

CZECH AND SLOVAK CRYSTALLOGRAPHIC ASSOCIATION

The Czech and Slovak Crystallographic Association (CSCA) organized or co-organized several conferences and traditional one-day seminars in 2008-2011.

Seminars on problems of X-ray and neutron structure analysis (Rozhovory)

276th Seminar

Institute of Molecular Biology, Slovak Academy of Sciences, Bratislava, 22. 1. 2008

Protein Crystallography: News from our Laboratories

Lectures:

V. Hlinková: Ribonuclease - catalytic mechanism of RNA fission and recognition, P. Řezáčová: Structural studies of catabolic repressors of *Bacillus subtilis*, J. Brynda: Structural studies of quinon reductase from *E. coli*, N. Kostlánová: Structural studies of saccharides binding proteins, G. Ondrovičová: Structural studies of ATP dependent proteases, P. Florek: Biochemical studies of SpoIIISA-SpoIISB toxin-antitoxin system from *Bacillus subtilis*, Vernon Smith: Fast track to a 3D protein Structure using Automated Crystal Imaging, Screening and Data Collection, I. Baráth: Can nuclear receptor HNF4 bind synthetic ligands?, J. Hašek: Projects of protein structure analysis solve in Institute of Macromolecular Chemistry, Academy of Sciences of the Czech republic. *Excursion*.

Organization: L. Urbániková

277th Seminar

Institute of Physics, Academy of Sciences of the Czech Republic, 28. 5. 2008

A new diffractometer Bruker D8 in Laboratory Rotan and lecture of Prof. Hartmut Fuess

Lecture:

Z. Šourek: Introduction of installed version of the diffractometer D8 DISCOVER SUPER SPEED SOLUTION, O. Pacherová: Investigation of crystal structure of thin single crystalline layers with D8 – DISCOVER, P. Vaněk: Preparation of ceramics EuTiO_3 with the use of mechanochemical activation and its characterization, Dieter Bertelmann: Thin films and X-ray diffraction, H. Fuess: In-situ characterization of materials for piezoceramics, Li-ion batteries and fuel cells, F. Fendrych: Nanostructured magnetic layers: preparation, characterization, use. J. Kub: Measurements of reflectivity and temperature dependence of lattice parameters

Organization: Z. Šourek

278th Seminar

Zentiva, a.s., 26. 11. 2008

Structure Analysis in Pharmacy

Lectures:

Importance of API crystal structure for pharmaceutical industry

H. Brusová: Polymorphism – new trends in development, M. Hušák: Phase transitions in pharmaceuticals studied by synchrotron radiation/ structure solution from powder diffraction data/ polymorph predictor, J. Brus: NMR crystallography of pharmaceutically active compounds, N. Minks: Patents, T. Pekárek: Tools for monitoring of particle size in pharmaceutical forms

Importance of protein structures for pharmaceutical industry

J. Brynda: X-ray structure analysis of proteins as a tool for drug design, P. Kolenko: Glycosylation modulating efficacy of antibody-based therapeutics, R. Hrabal: Role of NMR spectroscopy in structural biology, P. Řezáčová: HIV protease inhibitors derived from metalocarborans, Jindřich Hašek: Use of synchrotron radiation for diagnostics and development of new drugs.

Excursion

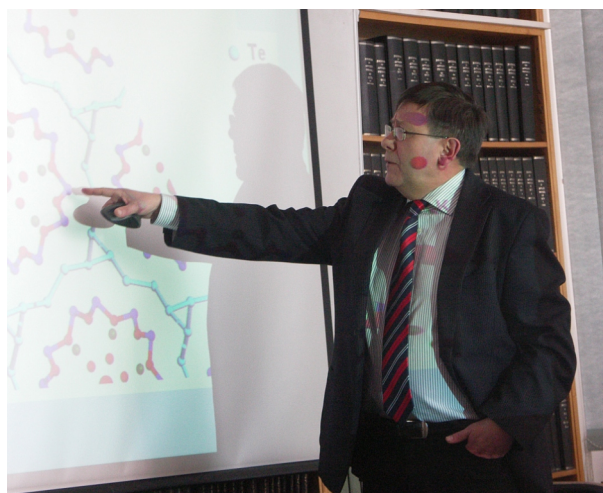
Organization: H. Brusová

279th Seminar

Institute of Macromolecular Chemistry, Academy of Sciences of Czech republic, 19. 3. 2009

X-ray structure analysis in Chemistry

V. Langer: Structural chemistry in practise, B. Kratochvíl: Pharmaceutical cocrystals, E. Smrček: On co-existence of crystallography and quantum chemistry, E. Scholtzová: NBO analysis - a useful tools for analysis of crystal structure, J. Kožíšek: Obtaining of physical-chemical properties from diffraction data, R. Černý: Hydrides: Achievements and traps of powder diffraction, J. Fábry: Dependence of frequent space group types of organic and organometallic compounds on reduced cell volumes,



279th Rozhovory, V. Langer



279th Rozhovory, E. Scholtzová



279th Rozhovory

ture of transition metal complexes, J. Fiala: X-ray diffraction in mechanochemistry

Organization: L. Smrčok

281st Seminar

Institute of macromolecular chemistry, Academy of Sciences of the Czech Republic, 20. 7. 2009

Compact Light Source

Lectures:

J. Dohnálek: Compact Light Source and its possibilities

General discussion on the source

Discussion on the research project BIOCEV (Structure biology and protein engineering)

Organization: J. Hašek

282nd Seminar

Research institute of inorganic chemistry, Ústí nad Labem, 4. 11. 2009

Lectures:

M. Petrák: History of X-ray laboratory in the Research institute of inorganic chemistry, Ústí nad Labem, P. Ryšánek: Use of powder diffraction for analysis of asbestos and their liquidation, N. Ganev: Application of X-ray tensorometry in mechanical engineering and material research,



279th Rozhovory, from the left: Z. Šourek, B. Kratochvíl, V. Langer

J. Hašek: Use of synchrotron radiation for study of structure and dynamics of macromolecules

Organization: J. Hašek

280th Seminar

Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, 11. 6. 2009

at the occasion of anniversary of S. Ďurovič

Lectures:

E. Makovický: How old are quasicrystals - excursion to cultural and archeological crystallography, M. Rieder: Silicate phases able of binding radioactive Cs: synthesis and crystal structures, J. Hybler: OD character and polytypism of mineral kettnerite, CaBiOFCO_3 , J. Majling: New regions of interest in arena of thermo-optical measurements, V. Petříček: Tradition of structure solution of difficult structures in our countries, T. Havlík: On possible applications of X-ray diffractometry for recycling of wastes, J. Kameníček: Quo vadis, X-ray structure analysis, D. Tunega: Activity of cationic absorption sites in zeolites and smectites - comparison, J. Kožíšek: Electronic struc-



280th Rozhovory



284th Rozhovory



M. Klementová



L. Palatinus



J. Fábry



S. Nazzareni



P. Comodi



R. Gyepes

the 2nd and 3rd generation in the Scientific center New Technologies in Pilsen, J. Kameníček: X-ray diffraction at the Faculty of Science, Palacky University - history and presence, R. Pažout: Chemistry and crystal structures of selected natural sulphosalts Ag-Pb-Bi-Sb, P. Bezdička: Ordinary day of one X-ray diffractionist

P. Antoš: Use of X-ray methods for characterization of pigments and organic coatings, O. Bortnovskiy: Use of powder diffraction for development of geopolymers, P. Koutník: Use of powder diffraction for development of production of calciumaluminates

Organization: P. Ryšánek

283rd Seminar

Institute of macromolecular chemistry, Academy of Sciences of the Czech Republic, 10. 12. 2009

Structure analysis

Lectures:

A. Fingerland: How to escape the science, J. Dubský: Use of diffraction for the study of plasma spraying, P. Šutta: Investigations of materials for photovoltaic technologies of

Organization: J. Hašek, R. Kužel

284th Seminar

Institute of Physics, Academy of Sciences of the Czech Republic, 18. 5. 2010

at the occasion of anniversary of M. Rieder

Lectures:

I. Kraus: Laudacio, M. Klementová: From the precession to the precession, L. Palatinus: How bad is too bad?, P. Comodi, HP-HT mineral physics and the implication for geosciences, S. Nazzareni: High pressure behavior of gypsum, F. Laufek: Application of experimental mineralogy to the systems containing Te and Se, E. Smrčok: Dynamics of hydrogens in 1:1 and 2:1 layered silicates with the aid of neutron inelastic scattering, R. Gyepes: Single crystal structure successfully solved - do we know everything?!,



284th Rozhovory. M. Rieder

J. Fábry, Notes on configuration of amine group-NH₂, R. Skála: Experimentally shock-loaded dolomite: TEM and XRD study, M. Rieder: Distressful ways to discoveries, M. Dušek: About department of structure analysis

Excursion

Organization: M. Klementová, J. Hybler

285th Seminar

Institute of macromolecular chemistry, Academy of Sciences of the Czech Republic, 20. 9. 2010

Prediction of Structure and Dynamics of Biomacromolecules

Lectures and short courses:

Samuel Coulbourn Flores: Prediction of Hinge Regions in Proteins. The Hinge Atlas, MolMovDB servers, and Molecular Motion Database.

B. Schneider, F. Pavelčík: Local Nucleic Acid Conformations from Experimental Data

Samuel Coulbourn Flores (Stanford University): Tutorial on the RNABuilder. Fundamentals and Applications.

Organization: J. Hašek

286th Seminar

Institute of macromolecular chemistry, Academy of Sciences of the Czech Republic, 13. 12. 2010

Lectures:

J. Kuběna: Curiosities about silicon, J. Fiala: Study of real structure by X-ray diffraction, M. Černík: Textures of hexagonal metals, X-ray analysis of meteorites, R. Kužel: Analysis of residual stresses and textures in thin films, selected non-routine cases, J. Hašek: Use of Cambridge structure database in science and teaching. New software in 2011.

Organization: J. Hašek



287th Seminar

U. S. Steel Košice, 4. 11. 2011

40 years of X-ray laboratory in U. S. Steel Košice

Lectures:

K. Lacková: Complex compounds Cu(II) containing tricyanmetanide and N-donor chelate ligands, L. Váhovská, Preparation and structure analysis of coordination compounds Fe(II) and Co(II) with N-donor bidentate ligands, P. Vranec: Square-planar Pd-complexes – analogues of cisplatin and carboplatinum, M. Almáši Study of structure of complexes of [Ln(OR)₃]_n type with the use of HE-XRPD, N. Pavlišáková, Structure of selected complexes of nickel and cobalt with 2'-dipyridylamin as blocking ligand, I. Větvička: Influence of flow on texture of wrapping pipes from Zr1Nb alloy investigated by neutron diffraction. L. Hrabčáková: Application of EBSD in U. S. Steel, M. Černík: History of X-ray lab since 1971. Activities, results, and interesting solutions - textures, residual stresses and pphase analysis.

Organization: M. Černík

288th Seminar

Institute of macromolecular chemistry, Academy of Sciences of the Czech Republic, 2. 12. 2011

Lectures:

I. Kraus: X-rays in history of the development of the Czech physics, L. Pina: X-ray optics in the Czech Republic - history and presenc, M. Čerňanský: Sgnificance of moments in profile analysis, V. Sklenář: Quo Vadis? NMR as an eminent tool for structural and systems biology, J. Maixner: Laboratory of X-ray diffractometry and spectrometry - history and presence, D. Gyepesová: Some aspects of structure research of selected inorganic compounds, F. Valach: Structure correlations in chemical crystallography, M.



I. Kraus

288th Rozhovory.

Petrák: Institute of Inorganic Chemistry in Ústí nad Labem,
R. Kužel: A tribute to Prof. Petera Klimanek and Prof.
Roberta L. Snyder

Organization: J. Hašek

Colloquium - Struktura 2008

Hotel Huberts, Valtice
16. - 19. 6. 2008

Main topics: Use of synchrotron radiation,
project CESLAB

Lectures:

Z. Pokorná: Synchrotron - physical principles and problems, P. Mikulík: CESLAB -project of central european synchrotron laboratory, J. Hrdý: Wigglers, undulators and othe sources of X-rays, P. Oberta: Synchrotron optics, R. Vašina: Construction of monochromators and focusing optics for infrared to soft X-ray radiation, P. Vagovič: Monochromatization of hard X-rays, V. Procházka: Nuclear resonant scattering and Mossbauer spectroscopy using synchrotron radiation, V. Holý: Study of nano-structures with sychrotron radiation, V. Holý, J. Dohnálek: Alternative small sources of intense X-rays, J. Hašek: Diffracton measurement for biocrystallography at synchrotrons, Y. Chuskin: Application of X-ray photon correlation

spectroscopy to soft matter, R. Mokso: Imaging methods, J. Roithová: VUV and chemistry in gas phase, J. Žabka: Application of synchrotron radiation for study of ionosphere of planets, G. Schoenhense: X-ray photoemission electron microscopy using synchrotron radiation - a powerful approach to chemical nanoanalysis, surface magnetism and ultrafast dynamics, M. Dopita, R. Kužel: Synchrotron radiation for materials research and powder diffraction, M. Vondráček: Czech Materials Science Beamline on synchrotron ELETTRA

Short Lectures:

M. Jergel: Real-time tracking of fast superparamagnetic nanoparticle self-assembling by focused synchrotron beam, P. Klang: Structure of GaAs whiskers grown on Si nanowires, M. Barchuk: Monte-Carlo simulation of diffuse x-ray scattering from dislocations in epitaxial layers, B.



Valtice



Struktura 2008



Schneider: Conformations of nucleic acids, A. Stsiapanava: Crystallization and preliminary X-ray characterization of DhaA mutants from *Rhodococcus rhodochrous*, A. Štěpánková: Beta-Galactosidase from *Arthrobacter* sp. C2-2 inhibited by galactonolactone; crystal structure with 2.2 Å resolution

Instruments

J. Dohnálek: Projects BIOCEV and INSTRUCT, J. Dohnálek: The first experience of a protein crystallographer with the Oxford Diffraction Enhanced Ultra source and the Atlas CCD detector, V. Smith: Bruker Latest Advances in Protein Crystallisation & Screening, M. Benson: Rigaku Automated crystal growth, transport, orientation and retrieval from Rigaku, V. Smith: Bruker Highest signal - Lowest noise: Detectors for X-ray crystallography, P. Munk: X-ray Diffraction analysis of packaged counterfeit drugs and controlled substances (narcotics), Peter Munk: Determination of Specific Surface Area and Nanoparticle Size Distribution by SAXS

WWW pages: <http://www.xray.cz/xray/csca/kol2008/>

Number of participants: 95

Organization: P. Mikulík, R. Kužel

17th Regional powder diffraction conference

Valtice, 19. - 20. 6. 2008

co-organized with colloquium

Lectures:

S. Daniš: Study of magnetic structures, V. Petříček: Refinement of magnetic structures by the system Jana2006, J. Maixner: Experience with automatic sample changer for XPert Pro, J. Drahoukoupil: Measurement of single crystal on powder diffractometer, D. Šimek: Transformation of NiTi wires with shape memory studied by synchrotron radiation, P. Roupčová: Analysis of phase composition of Zr-Fe-V after repeated charging and discharging by hydrogen, J. Hamza: Influence of real structure on quantitative phase analysis, L. Smrček: Structure of K_2TaF_7 at 720 °C - combined synchrotron powder diffraction and DFT calculations of solid phase, F. Laufek: Crystallographic studies of pyrite phases PtSnS, PtSeSe and PtSnTe, A. Buchal: Steel ČSN 14 331, 10 years after processing, M. Čerňanský: Cumulants in profile analysis, Z. Pala: Study of surface layers of large specimens by diffractometer X'Pert Pro, Z. Matěj: Coplanar grazing exit X-ray diffraction on thin polycrystalline films, L. Nichtová: Study of crystallization of TiO_2 thin films

Number of participants: 21

WWW <http://www.saske.sk/RPDK/>

Organization: V. Kavečanský, S. Jurečka, E. Čaplovič, R. Kužel

Colloquium - Struktura 2009

Parkhotel Hluboká, Hluboká nad Vltavou

22. - 25. 6. 2009

Main topics: structure analysis, biocrystallography, X-ray instrumentation, imaging, sources, surfaces, real structure, chemical crystallography

Lectures:

P. Vojtíšek: Stereochemistry of lanthanoid complexes used in medicine. Relation between structure and function, F. Laufek: Structure types of inorganic compounds in ICSD database, P. Řezáčová: Contemporary problems in protein crystallography, B. Schneider: New group of protein crystallography in Biotechnological Institute, S. Daniš: Coherent diffraction, J. Fiala, I. Kraus: Surfaces and interfaces, M. Dopita: Electron backscattered diffraction - principles and applications, P. Mikulík: Mapping of misorientation of crystal lattice by rocking curve mapping, M. Kotrlý: Micro and nanomaterials in forensic science, M. Šlouf: Electron diffraction, microanalysis and image analysis of nanocrystals, M. Klementová: Electron diffraction - SAED, CBED, NBED, PED

Short Lectures:

J. Drahoukoupil: Calculation of instrumental function, M. Čerňanský: Notes to the moments of diffraction lines, P. Roupčová: Influence of protective gas on the phase composition of Mg-Ni-Fe-H based nanocomposite prepared by Spark synthesis, J. Kopeček: Ferromagnetic shape memory alloy $Co_{38}Ni_{33}Al_{29}$ - single-crystal preparation and characterization, P. Vojtíšek: Useful disorder, J. Moncol: Polymorphism, isomorphism, distortion and supramolecular isomerism of complexes $[Cu(RCOO)_2(dena)_2(H_2O)_2]$ (dena = N,N-diethylnicotinamide), J. Hašek: Structure of valinomycin and its complexes, V. Goliáš: Experience with testing of XRD microdiffraction techniques for forensic science, P. Kacerovský: Microscopy of nanoparticles and layers with nanoparticles, P. Klang: X-ray characterization of GaAs nanowires on Si Nanowires



Struktura 2009.

M. Barchuk, the winner of the student presentations.



Struktura 2009, Student presentations
(P. Řezáčová, J. Wolfová)

J. Jiša

E. Sviridova



J. Krčmář

L. Horák



P. Pachtl



S. Bernátová



I. Kishko



A. Stsiapanava



A. Štěpánková

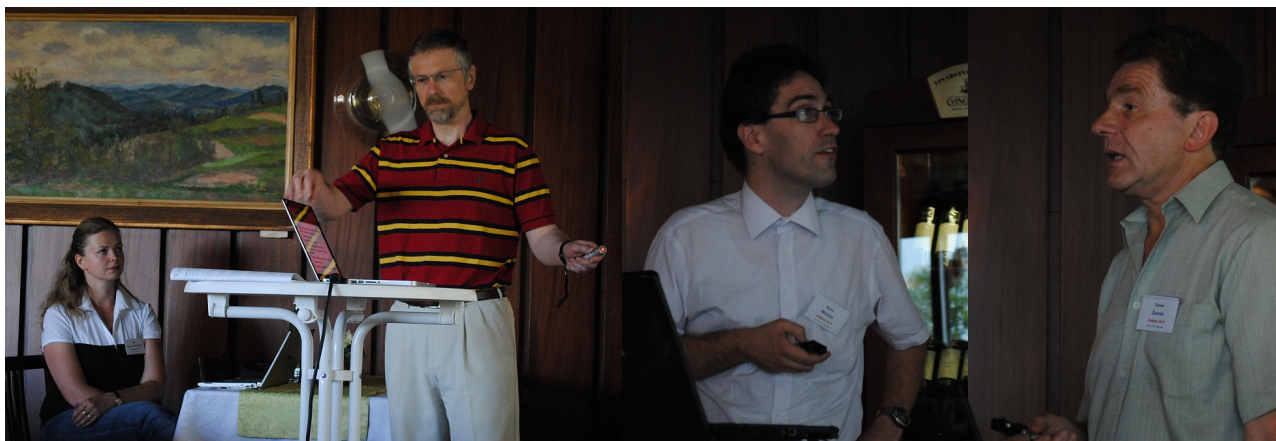
Instruments

L. Pína: Diffracted-beam analyzer with multiple single crystals for high resolution parallel-beam X-ray diffraction, B. Míč: Bruker products, J. Maixner: Experience with position sensitive detector LynxEye, P. Beran: Neutron powder diffraction in Institute of Nuclear Physics, Rez near Prague, T. Samtleben: New Possibilities for X-ray Diffractometry: Bringing Light into Homelabs, D. Gotz: New applications of the PIXcel detector, O. Presly: Cu vs Mo in Treatment of a Non-merohedral Twin using CrysAlisPro, S. Prugovecki: Hard radiation, Pair Distribution Functions.

8th series of student presentations in the field of X-ray and neutron structure analysis.

Traditional symposium of student presentations was organized within the framework of the colloquium. Twenty students from different institutions in Czech Republic and Slovakia presented the results of their diploma and doctoral thesis in the field of X-ray and neutron structure analysis. Main topics of presentations: powder diffraction and PDF on nanocrystalline powders and thin films, residual stresses, X-ray analysis of epitaxial and polycrystalline thin films, structure solution, protein crystallography.

The best presentations were evaluated and awarded - *Michael Barchuk* (Faculty of Mathematics and Physics,



Struktura 2010, I. Kutá Smatanová, B. Schneider

M. Meduňa

Z. Šourek

Charles University, Prague): Monte Carlo simulation in thin layers of GaN, *Jan Krčmář* (Faculty of Science, Masaryk University, Brno): X-ray diffraction on polycrystalline multilayers in GID geometry, *Andrea Štěpánková* (Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic): The binding modes of ligands in the active site of β -galactosidase, *Jan Jiša* (Faculty of Science, Masaryk University, Brno): Limits of X-ray reflection methods, *Petr Kolenko* (Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic): Design of novel polymers for macromolecular crystallography.

Courses:

Jana 2006 (V. Petříček, M. Dušek)

CCDC database (J. Hašek)

Real structure of polycrystalline materials (R. Kužel)

WWW pages: <http://www.xray.cz/xray/csca/kol2009/>

Number of participants: 84

Colloquium - Struktura 2010

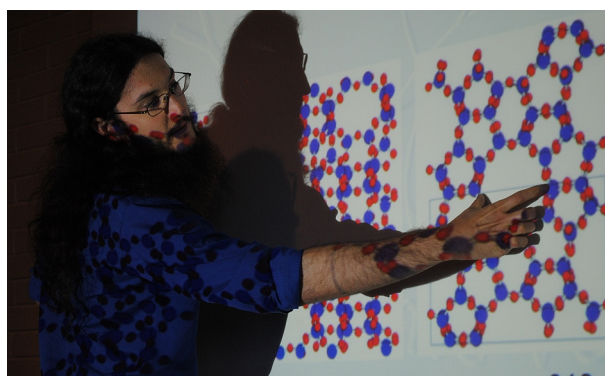
Hotel Soláň, Soláň

14. - 17. 6. 2010

Main topics: presentation of laboratories

Lectures:

J. Marek: Production of X-ray instruments in Czechoslovakia, Z. Šourek: Laboratory ROTAN, E. Dobročka: X-ray laboratory with rotating anode of consortium SAV MULTIDISC - possibilities of Bruker D8 DISCOVER SSS, M. Jergel: X-ray laboratory for coplanar and non-coplanar reciprocal space mapping on solid and liquid surfaces on FU SAV, M. Meduňa: X-ray structure methods at Institute of condensed matter, Faculty of Science, Masaryk University Brno, G. Demo: Current technological background for macromolecular crystallography in National center for research of biomolecules, B. Schneider: Structural biology at Biotechnological Institute, Academy of Sciences of the Czech Republic, I. Kutá Smatanová: Protein crystallography at University of South Bohemia, J. Hašek: Structure analysis of molecular systems in Institute of Macromolecular Chemistry Academy of Sciences of the Czech Republic, J. Ševčík: History and present of protein crystallography at ÚMB SAV, V. Goliáš: X-ray diffraction in geological branches at the Faculty of Science UK in Prague, L. Čaplovič: Laboratory of structure analysis in Institute of materials MTF STU Trnava, M. Černík: X-ray diffraction in U.S.Steel - residual stress, texture, and phase analysis, N. Ganev, Z. Pala: X-ray and neutron diffraction at Czech Technical University in Prague, M. Dušek: Department of structure analysis in the Institute of Physics, Academy of Sciences of the Czech Republic, J. Hybler: Laboratory for single crystal orientation at Institute of Physics, Academy of Sciences of the Czech Republic, M. Šlouf: Electron microscopy,



J. Drahokoupil



G. Demo



F. Eichler



F. Laufek

J. Hybler

M. Dopita

J. Rohlíček

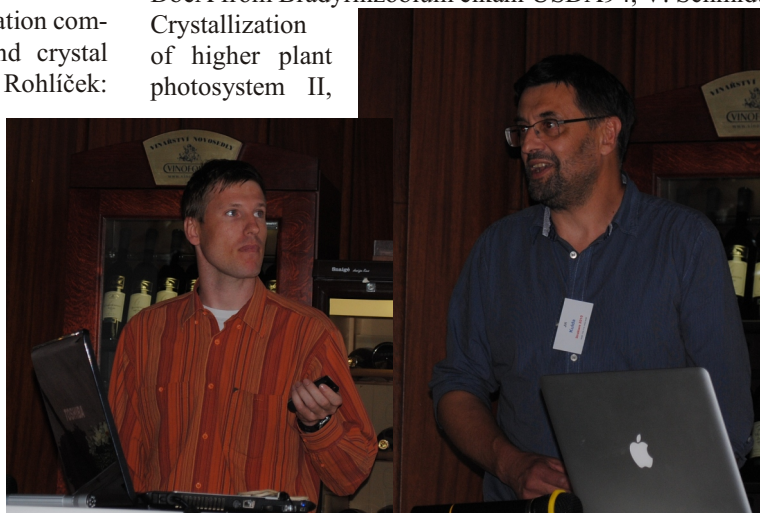
microanalysis and diffraction at ÚMCH AV ČR, v.v.i., L. Palatinus: Laboratory of electron precession diffraction FZÚ AVČR, J. Kulda: European infrastructures for neutron scattering studies, P. Beran: Neutron diffraction experiments on equipment MEREDIT, M. Kotrly: X-ray methods in criminalistic-technical a expert practise of Criminalistic Institute, Prague, M. Koman: Influence of X-ray structure on the development of coordination chemistry, J. Kožíšek: Electronic structure of coordination compounds, I. Císařová: Center of molecular and crystal structures in Faculty of Science, UK, Prague, J. Rohlíček: Structure analysis at Institute of solid state chemistry at Institute of Chemical Technology Prague, J. Filip: X-ray diffraction of nanomaterials at Faculty of Science, Palacky University Olomouc, R. Kužel, S. Daniš: Study of thin films and nanometaterials at MFF UK, M. Pospíšil: Use of molecular simulations for structure solution

Short Lectures:

F. Eichler: Possibilities of prediction of stability of sulphides to weathering from Rietveld analysis, P. Roupcová: Changes Of Phase Composition Of NaAlH_4 Based Complex Hy-

dride Exposed In The Air, R. Skála: On the elastic behavior of zeolite paulingite: a synchrotron powder diffraction study, F. Laufek: Synthesis and structure Pd_3AgSe a $\text{Pd}_3\text{Pb}_2\text{Te}_2$, J. Drahokoupil: Zeolite membranes - ZSM-5,

L. Urbániková: Structure-function relationship of xylanase A from *Erwinia chrysanthemi*, T. Prudnikova: Structure-functional analysis of a haloalkane dehalogenase DbeA from *Bradyrhizobium elkanii* USDA94, V. Schmidt: Crystallization of higher plant photosystem II,



P. Beran

J. Kulda



J. Maršík



M. Koman



S. Prugovečki



M. Čerňanský



M. Dušek



N. Ganev

J. Haníková: Structure of coordination compounds Cu(II) S N metylderivates of ethan; diamine and tetrafluoroboritan anion, P. Vranec: Complexes of Ni(II) and Pd(II) with 8-hydroxyquinoline derivatives, I. Kočanová: Contribution to study of crystal structure of Cu-Ni heterobimetalic coordination compounds,

M. Čerňanský: Method of two wavelength for determination of crystallite size and microstrain, J. Kopeček: Structural evolution in ferromagnetic shape-memory alloy Co₃₈Ni₃₃Al₂₉, D. Šimek: Investigations of properties of perlite steel in X-ray diffraction, M. Klementová: SiGe products prepared by CVD, P. Klang: Structural analysis of GaAs/Si nanowires, T. Čechal: Periodic modulation of deformation field and magnetic anisotropy in (Ga,Mn)As/InAs/GaAs structures.

Instruments

T. Samtleben: Clever diffractometers with the Incoatec microfocuss source, B. Míč: Bruker presentation, S. Prugovečki: Panalytical 2D and 3D detector), E. Sarakinou: New techniques for TEM nano-analysis : precession diffraction and 3D diffraction tomography for structure determination and (EBSD-TEM like) high resolution phase/orientation maps, L. Pina: X-ray Detector with Submicron Resolution



L. Čaplovič

Courses:

Protein crystallography (J. Dohnálek, J. Brynda, J. Hašek), Program MAUD (M. Dopita, M. Černík), Program MStruct (Z. Matěj).

WWW pages: <http://www.xray.cz/xray/csca/kol2010/>

Number of participants: 84



Struktura 2011 (more pictures can be found in issue 4).



Colloquium - Struktura 2011

Hotel Karel IV, Turnov
20. - 23. 6. 2011

Nanomaterials: M. Šlouf: Nanoparticles for multiple immunomarking and nucleation of crystallization of polymers, P. Roupcová: Nanocrystalline materials containing 3d metals for hydrogen storage, P. Brázda: $-\text{Fe}_2\text{O}_3$ - shape and distribution of size of nanocrystals prepared in SiO_2 matrix;

Materials: J. Drahokoupil: Analysis of highly mobile twin boundary in NiMnGa martensite by X-ray diffraction, J. Kopeček: Ferromagnetic shape-memory alloys, D. Šimek: The exploitation of X-ray diffraction in characterization of strength of hot-rolled and cold-drawn ferritic-pearlitic steel, M. Černík: X-ray diffraction analysis of ruins. EBSD analysis of wrapping sheets

Phase analysis, transformations:

J. Fiala: Qualitative and quantitative phase analysis, M. Kotrlý: Experience with powder microdiffraction in forensic practice, A. Zorkovská: Transformation of calcite to aragonite in the process of grinding egg-shell, J. Polák: Growing sapphire profiles by the EFG method and their use for structure analysis

Chemical analysis:

V. Starý: Electron probe microanalysis and some other methods of chemical analysis, S. Daniš: X-ray fluorescence, K. Mašek: Methods of surface and thin film chemical analysis (XPS, AES, SIMS), photoelectron diffraction, V. Havránek: Introduction to the use of ion beams, Ion scattering, PIXE, PIGE, proton microprobe. RBS, ion channeling, J. Dohnálek: Identification of ions in proteins

Structures:
M. Dušek: Constitution isomers of $[\text{Cp}^*_2\text{Mo}_2\text{P}_2\text{Se}_3(\text{CuI})_3(\text{CH}_3\text{CN})_n]$, J. Hašek: Interaction of polymers with proteins - Polymer structure database, J. Brynda: Aspartate proteases of pathogenic yeast cell *Candida parapsilos*, M. Pospíšil: Intercalated hydroxaltes, diffraction and modeling, F. Laufek: Crystallographic study of ternary systems with Pt-metals,

L. Sodomka: 116 years of use of X-rays, Determination of perfection of TiC and BN grains prepared with self-propagating high temperature synthesis (SHS), M. Čerňanský: Method of two radiations - experiment, R. Kužel: Textures and stresses in thin films

Instruments

J. Maršík: New possibilities of Smartlab diffractometer, B. Míč: Bruker products, T. Samtleben: High-brilliance low-maintenance microfocus sources for diffractometry

9th series of student presentations in the field of X-ray and neutron structure analysis.

Traditional symposium of student presentations was organized within the framework of the colloquium. Thirteen students from different institutions in Czech Republic and Slovakia presented the results of their diploma and doctoral thesis in the field of X-ray and neutron structure analysis. Main topics of presentations: protein crystallography, nanomaterials and thin films, residual stresses, textures

The best presentations were evaluated and awarded - *Zdeněk Pala* (FJFI CVUT - Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University, Prague): Investigations of real structure depth distributions using diffraction, *Monika Krůželová* (FJFI CVUT): Neutron diffraction study of Zr-based alloys, *Jan Drahokoupil* (FJFI CVUT): Phase transition in austenitic steel induced by plastic deformation, *Lukáš Horák* (Faculty of Mathematics and Physics, Charles University, Prague): Study of Mn interstitials in (Ga,Mn)As using HRXRD, *Andrea Štěpánková* (Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague): Structural and functional study of bi-functional anhydrolase.

Courses:

Phase analysis (P. Bezdička)

WWW pages: <http://www.xray.cz/xray/csca/kol2011/>

Number of participants: 63



7th Discussions in Structural Molecular Biology

Academic and University Center, Nové Hradky,
12. - 14. 3. 2009

Main lectures:

R. Ettrich: Structure of the motor subunit and translocation model for EcoR124I restriction-modification complex, J. Dohnálek: The Small Laccase from *Streptomyces coelicolor*, Z. Jiroušková: Electronegativity Equalization Method - Fast Method For Charge Calculation, J. Kmuňiček, M. Kuba: Metacentrum: e-infrastructure for solving structural biology research challenges, J. Burda: Quantum chemical description of the properties and reaction mechanisms of selected anticancer metallodrugs with biomolecule, J. Přecechtělová: The influence of backbone and solvent dynamics on ³¹P chemical shift tensors in Dickerson dodecamer: A combined MD/DFT study, B. Schneider: DNA local conformations and their sequence preferences, I. Kratochvílová: Conductivity of natural and modified DNA measured by Scanning Tunneling Microscopy. The effect of sequence, charge and stacking, V. Sklenář: Quo vadis? NMR as an eminent tool for structural and systems biology, T. Obšil: Role of 14-3-3 proteins in the regulation of G-protein signaling, J. Jonák: Proteosynthetic elongation factor EF-Tu domains: thermal adaptation and functions

Short contributions:

P. Florek, J. Hašek, A. Štěpánková, T. Koudeláková, J. Vondrášek, M. Krupička, A. Fořtová, V. Štumbauer, V. Sychrovský, I. Beššeová, J. Černý, P. Pachel, F. Lankáš, R. Chaloupková, V. Bauerová, Z. Halbhuber, J. Vlach, P. Plevka, D. Štys

WWW - <http://www.structbio.eu/>

Number of participants: 109

Number of posters: 42

Abstracts in *Materials Structure* vol. 16 (2009), č. 1a.



P. Řezáčová, J. Vondrášek

8th Discussions in Structural Molecular Biology

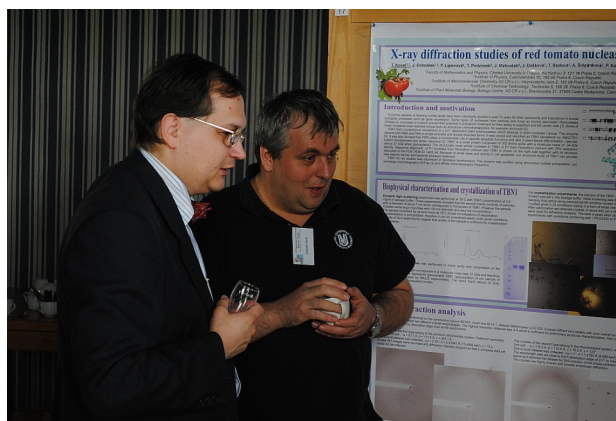
Academic and University Center, Nové Hradky,
18. - 20. 3. 2010

Main lectures:

P. Jungwirth: The interface between oxidized phospholipid bilayers and aqueous solutions, R. Ettrich: Was binding of free amino acids an early innovation in the evolution of allostery? J. Koča: Computational methods as a component of modern structural biology, I. Barák: Molecular and structural mechanisms of cell division site recognition in *Bacillus subtilis*, B. Schneider: Bioinformatic analyses of the first solvation shell of nucleic acids, M. Kuba: MetaCentrum - On the Way from Distributed Computing to Cyber Infrastructure for Research, D. Štys: Three dimensional information structure of living cell fate, V. Motáčková: Structure and dynamics of RNA polymerase delta subunit from *Bacillus subtilis* determined by NMR spectroscopy, K. Kubíček: Structural insights into recruitment and dissociation of RNA polymerase II termination factors, V. Veverka: Structural insight into regulation of the Wnt/b-catenin signalling pathway by sclerostin: implications for osteoporosis treatments.



V. Sklenář, B. Schneider



V. Kopecký, Z. Kříž



D. Antoř, I. Křenková, J. Dohnálek

Short contributions:

Z. Tořner, P. Srb, J. Prchal, V. Kopecký, V. Andruschenko, I. Kratochvílová, B. Minofar, V. Štěpánková, T. Mozga, V. Spiwok, R. Svobodová-Vařeková, J. Černý, L. Benda, C.M. Ionescu, J. Alán, T. Obřil, K. Procházková, P. Mader, D. Kopečný, J. Wolfová, T. Klumpler, J. Hařek F. Hóbor, J. Houser, R. Dvorský

WWW - <http://www.structbio.eu/>

Number of participants: 113

Number of posters: 44



V. Sklenář

9th Discussions in Structural Molecular Biology

Academic and University Center, hotel Residence, Nové Hradý, 24. - 26. 3. 2011

Main lectures:

I. Barák: Lipid helices formation in *Bacillus subtilis* cell membrane, P. Malý: Generation of artificial binders with affinity to human cytokines via computer-assisted mutagenesis of a stable protein scaffold and ribosome display selection, J. Přecech elová: Torsion angle dependence of phosphorus chemical shifts in a nucleic acid backbone from combined molecular dynamics and density functional calculations, P. Řežáčová: Crystal structures of two protease inhibitors from tick saliva, L. Urbániková: Structural basis for substrate recognition by GH30 glucuronoxylanase from *Erwinia Chrysanthemii*, J. Brynda: Crystal structure of the mouse galectin-4 N-terminal carbohydrate recognition domain, R. Dvorský: Impact of Point Mutations on Protein Functions: Example Case of Ras GTPases

Short contributions:

P. Dvořák, J. Prchal, J. Dohnálek, D. Rozbeský, P. Hanc, V. Andruschenko, L. Řežábková, M. Šebela, P. Man, Z. Chval, V. Sychrovský, Z. Futera, V. profant, J. Hudecová, D. Řeha, I. Kishko, J. Hařek, A. Štěpánková, T. Koval, O. Kroutil, M. Krupička, P. Pahl, A. Křenek, M. Ruda, O. Skřehota, J. Houser, R. Ettrich

WWW - <http://www.structbio.eu/>

Number of participants: 122

Number of posters: 46

Czech Society for Structural Biology

During the 8th Discussions the Czech Society for Structural Biology was founded, bylaws were accepted and a board elected

The official address is

The Czech Society for Structural Biology
(Česká společnost pro strukturní biologii)
Videňská 1083
CZ-142 20 Praha 4, Czech Republic
fax: +420 296 443 610
IČO: 0022869433

Board:

Ing. Jan Dohnálek, Ph.D., chair
Prof. RNDr. Vladimír Sklenář, DrSc., vicechair
Ing. Bohdan Schneider, DrSc., treasurer

Doc. RNDr. Rudiger Ettrich, PhD, RNDr. Jindřich Hařek, DrSc., Ing. Richard Hrabal, CSc., Doc. RNDr. Tomáš Obřil, Ph.D., members.



FEBS Advanced Course

Advanced methods in macromolecular crystallization III, IV

Academic and University Center, Nové Hradky, Czech Republic, October 3–10, 2008 and June 25–July 2, 2010

The practical and lecture courses were organized as continuation of two previously successful FEBS advanced crystallization courses in 2004 and 2006. Both courses were organized under the main sponsorship of the FEBS, however, other companies also sponsored the courses mainly by contribution of material and providing their equipment for the lab exercises. Outstanding lecturers/tutors have accepted our invitation and thank to them, a high level of the courses was provided. Students, mainly those having previous experience in the field of macromolecular crystallization, were introduced to standard and advanced methods of protein isolation, purification, crystallization screening and optimization, crystal handling and dynamic light scattering as well as working with crystallization robot. Speakers together with organizers and company representatives gave more than 20 lectures aimed at topic of protein expression and purification, protein refolding and protein modification for crystallization, solution properties and phase diagrams, standard and advanced crystallization techniques, crystals manipulation, DLS and advanced light scattering methods, membrane protein crystallization, etc. During four hours afternoon practical exercises focused on twelve different topics, students trained freshly obtained knowledge and used standard and advanced crystallization methods to grow crystals of their own proteins. Participants were encouraged to present their projects as poster presentations. The posters were displayed during whole courses

and the poster sessions were organized as evening events. Most participants seemed to be very satisfied with scientific and social program of courses. The social program included a trip to Hluboká nad Vltavou (2008) and Český Krumlov (2010). The abstracts of all lectures, lab exercises and poster presentations were published in a special issues of *Materials Structure in Chemistry, Biology, Physics and Technology*, vol. 15, no. 3a (2008) and vol. 17, no. 3a (2010), available on-line at <http://www.xray.cz/ms>.

No of students: 30/25 graduate students and postdocs (2008/2010)

No of speakers/tutors: 18/21 invited speakers + 3 organizers (2008/2010)

WWW: www.img.cas.cz/igm/cc

Organizer: Ivana Kuta Smatanová

Co-organizers: Pavlína Řezáčová, Rolf Hilgenfeld



FEBS course 2010.



12th Heart of Europe bio-Crystallography Meeting (HEC)

Třeš , September 24-26, 2009

In good tradition since 1998, mainly PhD students presented their results (and problems) in 20 min talks including discussion. The meeting was held in the Caste Hotel Třeš , which provided an elegant atmosphere for the talks and breaks. Most participants were accomodated in the building, which was transformed from a fortress into a castle during the 15th century. Pavlína Řezáčová and her structural biology group from Prague organized a stimulating scientific meeting and a pleasant stay for the participants. A highlight of the meeting is traditionally the invited HEC lecture, which was given by Paul Emsley (University of Oxford, UK). In a vivid and diverting talk, he reported about the development of the Coot program and provided insight into the many helpful functions for model building.

The free time on Friday afternoon a trip to Telc. A price for the best presentation was kindly sponsored by the IUCr: the book "Crystallography across the sciences". This year even two participants could be awarded with the price: P. Mader (IMG, Prague) and E. Ch. Schulz (Göttingen). Additional prizes were awarded for the best pronunciation of the name "Třeš ". The lucky winners received a bar of the favourite Czech chocolate 'Studentska pecet' (Student's seal). Linda Schuldt (EMBL Hamburg) was also rewarded with this chocolate for her active participation in the discussion after the talks. The HEC organizers hope for a stronger participation of the PhD students in the discussions in the future. Altogether, HEC-12 presented another highlight in the long history of the HEC-meetings.

Number of participants: 107

CSCA Scientific board 2007-2010

Members

Ing. Hana Brusová

Laboratory of solid state and optical purity
Zentiva, a.s.

Assoc. Prof. Jiří Brynda, CSc.

Institute of Molecular Genetics
Academy of Sciences of the Czech Republic, Prague

Dr. Antonín Buchal

Institute of Materials Engineering,
Technical University, Brno

Assoc. Prof. Ing. Lubomír Čaplovič

Faculty of Materials Science and technology,
Slovak Technical University, Trnava

Prof. Jaroslav Fiala

Faculty of Mechanical Engineering
West Bohemian University, Plzeň

Assoc. Prof. Nikolaj Ganev

Faculty of Nuclear Engineering
Czech Technical University, Praha

Dr. Jindřich Hašek

Institute of Macromolecular Chemistry,
Academy of Sciences of the Czech Republic, Praha

Prof. Václav Holý

Faculty of Mathematics and Physics,
Charles University, Prague
Faculty of Mathematics and Physics,
Charles University, Prague

Dr. Jiří Hybler

Institute of Physics,
Academy of Sciences of the Czech Republic, Praha

Dr. Jiří Kulda

Institute of Laue-Langevin
Grenoble, France

Dr. Ivana Kutá Smatanová

Institute of Physical Biology, South Bohemian
University at České Budějovice

Assoc. Prof. Radomír Kužel

Faculty of Mathematics and Physics,
Charles University, Praha

Dr. Zbyněk Šourek

Institute of Physics, Academy of Sciences of
the Czech republic, Praha

CSCA Scientific board elected for the period 2010-2013

Members

Ing. Hana Brusová

Laboratory of solid state and optical purity
Zentiva, a.s.

Assoc. Prof. Jiří Brynda, CSc.

Institute of Molecular Genetics
Academy of Sciences of the Czech Republic, Prague

Ing. Lubomír Čaplovič

Faculty of Materials Science and technology,
Slovak Technical University, Trnava

Prof. Jaroslav Fiala

Faculty of Mechanical Engineering
West Bohemian University, Plzeň

Prof. Nikolaj Ganev

Faculty of Nuclear Sciences and Physical Engineering
Czech Technical University, Praha

Dr. Jindřich Hašek

Institute of Macromolecular Chemistry,
Academy of Sciences of the Czech Republic, Praha

Dr. Jaromír Hrdý, DrSc.

Institute of Physics,
Academy of Sciences of the Czech Republic, Praha



- Dr. Jiří Hybler
Institute of Physics,
Academy of Sciences of the Czech Republic, Praha
- Dr. Jiří Kulda
Institute of Laue-Langevin
Grenoble, France
- Dr. Ivana Kutá Smatanová
Institute of Physical Biology, South Bohemian
University at České Budějovice
- Assoc. Prof. Radomír Kužel
Faculty of Mathematics and Physics,
Charles University, Praha
- Assoc. Prof. Petr Mikulík
Faculty of Science, Masaryk University,
Brno
- Ing. Bohdan Schneider
Biotechnological Institute
Academy of Sciences of the Czech Republic, Praha
- Dr. Zbyněk Šourek
Institute of Physics, Academy of Sciences of
the Czech republic, Praha

CSCA Information Centre

CSCA Journal

The journal "Materials Structure in Chemistry, Biology, Physics and Technology", ISSN 1210-8529. Contributions can be published in English, Czech or Slovak. Scientific papers are reviewed usually by two independent referees.

Web page of the journal: <http://www.xray.cz/ms>.

Other Journals and Proceedings

IUCr (International Union of Crystallography) Newsletter is quarterly distributed to all CSCA members.

Databases installed

The latest versions of crystallographic databases are installed in Institute of Physics and Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Faculty of Mathematics and Physics, Charles University, Slovak Technical University Bratislava

INTERNET

The association would like to extend the use of Internet.

Address of WWW page: <http://www.xray.cz>

Regional Committee of the IUCr

- Assoc. Prof. Radomír Kužel (Chair)
Faculty of Mathematics and Physics,
Charles University, Praha
- Prof. Marian Koman (Vice-chair)
Department of Inorganic Chemistry,
Faculty of Chemical and Food Technology,
Slovak Technical University, Bratislava
- Assoc. Prof. Dr. Ľubomír Čaplovič
Faculty of Materials and Technology
Slovak Technical University, Trnava
- Prof. Juraj Černák
Faculty of Nature, Safarik University, Košice
- Assoc. Jozef Kožíšek
Faculty of Chemical and Food Technology
Slovak Technical University, Bratislava
- Dr. Petr Mikulík
Faculty of Science, Masaryk University, Brno
- Dr. Ivana Kutá Smatanová
Institute of Physical Biology, South Bohemian
University at České Budějovice
- Prof. Nikolaj Ganev
Faculty of Nuclear Sciences and Physical Engineering
Czech Technical University, Praha

Addresses of the CSCA officials

President:

Dr. Jindřich Hašek

Institute of Macromolecular Chemistry
Heyrovského nám. 2, 162 06 Praha 6
Tel. 00420- 296 809 390,
Fax: 00420- 296 809 410
E-mail: hasek@imc.cas.cz

Vice Presidents:

- Dr. Ivana Kutá Smatanová
Institute of Physical Biology, South Bohemian
University at České Budějovice
- Dr. Zbyněk Šourek
Institute of Physics, Academy of Sciences of
the Czech republic, Praha

Secretary:

Assoc. Prof. Radomír Kužel
Faculty of Mathematics and Physics
Ke Karlovu 5, 121 16 Praha 2
Tel: 00420-221911394
Fax: 00420-224911061
E-mail: kuzel@karlov.mff.cuni.cz

J. Hašek, R. Kužel, I. Kutá Smatanová