their organisations' progress. The decision on the venue of ECM30 2016 will be made in Bergen.

At ECM27 in Bergen Danial Schechtmann, Nobel Laureate in Chemistry 2011, will deliver a Plenary Lecture as part of a special microsymposium on quasicrystals funded by the Nobel Foundation, a Laue Centennial Lecture will be given by Dieter Schwarzenbach, and the Max Perutz and the Bertaut Prize Lectures will be delivered.

New Officers and Members of the EC will be elected in 2012. Nominations are welcome (www.ecanews.org/statute.php). To join the association or report any change in your membership data, go to (www.ecanews.org/membership.php). For additional information on the ECA go to www.ecanews.org.

Petra Bombicz

MEETING REPORT

High-Pressure Single-Crystal and Powder Diffraction Workshop

Poznań, Poland, April, 2011
www.crystal.vt.edu/crystal/hpworkshop.html



Participants of the 4th Frolic Goats High-Pressure Workshop in Poznań (l to r): Andrzej Katrusiak, Marek Szafrański, Witold Zieliński, Weizhao Cai, Maciej Hodorowicz, Wojciech Nitek, Barbara Wicher, Anita Owczarzak, Tomasz Manszewski, Armand Budzianowski, Jarosław Chojnacki, Reza Kia, Katarzyna Kurpiewska, David Allan, Anna Olejniczak, Marcin Podsiadło, Michał Kaźmierczak, Michalina Anioła, Ewa Patyk, Kamil Dziubek, Hanna Pawłowska, Dorota Stępień, Marcin Stachowicz, Magdalena Sikora, Artemis Kladi, Marek Daszkiewicz, Ezgi Tulukcuoglu, Michał Dobrowolski, Julia Bąkowicz, Marcin Jarek, Damian Paliwoda, Marek Tkacz, Maciej Bujak, Mirosław Szafran, Rafał Czarnecki; absent from the photo: Zofia Dega-Szafran, Andrzej Okuniewski, Michał Andrzejewski, Waldemar Nowicki, Jolanta Darul, Paweł Piszora, Małgorzata Ratajczak-Sitarz.





Two teams of high-pressure crystallographers taking part in the race on historical draisine handcars.

Over 40 participants from 7 countries attended the 4th Frolic-Goats High-Pressure Diffraction Workshop, held at the Faculty of Chemistry, Adam Mickiewicz U. in Poznań, April 17-19, 2011. The Workshop name derives from one of the city symbols, Frolic Goats ramming their horns on the city-hall tower at high noon every day; the logo of the Workshop is composed of the Frolic Goats and opposed diamond anvils of a high-pressure cell. The Frolic Goats is a low-budget event, but a very efficient one: since it was started in 2007 several groups introduced high-pressure studies in their laboratories. High pressure is increasingly more often applied in research on physical, chemical, biological, and structural and materials chemistry projects, not to mention the traditional applications of geologists and astrophysicists. The lecturers (D. Allan, M. Tkacz, M. Bujak, M. Podsiadło, A. Olejniczak, K. Kurpiewska, K. Dziubek, D. Paliwoda, W. Zielinski, M. Sikora, Cai Weizhao, A. Budzianowski and A. Katrusiak) spoke about high-pressure techniques and structural studies in laboratories and synchrotron facilities, equations of state, phase diagrams and high-pressure structures, as well as on implementation of high-pressure equipment and methods in laboratories. Afternoon laboratories were dedicated to practical exercises with the diamond-anvil cell (DAC), its assembling and loading with samples, centering the DAC on a CCD diffractometer, diffraction data collection and processing, IR spectroscopy and auxiliary high-pressure equipment. Isothermal and isochoric crystallizations were applied for growing single crystals of new phases of substances brought in by participants. The Workshop excursion included a small Railway Station Museum in Kunowo, near Poznań, and an 8 km railway stretch between Kunowo and Bieżyn. Participants experienced the effort of driving human-powered historical draisines, produced between 1920 and 1950 – only one team managed to cover the entire 8-km distance through the picturesque, but hilly (particularly on the uphill sides), landscape. The workshop was sponsored by the Faculty of Chemistry, Agilent Technologies, Bruker Poland and Olympus Poland, and was organized under auspices of Polish Foundation for Science.

Andrzej Katrusiak

MISCELLANY

What? Where? When? Who?







The IUCr website is building a library of photographs of crystallographers from around the world over the past 30 years. If you go to the website and search on a meeting and your name, chances are you will get a dozen hits of photos of you at crystallographic meetings somewhere in the world.

We are asking you to help identify the people in these photos and the crystallographic meetings they were taken at. The first person who can correctly identify the meeting sites and at least five people in each photo will receive a prize of a $50 donation to their preferred crystallographic charity (*i.e.* Student travel fund for ACA, ECA or AsCA annual meeting).

MEETING REPORT

Multi-Pole Approach to Structural Biology

Warsaw, Poland, November 2011
http://genesilico.pl/MultiPole/



The 'Multi-Poles' pose for a family photograph (photo Roman Szczepanowski).

Two-hundred and sixty scientists, most of them very young, representing macromolecular crystallography, bioinformatics and related biological and chemical disciplines, flocked from all over the world for a gathering entitled Multi-Pole Approach to Structural Biology. The conference was truly international but the idea was to bring together a core of some 40 eminent structural biologists with Polish roots to discuss the advances of the field and to promote science, science education and scientific careers in Poland. The program committee was dominated by protein crystallographers (Zbyszek Dauter, Argonne, USA; Mariusz Jaskolski, Poznan, Poland; Wladek Minor, Charlottesville, USA; and Alex Wlodawer, Frederick, USA) but it was chaired by an extremely energetic and efficient bioinformatician of the younger generation, Janusz Bujnicki (Warsaw). Under Janusz's direction, this very unique scientific meeting went absolutely flawlessly and in a truly friendly atmosphere. The scientific level of the presentations was very high; this would be no surprise in the case of the eminent scholars, but the lectures by the young scientists were of matching quality. The scientific spirits remained high throughout the entire conference: at the closing session on Saturday afternoon, the large lecture hall was almost as full as at the beginning. Lectures were followed by animated discussions despite the tightly packed program: on Friday alone, there were 27 oral presentations! This hard-work day was concluded with a banquet; the excellent food and drinks created an atmosphere for personal remarks from a pioneer of synchrotron protein crystallography (Alex Wlodawer) and even for a small recital of limericks composed for the occasion by yours truly. The conference was covered by the media and was highly advertised with policy makers and science administrators. It was held under the honorary patronage of the Polish Minister of Science and Higher Education and the US Ambassador to Poland and his counterpart in Washington, D.C. The conference was inaugurated by the President of the Polish Academy of Sciences, the Rector of the U. of Warsaw, and the Director of the Int'l Inst. of Molecular and Cell Biology, the hosting institution. One afternoon was devoted to an open panel discussion on the future of science in Poland, animated by the Foundation for Polish Science, which included top government officials responsible for science policy in Poland. It is very much hoped that the conclusions formulated during the discussion will help to reverse the regrettable negligence, often shown by policy makers in Poland, of scientific research and of its educational, technological and cultural role for the society at large. As this conference has clearly demonstrated, investing in science and education is about the best thing a progressive government can do.

Mariusz Jaskolski

MEETING REPORT

Heart of Europe bio-Crystallography

Zagan, Poland, September 2011
www.staff.amu.edu.pl/~andrzejz/hec14/



Participants of the HEC-14 Meeting (photo Milosz Ruszkowski).

Protein crystallographers from Poland, Czech Republic, Germany and Austria gathered for the 14th Heart of Europe bio-Crystallography Meeting (HEC-14) in late September 2011. The meeting venue was chosen by Mariusz Jaskolski and his co-organizers from the Polish Academy of Science and the Polish Synchrotron Radiation Society, since Johannes Kepler, the famous astronomer (1571-1630), spent the last years of his life in Zagan (Sagan). In his opening remarks, Mariusz pointed out that Johannes Kepler's book: 'De Nive Sexangula' ('On the Six-Cornered Snowflake'), published 400 years ago in 1611, foresaw concepts of modern crystallography. As a tribute to this accomplishment, and also in anticipation of the 100th anniversary of the Laue experiment, the venue was perfect for a crystallographic meeting. The meeting provided a platform for both students and experienced researchers to share recent results on a wide range of bio-crystallographic studies. At the heart of the gathering were 32 short scientific talks given by either PhD students or young postdoctoral researchers. With only slightly more than 100 participants, HEC-14 succeeded in maintaining a family atmosphere and preserving the original HEC founding idea, namely to provide ample room for experienced and less experienced students to discuss ideas and solutions to individual crystallographic problems and questions. The official HEC lecture was delivered by Zygmunt Derewenda (U. of Virginia, USA). Zygmunt pioneered the method of entropy reduction, which greatly improves the success rate for the crystallization of difficult proteins. His achievements became obvious as the meeting progressed, since quite a few speakers had used this method in their studies. The HEC prize for the best talk, which was a collection of several crystallography books generously provided by the IUCr, was awarded to Christoph Parthier (U. of Halle). Christoph showed that with protein crystallography, quite unexpected and detailed insights can be gained into the mechanism of enzymes without having to await the results from extensive enzymatic studies. The success and continuity of the HEC meetings would not be possible without the enthusiasm of all the participants and, of course, the commitment and dedication of the organizers. I therefore want to extend my thanks to Mariusz Jaskolski and his coworkers on behalf of all the attendees for this very enjoyable and highly successful meeting. We are also always grateful for the support from companies that make this annual meeting affordable and the European Crystallographic Assn (ECA) that sponsored nine one-year ECA memberships and bursaries for attendance of young crystallographers. We may not be sure where the HEC meetings will be heading over the next 400 years, but there is certainly more road ahead for the bio-crystallography community in the heart of Europe.

Yves Muller

MEETING REPORT

Croatian–Slovenian Crystallographic Meeting

Baška, Croatia, June, 2011
www.hazu.hr/kristalografi



Saša Petriček and plenary lecturer Andrej Pevec.

The 20th Croatian-Slovenian Crystallographic Meeting (CSCM20) was held in the small town of Baška, on the island of Krk, Croatia, in June 2011. The Meeting was organized by the Croatian Crystallographic Association and the Slovenian Crystallographic Society, under the auspices of the Dept. of Mathematical, Physical and Chemical Sciences of the Croatian Academy of Sciences and Arts.



Audience during a meeting session.

Five plenary lecturers and 56 oral contributions from 150 contributing authors were given. 74 participants and 13 accompanying persons came from Austria, Czech Republic, Germany, Japan, Macedonia, Montenegro, Poland, Russia, Ukraine, UK, Croatia and Slovenia. The plenary lecturers were: Mario Cetina (Zagreb), 'From self-inclusion and host-guest complexes to channel structures'; Tomislav Friščić (Cambridge), 'How to be efficient and environmentally-friendly at the same time: solid-state routes to materials and molecules'; Vaclav Holy (Prague), 'Synchrotron-related methods of investigation of nanostructures'; Andrej Pevec (Ljubljana), 'Structural studies of some organotitanium(IV) complexes'; Ana Šantić (Zagreb), 'Charge carrier transport in materials with disordered structures'. Short oral contributions dealt with biologically active molecules, proteins, organometallic compounds, pharmaceuticals, microstructure of composites and its relation to properties.



Slo-Cro team: Ivan Leban, Danica Šegedin, Janja Leban, Božena Popović, Stanko Popović and Primož Šegedin.

The meeting was financially supported by the Ministry of Science, Education and Sport of the Rep. of Croatia. Sponsors included: PLIVA, Pharmaceutical Co., Bruker, Mikro+Polo, Zagrebačka Banka, Unicredit Group, Agilent Technologies, Renacon, Panalytical, Scan, Dectris, Incoatec, Alfa, Publishing Co., Hotelibaska, Baška. The meeting was organized without a registration fee.

The members of the Organizing Committee were: Honorary Chair B. Kamenar (Zagreb,) Chairs S. Popović (Zagreb), and I. Leban (Ljubljana), members M. Bijelić, M. Cetina, M. Luić, D. Matković-Čalogović, J. Popović, Ž. Skoko, Z. Štefanić, A. Tonejc, A. Višnjevac, (Zagreb), B. Kozlevčar, N. Lah, A. Meden, (Ljubljana).



Plenary lecturer Ana Šantić, Marijana Đaković, Andrea Moguš Milanković, Krešimir Molčanov.

An excursion was organized to Jurandvor and the old town of Krk, well known for its cathedrals, castles and walls. Refreshments were provided in a bar-museum, Volsonis, showing excavations of Roman monuments. The participants visited the church of St. Lucy in Jurandvor, which was built in 1100 AD on the ruins of a Christian church from the 7th century. The church houses the mythic Baška tablet which bears the earliest known inscription in the Croatian language, in glagolitic script, also dating to 1100 AD. The word Croatian and the name of a Croatian king, Zvonimir, are mentioned in the script.



Plenary lecturer Tomislav Friščić and Nenad Judaš



Plenary lecturers Tomislav Friščić and Mario Cetina

The meeting closed with the Band Zvonimir and the Folklore ensemble Šoto, Jurandvor, performing Croatian dances and songs typical for the island of Krk.

The 21st Meeting will be held next year in Slovenia. Details are available at www.hazu.hr/kristalografi.

Stanko Popović and Ivan Leban

MISCELLANY

Inorganic Crystallography

Taken from *C and E News*, Sept 26, 2011

The journal *Inorganic Chemistry* published by the American Chemical Society recently celebrated its 50th year of publication. An article in *Chemical and Engineering News* (**89** (39), 33-35, 2012) reviewing highlights from the past 50 years included extensive coverage of comments by James Ibers who was an associate editor of the journal in the 1960s. Ibers stated that the greatest impact on inorganic chemistry over the course of the journal's history has been in chemical structure determination. He noted that the first issue in 1962 had 38 papers, none of which presented X-ray crystal structures, although a few had powder diffraction data. In the August 15 2011 issue there were 64 papers reporting 44 crystal structures, clearly illustrating the evolution of techniques and concurrent software development for single-crystal X-rays studies of inorganic molecules. Ibers himself is one of the most prolific autors in *Inorganic Chemistry*, with 245 papers to his credit. His first paper was published in 1964 when he was at Brookhaven National Laboratory. It centered on the crystal structure of sodium perxenate octahydrate, $Na_4XeO_6.8H_2O$ (*Inorg. Chem.* 1964, **3**, 1412).

NOTICE

CCDC now accepts structure factors

www.ccdc.cam.ac.uk/

The Cambridge Crystallographic Data Centre (CCDC) is pleased to announce that structure factors are now being accepted with CIFs for deposition to the Cambridge Structural Database (CSD).

Colin Groom, Executive Director, commented that 'The CCDC supports the IUCr in highlighting the importance of retaining and validating experimental data. We strongly recommend that all journals publishing crystal structures should encourage their authors to provide these data in electronic CIF format.'

'The deposition of structure factors to the CSD is extremely welcome and will greatly facilitate the work of reviewers', said Sylvain Bernès, co-editor Acta Cryst. Section E. 'Archived structure factors also promise to be a rich source of data for research related to statistical bias in X-ray structures and in detection of systematic errors in data collections'.

CIFs and structure factors can now be deposited with the CCDC *via* our web-based deposition form at www.ccdc.cam.ac.uk/services/structure_deposit.

Further information on publication standards can be found on the IUCr website www.iucr.org/index.html/leading-article/2011/2011-06-02.

AWARDS AND PRIZES

Max Perutz Prize Awarded to Fuess



The sixth Max Perutz Prize of the European Crystallographic Assn goes to Hartmut Fuess from the Dept. of Materials Science at the U. of Technology in Darmstadt, Germany.

Hartmut Fuess is recognized for his outstanding contributions to structure research of functional materials such as zeolites, fuel cells and magnetic materials, the construction of scientific instruments at large-scale synchrotron and neutron facilities, and the skilled and enthusiastic service to crystallography in Europe and the broader international community.