INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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Contents

> Extraction incomplete: missing article positions 1, 14.

IUCr journals news

The development of Laue techniques for single-pulse diffraction of chemical complexes: time-resolved Laue diffraction on a binuclear rhodium metal-organic complex 3

Structure analysis of titanate nanorods by automated electron diffraction tomography 4

The pentacoordinated [Cr(CO)5]2- dianion in [2,2,2-crypt-K]2[Cr(CO)5] ethylenediamine monosolvate 5

Using the conformation-dependent geometry paradigm improves atomic resolution refinements 6

Bis(8-methyl-2,8-dicarba-closo-dodecaboran-2-yl) triselenide 7

In silico identification and crystal structure validation of caspase-3 inhibitors without a P1 aspartic acid moiety 8

Mitigation of errors in pair distribution function analysis of nanoparticles 9

Hard X-ray Fourier transform holography from an array of oriented referenced objects 10

Special report

Crystallography in South-Eastern Europe 11

Meeting report

So long IUCr2011... 31

IUCr activities

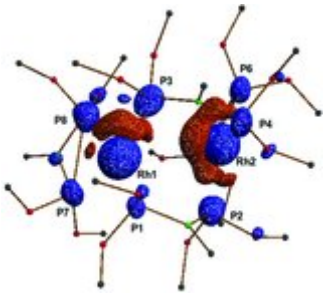
2011-2013 Executive Committee 33

IYCr 2013 logo design competition 34

IUCR JOURNALS NEWS

The development of Laue techniques for single-pulse diffraction of chemical complexes: time-resolved Laue diffraction on a binuclear rhodium metal-organic complex

Acta Cryst. **(2011). A67, 19–326 (dx.doi.org/10.1107/S0108767311011883)**



Photodifference maps showing instantaneous changes on excitation with isosurfaces of ±0.25 e$Å^{-3}$ (red positive, blue negative).

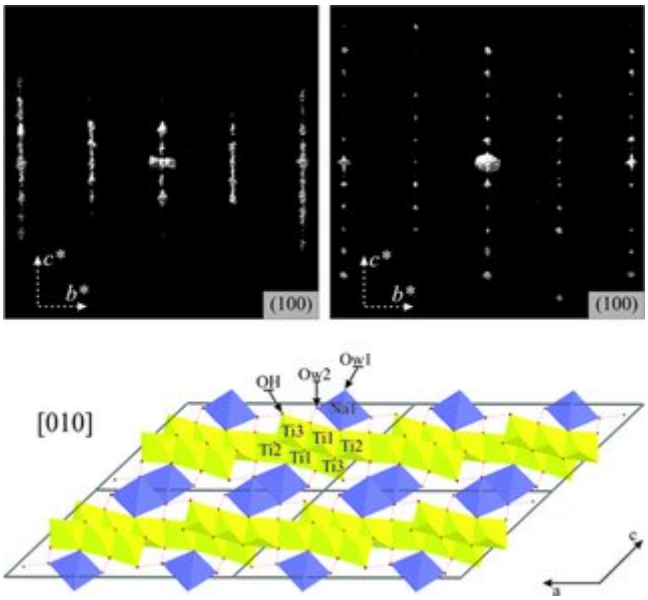
Laser-pump/X-ray probe experiments at synchrotron sources can reveal the structure of very short-lived chemical complexes at atomic resolution. It is crucial in such experiments to maximize both the time resolution and the accuracy of the results. The former requires single-pulse diffraction which can be achieved with the polychromatic Laue technique, the latter requires detailed modification of existing Laue procedures, which are described in the article together with results of their application at APS beamline ID-14 and comparison of the results with theoretical predictions.

A. Makal, E. Trzop, J. Sokolow, J. Kalinowski, J. Benedict and P. Coppens

IUCR JOURNALS NEWS

Structure analysis of titanate nanorods by automated electron diffraction tomography

Acta Cryst. (2011). B67, 218–225 (doi.org/10.1107/S0108768111014534)



Projection of three-dimensional reconstructed reciprocal space from ADT data taken from two single nanorods. The reciprocal space is oriented along (100). Top left: strongly disordered rod, top right: almost ordered rod. Bottom: final model of sodium titanate $NaTi_3O_6(OH)$

- $2H_2O$ structure, obtained *ab initio* from the upper-right reconstruction.

A newly developed electron diffraction technique was used to solve *ab initio* an intermediate species in the synthesis of TiO_2 nanorods used for dye-sensitized solar cells. Automated diffraction tomography (ADT) allows scanning and 3D reconstruction of the reciprocal space from a single non-oriented nanocrystal. This new approach delivers intensity data sets with enhanced quantity and quality suitable for *ab initio* structure solution and in addition visualizes crystallographic specialties such as diffraction streaks caused by layer shifts. HRTEM analysis revealed more detailed understanding of the defects.

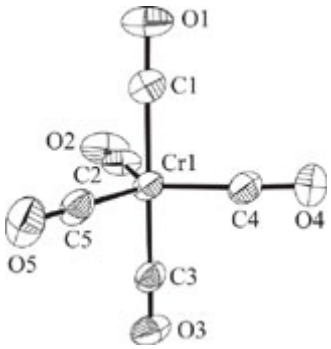
I. Andrusenko, E. Mugnaioli, T. E. Gorelik, D. Koll, M. Panthöfer, W. Tremel and U. Kolb

IUCR JOURNALS NEWS

The pentacoordinated [Cr(CO)5]2- dianion in [2,2,2-crypt-K]2[Cr(CO)5] ethylenediamine monosolvate

The pentacoordinated $[Cr(CO)_5]^{2-}$ dianion in [2,2,2-crypt-K]$_2$[Cr(CO)$_5$] ethylenediamine monosolvate

Acta Cryst. **(2011). C67, m202–m204 (doi.org/10.1107/S0108270111018233)**



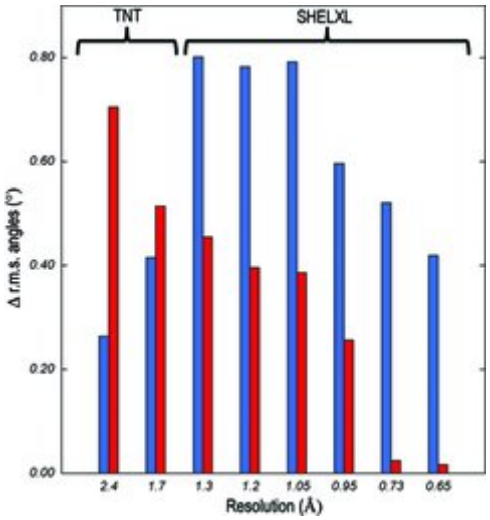
The first penta-coordinated chromium–carbonyl compound [2,2,2-crypt-K]$_2$[Cr(CO)$_5$]•$NH_2CH_2CH_2NH_2$ was obtained from the reaction of $K_3Cd_2Sb_2$ and $Cr(CO)_6$ in ethylenediamine in the presence of 2,2,2-cryptand. The central Cr atom is coordinated by five carbonyl ligands in a distorted trigonal bipyramidal geometry. In contrast to the case of the reported hexacoordinated $[Cr_2(CO)_{10}]^{2-}$ dianion, the pentacoordinated $[Cr(CO)_5]^{2-}$ dianion has a longer apical Cr–C bond length than the equatorial ones as a consequence of less electron back donation to the axial carbonyl ligands.

J. Zhai and L. Xu

IUCR JOURNALS NEWS

Using the conformation-dependent geometry paradigm improves atomic resolution refinements

Acta Cryst. (2011). D67, 699–706 (doi.org/10.1107/S090744491102292X)



Improved refinement behavior using the CDL. For a test case at each resolution, the bars show the decrease in r.m.s.d. for the main-chain bond angles resulting from the refinement against the CDL as opposed to the single-value Engh & Huber restraint library. Blue bars show the improvement in assessed quality. Red bars show the real improvement.

A script has been created to allow protein refinements with SHELXL to use a conformation (φ/ψ) dependent library (CDL) of restraints. Tests at resolutions between 1.4 and 0.8 Å showed that models created using the CDL restraints had much improved geometry. For resolutions better than 0.8 Å, use of the CDL made little difference to the models, but their assessed quality was much improved. Results indicate the CDL improves refinement behavior at all resolutions. The script can be accessed at http://pgd.science.oregonstate.edu/cdl_shelxl.

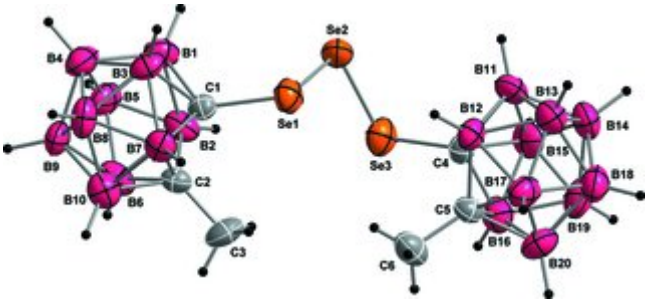
D. E. Tronrud and P. A. Karplus

IUCR JOURNALS NEWS

Bis(8-methyl-2,8-dicarba-closo-dodecaboran-2-yl) triselenide

Bis(8-methyl-2,8-dicarba-*closo*-dodecaboran-2-yl) triselenide

Acta Cryst. (2011). E67, o1908 (doi.org/10.1107/S1600536811025712)



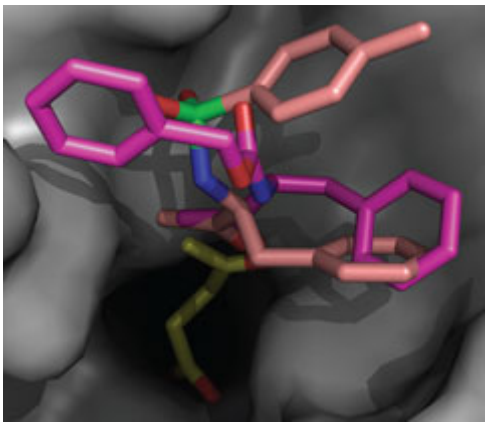
The structure of the title compound is reported, the first (to our knowledge) dicarboranetriselenide described so far. Two *closo*-C_2B_{10} icosahedra are linked by a chain of three selenium atoms: the Se–Se bond lengths suggest that they can be regarded as single covalent bonds. The geometry around the central Se atom is V-shaped, with an Se–Se–Se angle of 105.60 (4)°, and the C–Se–Se–Se torsion angles indicate a strongly twisted conformation for the linking triselenide grouping.

A. Ilie, A. Soran, A. Laguna and C. Silvestru

IUCR JOURNALS NEWS

In silico identification and crystal structure validation of caspase-3 inhibitors without a P1 aspartic acid moiety

Acta Cryst. (2011). F67, 842–850 (doi.org/10.1107/S1744309111018604)



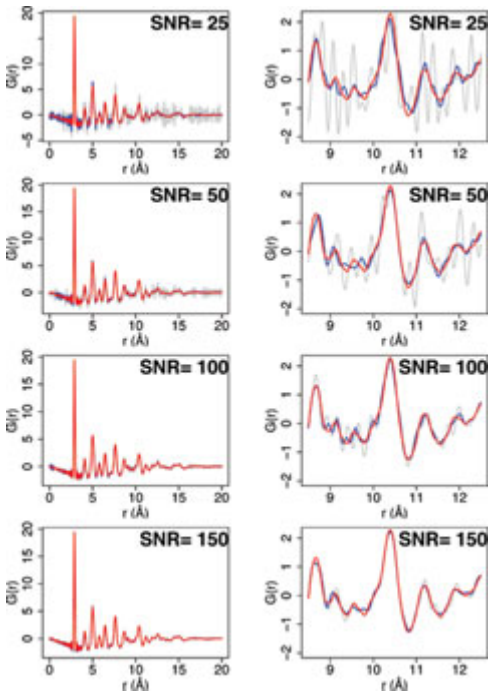
High-resolution crystal structures in combination with fragment-based docking procedures are powerful tools for the identification of novel inhibitors. By using the fragment-based docking suite *DAIM–SEED–FFLD* several novel caspase-3 directed inhibitors were identified. Interestingly many of those inhibitors are lacking an aspartic acid. Although aspartic acid diminishes cell penetration, it is almost ubiquitously present in caspase inhibitors because caspases possess a stringent requirement for this amino acid. The complex structures reveal that several inhibitors utilize interactions in the prime part of the substrate-binding site.

R. Ganesan, S. Jelakovic, P. R. E. Mittl, A. Caflisch and M. G. Grütter

IUCR JOURNALS NEWS

Mitigation of errors in pair distribution function analysis of nanoparticles

J. Appl. Cryst. (2011). 44, 788–797 (doi.org/10.1107/S0021889811014749)



PDFs (grey) generated using total scattering data representing counting statistics noise, with the signal-to-noise ratio indicated in the upper right corner of each plot. Smoothing the total scattering data results in approximations (blue) to the PDF (red) obtained from noise-free scattering data. The right plots represent selected ranges from the left plots.

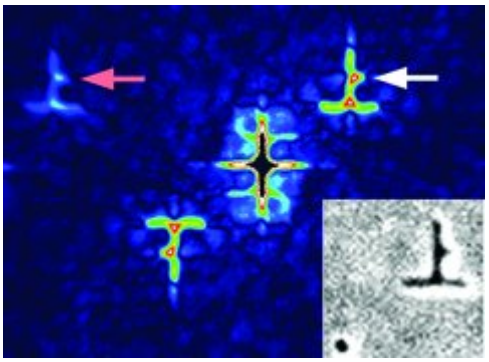
This paper discusses procedures for minimizing systematic errors in atomic pair distribution function (PDF) calculations for nanoparticles. The use of a Fourier-transformed small-angle scattering data set to model a baseline in the PDF calculated from wide-angle scattering data is shown to be a promising means of eliminating errors due to use of analytical baseline functions. It is also shown that smoothing noise due to counting statistics in reciprocal-space data can improve the precision of parameter estimates obtained from PDF analysis thus facilitating selection of the correct structural model.

K. Mullen and I. Levin

IUCR JOURNALS NEWS

Hard X-ray Fourier transform holography from an array of oriented referenced objects

J. Synchrotron Rad. (2011). 18, 564–568 (doi.org/10.1107/S0909049511009836)



Scanning ion microscope image of the test pattern (lower right, a Chinese character meaning 'up') and multiple images restored from a hard X-ray hologram.

The use of multiple, oriented and singly referenced objects was evaluated as a means to overcome the low scattering cross section inherent in hard X-ray Fourier transform holography. The nanofabricated test pattern consisted of identical characters, each with a reference dot, arranged in a 5 × 5 matrix. The image of each object was restored as in the conventional single-object case. This technique can be considered as a means to image biological macromolecules or their assemblies, which diffract weakly but of which identical copies are available.

H. Iwamoto and N. Yagi

SPECIAL REPORT

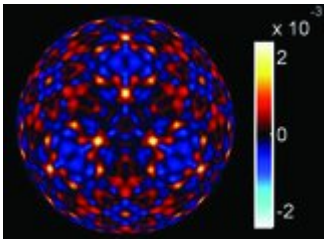
Crystallography in South-Eastern Europe

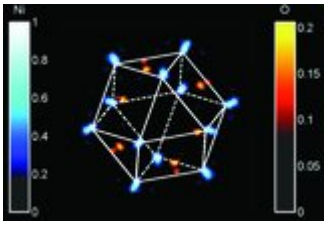


Part 2 **(see also Part 1 and Part 3)**

Crystallography in Hungary

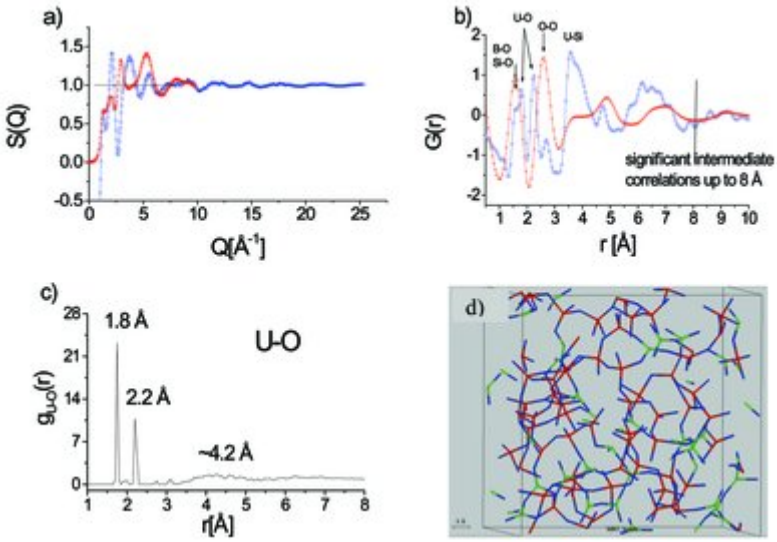
Crystallography Research





Left: X-ray hologram of NiO taken at 17.9 keV, and right: reconstructed atomic positions in 3D (bottom). (Tegze M., Faigel G., Marchesini S., Belakhovsky M., Ulrich O. *Nature*, **407**, 38, 2000.)

The Hungarian Academy of Sciences has many Research Institutes where crystallographic research is performed. The X-ray Laboratory of the Research Inst. for Solid State Physics and Optics (RISSPO) of the Hungarian Academy of Sciences (HAS) (www.szfki.hu) is led by G. Faigel (gf@szfki.hu). Six investigators in the group study phase retrieval methods, X-ray holography and single molecule imaging using powder and single crystal diffraction from liquid nitrogen temperature to 600 K. Significant recent results include structure determination of new fullerene compounds such as alkali-C60, cuban-C60 and C70 (G. Bortel, G. Oszlányi), atomic resolution X-ray holography (G. Faigel, M. Tegze), the introduction of the 'charge flipping' phase retrieval method (G. Oszlányi, A. Sütő) and the modeling of the Coulomb explosion of single molecules in a hard XFEL pulse (G. Faigel, Z. Jurek).

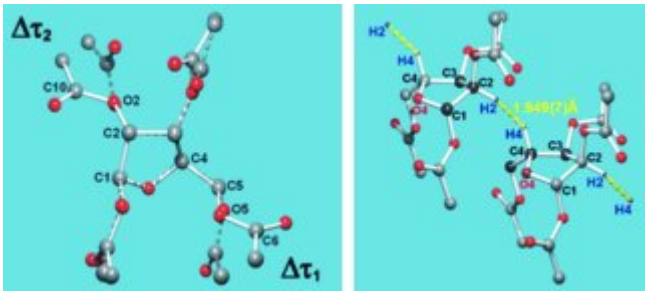


Uranium-containing multicomponent borosilicate waste glass: 30wt%($55SiO_2.10B_2O3.25Na_2O.5BaO.5ZrO_2$)+30wt%$UO_3$ measured by neutron (red cross) and hard X-ray diffraction (blue circle): a) Structure factor, b) Total distribution function, c) U-O partial correlation function, d) Si-B-O (red-green-blue) network structure. (Fábián M., Proffen Th., Ruett U., Veress E., Sváb E. *J. Phys.: Condens. Matter* **22**, 404206 (8pp), 2010).

The Neutron Diffraction Laboratory at the 10 MW Budapest research reactor of RISSPO in the Budapest Neutron Centre (www.bnc.hu) has eight researchers under the supervision of E. Sváb (svab@szfki.hu) and L. Pusztai (lpusztai@szfki.hu). Powder diffraction and reverse Monte Carlo computer simulation techniques are applied and developed for modeling disordered systems, such as alkali-borosilicate, chalcogenide, metallic glasses, molecular liquids, electrolyte solutions, and crystalline mixed oxides, and for internal stress investigations of bulk polycrystalline materials.

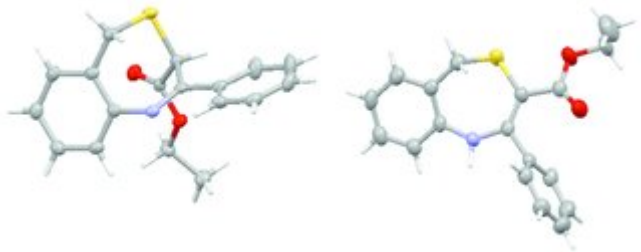
In 1928 Z. Gyulai and D. Hartly designed the first experiments to detect crystal imperfections. Gyulai observed that the tensile strength of NaCl whiskers depends on their diameters and can be nearly as high as that theoretically calculated for perfect crystals. He and I. Tarján grew synthetic quartz crystals in the early fifties. I. Tarján arranged for Hungary to join the IUCr in 1963 and was a co-author of the *Laboratory Manual on Crystal Growth* (1972). A pamphlet *An Introduction to Crystal Physics* was written by E. Hartmann (1984, 1998) for the Teaching Commission of IUCr. Currently, L. Kovács (lkovacs@szfki.hu) supervises sixteen researchers dealing with the growth and characterization of nonlinear optical crystals within the RISSPO.

Single crystal X-ray diffraction research was introduced in Szeged by I. Náray-Szabó (a student of L. Bragg, 1928-1930) in 1930. Together with K. Sasvári he solved several structures (e.g. cryolite) and with a generalization of crystal isomorphism he defined the descriptors of the 'sister structures' in 1943. In 1948 young physicists under the guidance of Sasvári started to work on various applications of X-ray diffraction at the Eötvös Loránd U. Since 1958 an X-ray laboratory (chaired by Náray-Szabó) in the Central Research Inst. of Chemistry, HAS, has studied inorganic and organic crystals, organosulfur compounds (spirosulfuranes), organo-silicon compounds (silatranes), clathrates, inclusion compounds and compounds of biological importance.



Polymorphism - intermolecular interactions - crystal architecture. The disappeared crystal form of 1,2,3,5-tetra-O-acetyl-β-D-ribofuranose reappeared in Budapest (solid line) of the conformational dimorphs. The structure contains the shortest H&ctdots;H intermolecular interaction ever found in organic crystal structures till today. (Bombicz P., Czugler M., Tellgren R., Kálmán A., *Angewandte Chemie, Int. Ed.* **17**, 1957, 2003.)

Beginning in the eighties, the study of polymorphic isostructurality and supramolecular chemistry became the focus of interest while the Dept. of X-ray diffraction was directed by A. Kálmán for thirty years. The reorganised X-ray diffraction laboratory in the Inst. of Structural Chemistry, Chemical Research Center, HAS (www.chemres.hu) is now under the supervision of M. Czugler (mcz@chemres.hu). The five members of the Laboratory (A. Kálmán, L. Párkányi, P. Bombicz, V. Hegedűs-Kudar and T. Holczbauer) are interested in crystal engineering, supramolecular chemistry, solid state reactions, and low resolution structures of 10-700 μ size crystals of organic, metal-organic, inorganic and protein structures, soft anionic system design and non-standard crystallization techniques with national and international collaborations. In the Laboratory for Powder Diffraction in the Inst. of Nanochemistry and Catalysis at HAS I. Sajó (sajo@chemres.hu) pursues structural research and phase analysis.



CH ↔ NH. An example for annular desmotropy of three pairs of seven-membered heterocycles confirmed by X-ray crystallography. Desmotropy (tautomerism in solid state) is uniquely demonstrated by three pairs of 4,1-benzodiazepines. The desmotropes are visibly distinguished by the puckering of the hetero-rings governed by the flopping (CH↔NH) hydrogen atoms. Holczbauer T., Fábián L., Csomós P., Fodor L., Kálmán A., *CrystEngComm* **12**, 1712, 2010.

The Laboratory for Single Crystal X-ray Diffractometry established in 1995 at the U. of Debrecen, Inst. of Chemistry. (puma.unideb.hu/~xray) is directed by A. Bényei (abenyei@delfin.unideb.hu). His main research concerns organometallics, guanidine salts of water soluble phosphanes and their transition metal complexes, and polymorphism of pharmaceutical compounds. A recent discovery of racemic conglomerates stimulated research into techniques to achieve spontaneous resolution of these enantiomers. Application of Continuous Symmetry Measures in the comparison of hydrogen bonds represents a new direction of supramolecular research in Debrecen. In the field of macromolecular crystallography, T. Barna (Dept of Genetics and Molecular Biology) has been studying reductases and their complexes with environmentally important substrates, antifungal (PAF, NMR structure in the PDB: 2KCN) and human proteins. Powder diffraction and nanolayer studies are performed by M. Kis-Varga in the Inst. of Nuclear Research of HAS and routine powder diffraction measurement is done at the TEVA Pharmaceutical Works Ltd, Debrecen. Several graduate and undergraduate students including G. Paragh, Z. T. Nagy, C. Fekete and R. Elek are engaged in crystallographic studies.

In the Liquid Structure Laboratory at HAS (www.chemres.hu) T. Megyes, I. Bakó and S. Bálint study liquid structures by experimental (X-ray and neutron diffraction), molecular dynamic simulation and *ab initio* methods. The focus of their studies includes intermolecular interactions, hydrogen bonding, and ion solvation in pure solvents and their mixtures. Bulk solvent structures in complex solutions are compared with pure solvent structures and the changes in the orientation of solvent molecules in the first coordination shell are analyzed. Self-assembling supramolecules are another focus.

At the Thin Film Physics Laboratory, Research Inst. for Technical Physics and Materials Science, HAS (RITPMS) (www.mfa.kfki.hu), the research group of J. Lábár (labar@mfa.kfki.hu) investigates solid state reactions, ordering in crystals and thin films physics by analytical electron microscopy and quantitative

electron diffraction in the TEM. Software was developed for processing electron diffraction ring patterns from polycrystalline samples and electron probe microanalysis. G. Radnóczi, head of Structural Research Dept. (RITPMS, HAS), studies thin films, surfaces, amorphous materials and crystalline C-N (alloyed by B, Si) and their structural and compositional characterization by TEM, as well as theoretical studies.

The research group of T. Ungár (ungar@ludens.elte.hu) Dept. of Materials Physics, Loránd Eötvös U. (ELTE) (metal.elte.hu/aft.elte.hu/Kezdolap_en.html) uses EXAFS and small angle scattering high resolution X-ray diffractometry and peak-profile analysis, to study dislocation structures and densities, microdiffraction, microstructure particle size determination, stored energy from dislocation density, crystallite size and size distribution. Current emphasis is upon the structure of metals and alloys, the dislocation model of strain anisotropy, and scanning microdiffraction to determine local variation of stored energy in heterogeneous microstructures. T. Weiszburg (weiszburg@ludens.elte.hu), I. Dódony and G. Lovas of the Dept. of Mineralogy, Centre of Geology and Environmental Physics (ELTE) (teo.elte.hu/fs/geoldirect.html) conduct investigations of natural and environmental solid materials, TOT-Fe layer silicates, archeometry, mineral topography, and the history of mineralogy.



Inhibitor molecule (shown in magenta with molecular surface) bound at the active site of prolyl oligopeptidase.

The Protein Crystallography Laboratory at ELTE was founded by G. Náray-Szabó and Z. Böcskei in 1993 with the acquisition of a diffractometer suitable for the biochemical and molecular biological research of many groups in Hungary including scientists in the Dept. of Biochemistry at LEU, the Inst. of Enzymology, and the Agricultural Biotechnology Centre where graduate and PhD students are trained in the field of protein crystallography. In 2006 the Laboratory joined the Laboratory of Structural Chemistry and Biology to study the structure, dynamics and interactions of proteins and peptides (www.chem.elte.hu/departments/protnmr). Targets for study have included metal preference, mechanism of action and substrate specificity of tryspin, chymotrypsin and prolyl oligopeptidase, the prototype of a new protease family, enzyme mechanisms and substrate specificity. Studies on proteases of the complement cascade system, an important element of innate immunity, have produced detailed models of their autoactivation mechanism, the first enzymatic event of the complement, and protein/protein interactions. C1-inhibitor, the natural inhibitor of these enzymes is of pharmacological interest. Its crystal structure shed light on the structural basis of the anti-inflammatory effect of heparin, which influences C1-inhibitor-protease complexes. In contrast to the conservative substrate hosting of the studied proteases, the prototype calcium sensor protein calmodulin showed protein/ligand interactions of a highly adaptive and promiscuous nature in its complexes with small molecular drugs and drug candidates explaining their different effects on calmodulin function. dUTPases have essential role in preventive DNA repair via exclusion of uracil and contribution of dTTP biosynthesis. Structures of dUTPase mutants and variants from different species help elucidate the role of conserved amino acid residues that could provide the basis of designing selective inhibitors.

Petra Bombicz (bombicz@chemres.hu)

National Organization

The chair of the National Committee of the IUCr in Hungary is G. Faigel. Past-Chair is A. Kálmán, Secretary is P. Bombicz. Members: A. Bényei, L. Kovács, L. Kőszegi, J. Lábár, G. Náray-Szabó, G. Radnóczi, I. Sajó, K. Simon, E. Sváb, T. Ungár and T. Weiszburg. The Hungarian Synchrotron Committee organizes meetings and workshops connected to X-ray crystallography. Both of these committees work under the auspices of the Physical Section of the HAS.

Petra Bombicz (bombicz@chemres.hu)

Facilities

The Inst. for Solid State Physics and Optics of the Hungarian Academy of Sciences has three traditional X-ray generators, a Huber-goniometer-based home made single crystal diffractometer with an Oxford cryomodule, a Huber 670 image plate Guinier camera, home made X-ray holography setup, a two-axis powder neutron diffractometer equipped with linear position sensitive detector system and a 4-circle neutron diffractometer. The Inst. of Structural Chemistry, Chemical Research Center, HAS, has a Rigaku R-AXIS RAPID image plate diffractometer, an X-Stream 2000 low temp unit, Enraf-Nonius turbo CAD-4 diffractometer, stereo microscopes, a Philips X'Pert diffractometer, a Philips PW1050 diffractometer, Philips PW1050 diffractometer equipped with an Anton Paar HTK 1200 high temperature chamber and a compact Kratky-type small angle camera, and is the Hungarian Affiliated Centre of the Cambridge Structural Database. The Laboratory for Single Crystal X-ray Diffractometry, Institute of Chemistry, U. of Debrecen has an Enraf-Nonius MACH3 CAD-4 diffractometer. The LEU has a Rigaku R-AXIS IV++ image plate diffractometer, an Oxford Cryosystems Cryostream 700 low temperature unit and a Cyberlab C-200 crystallization robot.

Petra Bombicz (bombicz@chemres.hu)

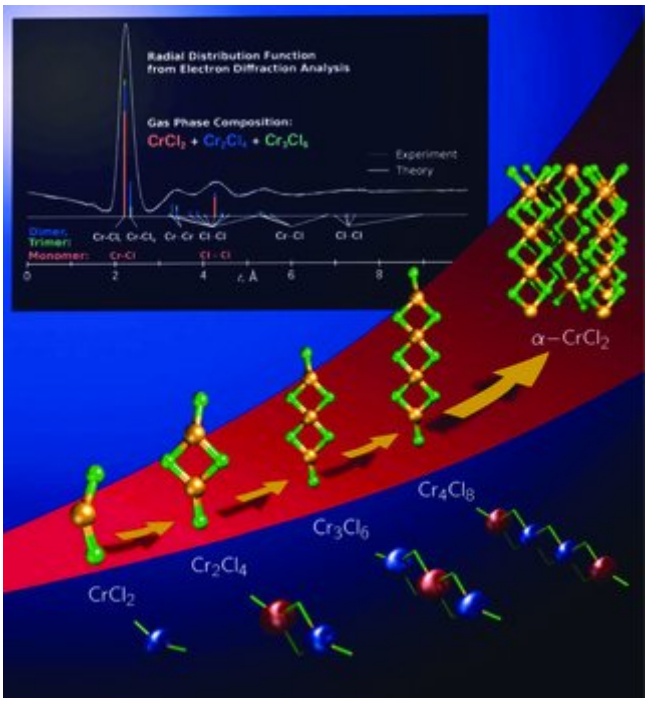
Awards and Current Appointments

A. Kálmán served the IUCr as a member of the Executive Committee from 1984, and was the Vice-President of the Union between 1990-1993. P. Bombicz has been a member of the IUCr Commission on Structural Chemistry since 2005, succeeding previous Hungarian representatives A. Kálmán and K. Simon. From 1990 to 2000 A. Kálmán co-edited *Acta Crystallographica B* and *C*, and M. Czugler has been a co-editor of *Acta Crystallographica E* since 2006.
The 2nd and the 22nd European Crystallographic Meetings were held in Hungary, in Keszthely in 1974 and Budapest in 2004. Other Crystallography-related conferences held in Hungary include the 20th General Meeting of the International Mineralogical Association (2010), the 5th Mid-European Clay Conference (2010), Conference on Reverse Monte Carlo Modelling (2003, 2006, 2009), Symmetry Festival (2009), Electron Crystallography: INNOVATIAL Process Diffraction School (2008), Ultra-high Pressure Metamorphism, the 5th EMU School & Symposium (2003), Energy Modelling in Minerals, the 4th EMU School in Mineralogy (2002), EPDIC (1998), 2nd Regional Workshop of EMAS (1996).

There is significant activity in the field of crystallography in the pharmaceutical companies Gedeon Richter, EGIS and Sanofi-Aventis (Chinoin). These industrial labs use mainly powder X-ray diffraction for analytical purposes. EGIS pharma company lately installed an R-Axis SPIDER for single crystal diffraction studies.

Petra Bombicz (bombicz@chemres.hu)

Electron Diffraction Research



Results from the electron diffraction study of chromium dichloride of complex vapor composition. Its structure illustrates all vibronic interactions: the monomeric molecule exhibits the Renner-Teller effect, its dimer the pseudo-Jahn-Teller effect, and its crystals the Jahn-Teller effect. The oligomers as well as the crystal display antiferromagnetic coupling.

A strong research group for molecular structure studies has developed since 1965 at the Hungarian Academy of Sciences - currently located at the Budapest Univ. of Technology and Economics under the name Materials Structure and Modeling Research Group. Its leading scientists are Istvan Hargittai (istvan.hargittai@gmail.com) and Magdolna Hargittai (hargittaim@mail.bme.hu). The group's main experimental technique has been gas-phase electron diffraction together with mass spectrometry. Their experimental data have been augmented by various spectroscopic information, and, increasingly, by quantum chemical calculations. The group focuses on the structural variations and modeling of free molecules, and has often performed joint work and comparisons with crystallographic studies.

Currently, one of their main interests is in structural peculiarities in metal halides under the leadership of Magdolna Hargittai. They have been involved with determining rare structural effects due to vibronic (vibrational-electronic) interactions - the Jahn-Teller, Renner-Teller, and pseudo-Jahn-Teller effects - and relativistic effects. They discovered several unexpected structural features, such as the effect of spin-orbit coupling and of the 4*f* orbital occupation on molecular geometry and found examples of antiferromagnetic coupling and spin-crossover in gas-phase metal halide structures combining data from a plethora of techniques. Lately they have also been involved with determining the structural relationship between the gas-phase and crystal-phase structures of metal halides.

The group, under the leadership of its founder Istvan Hargittai, has been involved in a number of international collaborations that have increased the accuracy of gas-phase electron diffraction studies and have expanded the field to include unstable species. The broad scope of their work can be seen in their publications in a wide spectrum of journals. They have also published several monographs including: their books on gas-phase electron diffraction (I. Hargittai, M. Hargittai, eds., *Stereochemical Applications of Gas-Phase Electron Diffraction*, Parts A and B, VCH Publishers: New York, 1988); symmetry (M. Hargittai, I. Hargittai, *Symmetry through the Eyes of a Chemist*. Third Edition. Springer, 2009; 2010; M. Hargittai, I. Hargittai, *Visual Symmetry*. World Scientific, 2009); molecular structures (A. Domenicano, I. Hargittai, eds., *Accurate Molecular Structures*. Oxford University Press, 1992; R. J.

Gillespie, I. Hargittai, *The VSEPR Model of Molecular Geometry*. Dover (reprint edition), 2011); and leading personalities in crystallography (I. Hargittai, M. Hargittai, B. Hargittai, *Candid Science I-VI*. Imperial College Press, London, 2000-2006; and I. Hargittai, *The DNA Doctor*. World Scientific, 2007).

Istvan Hargittai is the Editor-in-Chief of *Structural Chemistry* (Springer-Verlag), an international journal in its 22nd year of publication.

Find further information on the research groups at www.amkcs.ch.bme.hu.

Istvan Hargittai (istvan.hargittai@gmail.com) and Magdolna Hargittai (hargittaim@mail.bme.hu)

Crystallography in Turkey

Crystallography became an independent scientific discipline in Turkey in the 1960's. Crystal geometry and optics were taught in the Geology and Mineralogy Depts. to prepare students for microscopic investigation of crystalline materials. In some departments, including the Mineral Research and Exploration Inst. of Turkey (MTA), X-ray powder diffractometers were used for materials identification. In physics and chemistry departments, crystal symmetry, physical and chemical properties of crystals were taught without structure analysis.





Left: Some of the older equipment used for crystallography research in Turkey. Right: The participants of the 2nd National Meeting in Kayseri.

In the mid 1960's A. F. Cesur of Ankara U. started an X-ray crystallography laboratory which used photographic single crystal data collection techniques. In 1970, D. Ulku established a laboratory at Hacettepe U. in Ankara equipped with a 5 kW X-ray generator, a GE-SPG2 Spectrogoniometer with a quarter circle single crystal orienter, proportional and scintillation counters, and Wiessenberg, Buerger Precession and powder cameras. This laboratory has become the leading centre of X-ray crystallography in the country. The purchase of a CAD-4 diffractometer in 1992 attracted young scientists to do graduate work in X-ray crystallography. In 1999, a rotating anode X-ray generator was put in operation in the same department. Crystallography laboratories at Gazi, Erciyes, Ondokuz Mayıs and Atatürk U. were established by these young crystallographers who are very active in chemical crystallography today. Several X-ray single crystal and powder diffraction units are currently scattered across the country. University X-ray diffraction laboratories, dedicated to materials science research, also utilize crystallographic methods.

The SESAME (Synchrotron Light for Experimental Science and Applications in the Middle East) Project, developed by UNESCO, will further expand crystallographic research in Turkey. SESAME, based in Jordan, will provide opportunities for research in structural molecular biology, environmental, surface and interface science, microelectromechanical devices, X-ray imaging, archaeological microanalysis, and materials characterization. The founding members of the project are Bahrain, Cyprus, Egypt, Iran, Israel,

Jordan, Pakistan, the Palestine Authority and Turkey. Turkey will be involved in building the protein crystallography and powder diffraction beamlines. Young Turkish scientists have benefited from extensive training in accelerator technology and applications at different European, US and Taiwanese Light Source laboratories (for more information, see: www.sesame.org.jo).



Photos from the ECM25 Istanbul Meeting.

The Turkish Crystallographic Association (TCA; www.tucr.org), formed in 2001, presently has about 140 registered members, one fourth of whom are senior scientists. The TCA was accepted in the European Crystallographic Association at its General Assembly in Cracow in August 2001. TCA organizes biannual National Meetings and workshops. W. Duax, J. Glusker, G. Cascarano and P. Rizkallah attended the 2006 National Meeting held in Kayseri. The 25th European Crystallographic Meeting was organized in Istanbul in 2009 by TCA (*IUCr Newsletter*, Volume 18, Number 1, 2010).



The Crystallography group and laboratory at Hacettepe University in Ankara.

The Crystallography Laboratory of Hacettepe U. in Ankara (contact: kendi@hacettepe.edu.tr) specializes in organic and inorganic compounds such as polynuclear coordination complexes of transition metals with unusual magnetic properties, inclusion compounds such as Hoffmann clathrates and crown ethers, phosphazene derivatives, intermetallic compounds, synthetic metallic materials, and pharmaceutical compounds (flavones, oxime ether derivatives, indoles, benzimidazoles, triazole and thiosemicarbazones). Protein crystallography has also begun in the lab (contact: sozbey@hacettepe.edu.tr). The plant lectins have been studied at Daresbury Laboratory, UK in collaboration with P. Rizkallah. The structures of neurotoxic peptides extracted from Turkish scorpions have been studied in collaboration with J. R. Helliwell from Manchester U. The first Turkish small and wide angle X-ray scattering system (Hecus SWAXS) was installed in the laboratory in 2009. SWAXS analysis of multicompartment micelles, lamellar liquid crystals, hydrogels, polymer coated magnetic nanoparticles, stimuli-responsive block copolymers, marble dust, nanocomposites, membrane interactions, teeth and spider silks are in progress (contact: side@hacettepe.edu.tr).



The Advanced Materials Research Group, Hacettepe University.

The scientific activities of the Advanced Materials Research Group (AMRG, www.imal.hacettepe.edu.tr; contact: ozdas@hacettepe.edu.tr) include the following four major research areas: intercalation compounds, graphite-like compounds, nanocarbon, and high-pressure and superconducting materials. Materials science research at AMRG addresses understanding the relationships between structural and material properties using powder, high-pressure and electron crystallography, and developing new

synthesis and characterization techniques for advanced materials. The group is also in charge of the powder diffraction beamline at SESAME.





Left: The Material Research Laboratory, Ankara. Right: The Nonlinear Optics Laboratory, Ankara University.

The Material Research Laboratory at Ankara U., Ankara (contact: elerman@eng.ankara.edu.tr) collaborates with research centers in Germany on single and powder crystal diffraction analysis of electrical, magnetic and specific heat properties of mono- and hetero-crystals and rare earth alloys. They also perform research related to the production and characterization of rare earth-intermetallic magnetic compounds between 2 K and 350 K, magnetocaloric materials, hard and soft magnetic materials, magnetic sensor materials and nanomagnetism.

The Nonlinear Optics Laboratory (contact: elmali@eng.ankara.edu.tr) established in 2005 is equipped with a Spectra Physics femtosecond laser system, a Light Conversion Topas-C optic parametric amplifier, a Newport Helios spectroscopy system, a Quantel Briallant Nanosaniye laser system and a J. A. Woolaam M2000V spectroscopic ellipsometer for measurements of the second and third-order NLO properties and optical limiting behavior of organic thin films, carbon nanotubes, polymers, organic and organometallic compounds.



The Molecular Biology Research Laboratory at Sabancı University.

Studies in the Molecular Biology Research Laboratory at Sabancı U., İstanbul (contact: zehra@sabanciuniv.edu) are focused on determining mechanisms of fundamental processes in living organisms, prediction of function from the 3D structure, and for engineering new systems via cloning, purification, characterization, and 3D structure determination using synchrotron X-ray solution scattering and diffraction techniques. The current applications include environmental pollution remediation and pathogen resistance in plants.



X-ray crystallography research at Ondokuz Mayis University, Samsun.
The introduction of the IPDS II diffractometer with a low temperature apparatus in the Physics Dept. at Ondokuz Mayıs U. (OMU), Samsun, (contact: orhanb@omu.edu.tr) has allowed fourteen researchers from the academic staff as well as a number of MSc and PhD students to study organic crystals with non-linear optical properties, the biological activities of novel saccharin and acesulfame metal complexes, structural and magnetic properties of dimeric cyano complexes, supramolecular structures and crystal engineering. The academic staff in the Department cooperates with researchers from different areas of science.





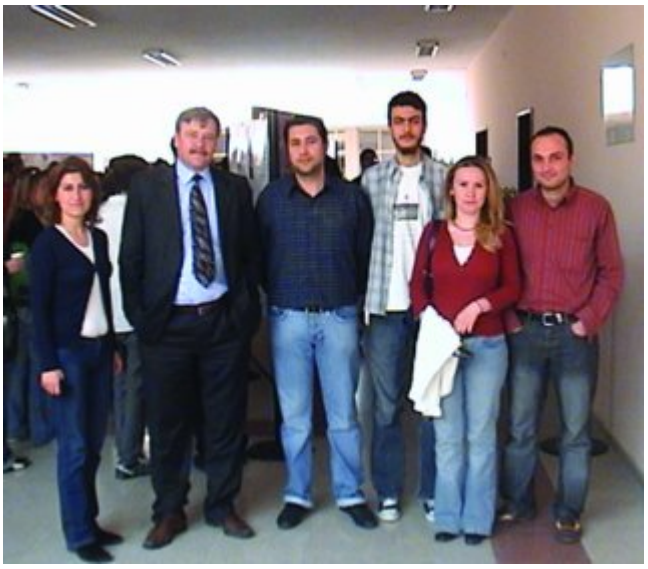
Left: The Advanced Thin Film Research Group at Anadolu University, Eskişehir. Right: Research facilities at the Anadolu University, Eskişehir.

The Advanced Thin Film Research Group at Anadolu U., Eskişehir (contact: rmoksuzoglu@anadolu.edu.tr) was established in 2008 at the Dept. of Material Sciences and Engineering to study spintronics (spin valves and tunnel magnetoresistance) and photovoltaics (wide band gap semiconductors, complex metal oxide thin films). A self-designed multi-chamber sputtering tool with magnetic annealing oven is used for production of nanoscale/ultra thin film systems containing metal, semiconductor and insulator materials. Facilities for structural characterization of thin films include instruments for grazing incidence X-ray diffraction, X-ray reflectivity and rocking curve measurements and a scanning probe microscopy (AFM, STM, LFM).

The Chemistry Dept. of Middle East Technical U., Ankara is involved in chiral synthesis of amino acids, drugs, biologically active compounds, biodegradable polymers, and natural products, the application of quantum chemical methods to spectroscopic studies, metal clusters and colloids, measurement and control of hazardous substances, and application and development of nuclear analytical, atomic spectroscopic and chromatographic techniques for pollution studies and for analysis of trace elements in biological materials. In addition, low energy atom diffraction (LEAD), X-ray photoelectron diffraction, scanning probe microscopy and quartz crystal microbalance studies of self-assembled monolayers (SAMs) and organic semiconductor thin films are performed. The Central Laboratory is equipped with Rigaku Ultima IV X-ray diffraction system and provides services for the university.

The X-ray Research Laboratory at Erciyes U., Kayseri (contact: akkurt@erciyes.edu.tr) operates an Enraf-Nonius Diffractis 583 X-ray generator, Weissenberg and Buerger Precession cameras, and one microdensitometer. The U. of Technology Research Center has a Bruker AXS D8 Advance X-ray powder diffractometer and a LEO 440 scanning electron microscope. The group members work on structures of organic and metal-organic compounds with medical and pharmacological properties, and quantum mechanical calculations of crystal phase identification and analysis.

In the X-ray Crystallography Laboratory at Kırıkkale U., Kırıkkale a full circle single crystal X-ray diffractometer Rigaku MSC/AFC-7s and a TEM were purchased in 1998 for studies including boron complexes obtained from acidic amines, amides and organics, Al and Cu based microstructures, and metallic borons.



Members of the X-ray Crystallography Laboratory, Dokuz Eylül University.

M. Aygün and his coworkers from the X-ray Crystallography Laboratory at Dokuz Eylül U., İzmir (contact: muhittin.aygun@deu.edu.tr) are interested in intermolecular interactions of N-Heterocyclic Carbene (NHC) complexes with transition metals and the theoretical foundations of classical crystallography (CCr) and quantum crystallography (QCr).

Researchers at Dokuz Eylül U. have improved the solution of the phase problem with a new methodology called Generalized Classical Crystallography (GCCr) in which the tangent formula was recast in terms of perturbative contributions from various orders with the aid of information theory and a generalized polynomial equation satisfied by electron density in the unit cell. From a generalized point of view, conventional crystallography, zeroth order crystallography and higher order crystallographic studies are possible. In addition, a novel iterative scheme was developed for the application of Generalized Quantum Classical Crystallography (GQCr).





Left: The research group at the Laboratory for Advanced Analysis, İstanbul University. Right: İstanbul University, İstanbul, Turkey.

Crystallographic work in İstanbul started in 2003 when the Advanced Analysis Laboratory was established at İstanbul U. (contact: ial@istanbul.edu.tr) with single crystal (Rigaku R-AXIS Rapid-S) and powder diffraction (Rigaku D-Max family) studies of natural and synthetic organic and inorganic molecules, and phase analysis of functional materials and clays.

A crystallography laboratory in Atatürk U., Erzurum was established in the Organic Chemistry Dept. in 2005, where the synthesis of natural products, synthetic organic chemistry studies, asymmetric synthesis and mechanistic studies are conducted. Together with organic and inorganic compounds from other working groups, an average of 40-50 structures are determined per year.



The X-ray research group at Balıkesir University.
A research group at Balıkesir U., Balıkesir (contact: hkara@balikesir.edu.tr) works on the structures and magnetic properties of novel polynuclear Schiff base transition metal complexes that have potential applications for storage of information at the molecular and nanoscale level. The group plans to develop new materials with novel magnetic properties, such as single molecule magnets, for technological applications.

Other institutions in Turkey that operate diffraction facilities

Some laboratories running X-ray diffraction facilities exist as research infrastructure of the Applied Physics and Material Science Depts. located at the Middle East Technical U. (Metallurgical & Materials Dept. and Central Research Laboratory), Anadolu U. (AUBIBAM, Eskişehir), Gazi U. (Semiconductor Tech. Adv. Research Laboratory), Harran U. (Urfa) and İzmir Inst. of Technology (Materials Research Centre, İzmir). In addition to these, there are many industrial institutions in Turkey including labs that perform powder diffraction for materials characterization and quality control, such as the Turkish Atomic Energy Agency, the General Directorate of Mineral Research and Exploration, the General Directorate of Highways and the General Directorate of State Hydraulic Works.

Engin Kendi (kendi@hacettepe.edu.tr)

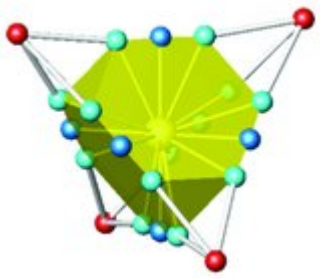
Crystallography in Serbia

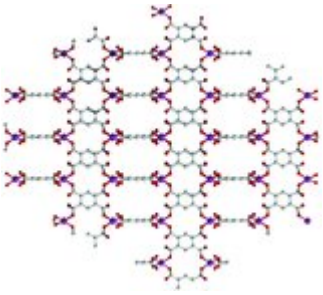
The former Yugoslav Centre for Crystallography in the Republic of Serbia has been reorganized by the Serbian Crystallographic Society. The SCS was founded in Belgrade on May 7, 1992 at the Faculty of Mining and Geology of the Serbian Academy of Science and Art. Bela Ribar was elected president, I. Krstanovič vice-president, and L. Karanovič secretary, and other members of first SCS committee were: B. Prelesnik, S. Stankovič, S. Janjič and D. Stojanovič.



Participants of the SCS Conference, Novi Sad, 2006.

The First Conference of the SCS was held in Belgrade in 1992. In 1993, at the 16th General Assembly of the IUCr in Beijing, China, SCS was accepted as a member of the Union. When the European Crystallographic Association was founded, Serbia became a member. The current president of SCS is A. Kremenovič (akremenovic@rgf.bg.ac.rs). The Society organizes annual Conferences each June and invites crystallographers from abroad as plenary lecturers. SCS receives financial aid for membership payments and conference organization from the Ministry of Science and Technological Development of the Republic of Serbia. The complete book of abstracts from the last conference can be found at: www.df.uns.ac.rs/skd.





Crystallography research at the University of Belgrade, Serbia.

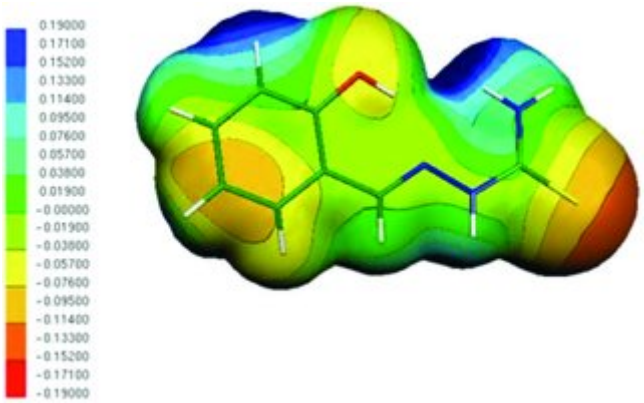
Several crystallographic research groups are active within Serbian Universities and research institutes. The group that initiated crystallographic research in Serbia became the Dept. for Crystallography at the Faculty for Mining and Geology of Belgrade U., now headed by L. Karanovič (ljkaranovic@rgf.bg.ac.rs). Since establishing the Chair for crystallography in 1991, the team has used X-ray, optical and geometrical crystallography to study mineralogy, chemistry, physics and material science of natural and synthetic materials. Crystallography is taught at this Faculty at Bachelor, Master and PhD levels.

A group lead by D. Poleti (dejan@tmf.bg.ac.rs) at the Faculty of Technology and Metallurgy studies the structure and functional chemistry of transition and post-transition elements. The laboratory for X-ray diffraction of the Dept. of Physics, Faculty of Sciences, U. of Novi Sad was founded in 1973 by the late B.

Ribar. Ribar formed a group of physicists involved in crystallography that is now led by S. Rakič (srdjan.rakic@df.uns.ac.rs), who together with senior scientists V. Divjakovič (divus@uns.ac.rs) and A. Kapor (akapor@df.uns.ac.rs) conducts powder, liquid crystal and single crystal analysis. Current instrumentation includes an Oxford Diffraction Xcalibur S, a Cryojet HT cooling system high-temperature equipment (Anton Paar HTK2), and an Edwards vacuum pump. Services provided include application of Rietveld and *SHELX* refinement programs. Research targets include ceramics, spinel type nanocomposites for application in new technologies, studies of crystallite size, microstrain, and phase transitions, and analysis of compounds potentially relevant for pharmacology.

Research groups at Novi Sad U. study the coordination of synthetic transition and metal complexes, and biologically active organic compounds. Courses on Crystallography are offered at the Bachelor and Master degree levels in the Departments of Physics and Chemistry.

In the Dept. of Chemistry of the U. of Kragujevac, crystal structures of synthetic compounds are determined in the group headed by S. Trifunovič (srecko@kg.ac.rs). In the Dept. of Chemistry, U. of Belgrade, research groups led by S. Zarič (szaric@chem.bg.ac.rs) study inorganic complexes, noncovalent interactions, theoretical energy of crystal formation and analysis of data derived from the Cambridge Structural Database.



Crystallography research at the Research Institute 'Vinča', Serbia.
Several institutes conduct crystallographic research on materials. The first group to use automatic single crystal diffractometry was started by R. Herak and B. Prelesnik in the Laboratory for Solid State Physics at the Inst. for Nuclear Science 'Vinča' in the 1950's. They published work in single-crystal and powder diffraction and secured an Enraf-Nonius CAD4 diffractometer. Current research by the group in the department headed by G. Bogdanovič (goranb@vin.bg.ac.rs) is focused on transition metal complexes, weak intermolecular interactions, hydrogen bonding, supramolecular structures and CSD database and experimental charge density studies. In the Condensed Matter Laboratory, research on synthesis and structural and magnetic characterization of nanosized and polycrystalline magnetic materials ($La_{0.7}Ca_{0.3}MnO_3$, ε-Fe_2O_3) is led by V. Spasojevič (vojas@vinca.rs) and diffraction measurement on a Bruker AXS D8 diffractometer are coordinated by M. Mitrič (mmitric@vinca.rs). The founder of this group was late D. Rodič. The SCS presents an annual award, named after Rodič, to a promising young crystallographer. Another crystallographic research group led by S. Boškovič (boskovic@vin.bg.ac.rs) in the Ceramic Department at 'Vinča' studies nanostructured carbon materials, ceramics and solid solutions for use in electronics, conducts synthesis, characterization, qualitative and quantitative analysis, and determines crystallite size and microstrain using Rietveld refinement and other techniques.

Agneš Kapor (akapor@df.uns.ac.rs)

Crystallography in Romania

An overview of the Romanian groups dedicated to crystallography reveals a variety of interests, from small molecule structure determination to materials science. The X-ray laboratories equipped with the necessary instruments are associated with universities and research institutes.





Left: National R&D Institute for Nonferrous and Rare Metals (IMNR), Bucharest. Right: X-ray Powder Diffraction Group, Analysis Laboratory.

The National R&D Institute for Nonferrous and Rare Metals (IMNR) founded in Bucharest in 1965 to conduct research in the field of nonferrous metallurgy, is currently focused on nanostructured materials, novel technologies and materials, ecotechnologies and environment protection.

The X-Ray Powder Diffraction Group has two researchers and several students. X-ray diffraction equipment consists of a Bruker D8 ADVANCE diffractometer in Bragg-Brentano geometry, using *DIFFRACplus* BASIC software and the ICDD PDF-2 Release 2006 database. Powder diffraction techniques are used for qualitative and quantitative crystalline phase identification in ores, industrial waste, alloys and inorganic substances, for microstrain and crystallite size determination of nanobiomaterials, ceramic matrix composites, and powders with core/shell structure. The X-Ray Powder Diffraction Group offers young students the opportunity to use its facilities under guidance of the laboratory specialists, in order to develop experimental projects.





(left) Researchers and (right) equipment at the National Centre for X-Ray Diffraction, Laboratory for Molecular Structure Determination, Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, Cluj-Napoca.

The National Centre for X-Ray Diffraction, Laboratory for Molecular Structure Determination, Babes-Bolyai U., Cluj-Napoca was established in 2000 as a multi-user center. The laboratory has a Bruker SMART APEX CCD diffractometer for single crystal structure determination, a KRIOFLEX low temperature system, NIKON SMZ1000 microscope and access to Cambridge Structural Database. The Center provides molecular structure determinations of inorganic, organic and organometallic compounds. User services include: unit cell determination, data collection and refinement, molecular structure determination, and supplementary refinement of molecular structures measured elsewhere. The group has four permanent members (richy@chem.ubbcluj.ro, cristi@chem.ubbcluj.ro; chem.ubbcluj.ro/~richy/).



The National Institute for R&D of Isotopic and Molecular Technologies, Cluj-Napoca.
The National Institute for R&D of Isotopic and Molecular Technologies, Cluj-Napoca crystallographic group has three researchers and several graduate students. A Bruker D8 powder diffractometer and a SuperNova single crystal diffractometer are used to determine structures of small molecules and for microstructural characterization of inorganic compounds using X-ray profile Fourier analysis, EXAFS and XANES absorption spectroscopy small angle X-ray scattering (SAXS) and structural study of amorphous materials. Materials investigated include: pharmaceutical compounds and their polymorphs, intermetallic compounds, metal supported catalysts, semiconductors, and inorganic oxides (contact: borodi@itim-cj.ro).





Left: West University of Timişoara. Right: Crystallography research at West University of Timişoara.

The Solid State Structure Characterization Lab at the West University of Timişoara, Timişoara was established in the early 70s, by the late O. Birau. A Bruker D8 diffractometer with a horizontal goniometer and an open Eulerian cradle are used for phase stress and texture analysis, and grazing incidence studies of powder samples and thin films. The research team of two permanent members and several students pursue interdisciplinary research studies of bulk, thin films or powder of semiconductors, oxides, zeolites, pharmaceuticals, and nanotubes. (contact: Paul Barvinschi; pbarvi@physics.uvt.ro, quasar.physics.uvt.ro/physics/ldccs/).





Left: National R&D Institute for Electrochemistry and Condensed Matter, Timişoara (NIRDECM). Right: Equipment at NIRDECM.

The X-Ray Diffraction Laboratory at the National R&D Institute for Electrochemistry and Condensed Matter, Timişoara (NIRDECM) (founded in 2008) possessing an X'Pert PRO MPD diffractometer with PixCEL detector. Activities of the laboratory includes single-crystal XRD, phase identification powder XRD at variable temperatures (−193°C to 1400°C) (mainly oxidic materials), and sensitive pharmaceutical samples in glass capillaries. The newly established laboratory has equipment for the study of texture, stress, reflectivity, thin films, transmission measurements, SAXS, and work under oxidizing/inert/vacuum atmosphere up to 900°C (reactor chamber). The laboratory has two researcher scientists and four PhD students, contacts with national and international education and research institutions and is pursuing certification, training personnel, developing partnerships and providing services (contact: Alexandra Bucur, alexandra.i.bucur@gmail.com, www.icmct.ro).

NIRDTP Iaşi



Crystallography at National Institute of Research and Development for Technical Physics, Iaşi.

The research group from the Department of Magnetic Materials and Devices at the National Institute of Research and Development for Technical Physics, Iaşi is designing and developing novel magnetic materials. The primary focus is on disordered, nanocrystalline nanocomposites and nanomaterials, and their applications in sensors, actuators or transducers. Using powder diffractometer from room temperature to 1400 K, the X-ray diffractometer at NIRDTP Iaşi allows the measurements in either Bragg-Brentano or Goebel mirrors configuration. There are facilities for X-ray reflectometry (XRR measurements on multilayered structures and estimation of the layer thickness. The department has twenty researchers, six engineers, five technicians, and several PhD students and postdocs (contact: nicole@phys-iasi.ro; hchiriac@phys-iasi.ro).

MSL Materials Science Laboratory

TECHNICAL UNIVERSITY OF CLUJ-NAPOCA ROMANIA



The Materials Science Laboratory (MSL) at the Technical University of Cluj-Napoca established in 1995 explores superconducting, dielectric and magnetic thin films and heterostructures grown both by physical and chemical methods. The laboratory is equipped with a modular high-resolution four circle diffractometer, high-resolution X-ray diffraction, reciprocal space mapping, X-ray reflectometry and grazing incidence diffraction characterization of epitaxial and polycrystalline thin films and multilayers. The group consists of five researchers, one post-doctoral fellow and five PhD students (contact: mihai.gabor@phys.utcluj.ro).

Other X-ray laboratories are in Bucharest (National Institute for R&D in Electrical Engineering ICPE-CA (www.icpe-ca.ro/); The National Institute of Materials Physics (www.infim.ro); U. of Bucharest, Faculty of Physics (www.fizica.unibuc.ro/fizica/Main.asp); U. of Bucharest, Faculty of Chemistry (contact: Marius Andruh, marius.andruh@dnt.ro); Horia Hulubei National Inst. of Physics and Nuclear Engineering - IFIN HH (www.nipne.ro/index.php), Brasov (Transilvania U., www.unitbv.ro/), Cluj-Napoca (Babes-Bolyai U., Faculty of Physics, phys.ubbcluj.ro/index_eng.htm) and Iaşi ('Petru Poni' Inst. of Macromolecular Chemistry, www.icmpp.ro/index.html).

Richard A. Varga (richy@chem.ubbcluj.ro)

(See also Part 1)

MEETING REPORT

So long IUCr2011...

IUCr2011 (www.iucr2011madrid.es/), the most important crystallographic event held in Madrid (Spain) since the IUCr was founded in 1948, ended happily looking forward to the International Year of Crystallography (IYCr2013) and to Montreal (IUCr2014).

The opening ceremony, including the presentation of the three Ewald awards, the congress dinner accompanied by Dixie-Land live music, and the closing ceremony, encompassing the handover of the IUCr's Presidency, were crowded events.



Madrid Local Committee. Front (left to right): Lourdes Infantes, Martin M. Ripoll, Marta Jiménez, Armando Albert. Behind (left to right): Julia Sanz, Avelino Martin, Pilar Gómez, Catalina Ruiz, Enrique Gutiérrez, Miquel A. Cuevas, Pascual Román, Marta E.G. Mosquera, and Sol López.



Thomas A. Steitz (left) and Venki Ramakrishnan (right).

The congress brought together nearly 2800 people (1880 standard participants, 360 students, 350 grantees, 65 exhibitors and 113 accompanying persons). 73 countries were represented by 2040 abstracts that were distributed across 98 Micro-Symposia with 490 oral and 1550 poster presentations, 20 of which were awarded prizes sponsored by 9 institutions or commercial companies.

In addition, 36 Keynote speakers covered the state of art in crystallography: very large macromolecular assemblies, ribosome complexes, membrane proteins, supramolecular chemistry, structural aspects of bacterial pathogenicity, the structural basis of cell regulatory processes, structural genomics, validation and errors in protein structures, XAFS as a new tool for protein structure-function investigations, ultrafast crystallography using X-ray free electron lasers, coherent X-ray diffraction, single-molecule and hybrid methods, new approaches to experimental phasing of macromolecules, automated electron diffraction tomography as an *ab initio* structure solution method, polycrystalline materials, powder diffraction at the nanoscale, magnetic neutron crystallography, commensurate and incommensurate structures, soft matter, solid gas materials, energy-related materials, crystal engineering, very recent advances in crystal growth, new topological structural characterization, high-pressure molecular crystals and

mineralogy, atomic resolution real-space imaging, and ornamental art of the Alhambra (from plane groups to quasilattices). In summary, the meeting showcased the most recent research being done all over the world in the extremely important scientific fields such mineralogy, chemistry, physics, material science, nanotechnology, biochemistry, biology and biomedicine.

Of the 4 plenary lectures at the congress three, based on the structural and functional aspects of the ribosome, were presented by the 2009 Chemistry Nobel Laureates, Thomas A. Steitz, Venki Ramakrishnan and Ada Yonath. The fourth lecture was given by Omar M. Yaghi on metal organic frameworks.

IUCR ACTIVITIES

2011-2013 Executive Committee



Front row: Sine Larsen, Gautam Desiraju, Hanna Dabkowska, Elena Boldyreva; back row: J. Mitchell Guss, J. Manuel Perez-Mato, Wulf Depmeier, Luc Van Meervelt, Claude Lecomte, Marvin Hackert

President Gautam Desiraju

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Immediate Past President S. Larsen

Ordinary Members J. M. Guss, J. M. Perez- Mato, M. L. Hackert, H. Dabkowska, and E. Boldyreva

IUCR ACTIVITIES

IYCr 2013 logo design competition



Michele Zema was presented with a certificate and an Apple iPad 2 by Sine Larsen at the IUCr Congress.

The winning entry in the competition for a logo for the International Year of Crystallography 2013 was submitted by Michele Zema from the U. of Pavia, Italy. The design emphasizes the role of diffraction in the development of crystallography as a branch of science, with the zero in the representation of the festival year coinciding with the central beam of a hypothetical diffraction experiment, and the extended diffraction pattern forming the background. His design is available at www.iucr.org/iycr/logocompetition.