



CZECH AND SLOVAK CRYSTALLOGRAPHIC ASSOCIATION

The Czech and Slovak Crystallographic Association (CSCA) organized or co-organized several conferences and traditional one-day seminars in 2006-7.

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

268th Seminar

Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, 18. 5. 2006

to the anniversary of Dalma Gyepesová

Lectures:

M. Koman: Importance of X-ray structure analysis for estimation of biological activity of compounds, J. Hašek: 40 years of Cambridge structure database of organic and organometallic compounds, F. Pavelčík: From coordination chemistry to structure genomics, J. Marek: A few examples of use of X-ray crystallography for anti-cancer research, D. Mikloš: Variability of binding of biologically active ligands in coordination compounds, Z. Žák: Basic nitrates of lanthanoids, J. Černák: Advances in study of cyanocomplexes, J. Fábry: Dependence of frequency of appearance of space group types on reduced volumes of unit cells of organic and organometallic compounds, D. Tunega: Modeling of adsorption processes on surfaces of minerals by method of molecular dynamics.

Organization: L. Smrčok

269th Seminar

Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, 29. 5. 2006

Position sensitive detectors of X-rays

Lecture:

J. Fiala: Comeback of position sensitive detector in powder diffraction, V. Kolařík: Real structure effects in FeCrAl alloys during initial oxidation at high temperature, M. Čerňanský: Determination of crystallite size from statistical fluctuations of azimuthal profile, J. Pechmanová: Recrystallization of austenitic steels, O. Vojtíšek: Digital imaging by imaging plates – principle and basic characteristics, Z. Porkert: Area-sensitive detectors in non-destructive materials testing, J. Hybler: Identification of polytypes with the aid of data from CCD detector, N. Ganey: Imaging plate in laboratory of X-ray diffraction, Fac. of Nuclear and Physical Eng., Z. Pala: Characteristics of imaging plate used in X-ray lab (Fac. of Nucl. Eng.), P. Sedlák: Precise

determination of single crystal orientation by Laue method for ultrasound spectroscopy, D. Novotný: Products delivered by Pragolab. New powder diffractometer.

Excursion in X-ray laboratory of Department of Solid State Engineering, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague.

Organization: N. Ganey

270th Seminar

Institute of macromolecular chemistry, Academy of Sciences of the Czech Republic, 15. 12. 2006

Lectures:

I. Kraus: Adéla Kochanovská and her fellows Petr Skulari and Jan Boehm, Z. Žák: Basic nitrates of lanthanoids, J. Černák: Magneto-structural correlation in compounds Cu(II) with cyanocomplex anions, A. Buchal: Powder diffraction on Technical University Brno, R. Králová: A few feedbacks from crystallographic life, L. Čaplovič: Application of diffraction techniques in materials engineering, M. Steinhart: Small-angle scattering under high pressures

Organization: J. Hašek, R. Kužel

271st Seminar

Centre of nanotechnologies, Technical university Ostrava, 22. 3. 2007

Nanomaterials based on intercalates and surface modifies structures

Lectures:

J. Bujdák: Optical properties of surface modified silicates, F. Kovanda: Mg-Al hydrotalcites - intercalated porphyrines, M. Pospíšil: Structure analysis of intercalates - molecular modelling and experiment, Z. Klika, P. Praus: Intercalates of layer silicates, V. Zima: New organic-inorganic hybrid materials based on arylphosphates of metals, P. Praus: Adsorption of cationic tensides on montmorillonite, L. Obalová: Catalysts based on hydrotalcites, M. Valášková: Photoactive nanoparticles in clay matrix, G. Simha Martynková: Nanocomposites polymer-silicate, K. Barabaszová: Mechanic procedures of preparation of silicate nanoparticles and characterization.

Organization: P. Čapková

272nd Seminar

Faculty of Science, University of P.J. Šafárik, Košice 17. 5. 2007

Application of diffraction methods in research and education in region Košice

Lectures:

I. Potočnák: Study of shapes of coordination polyhedra of complexes Cu(II), V. Zelenák: Use of X-rays for study of mesoporous materials, J. Ďurišin: Characterization of



nanomaterials by combination of X-ray powder diffraction and electron microscopy, V. Kavečanský: On crystal structure of perovskites of LaMnO_3 type, M. Černík: Texture of rolled steel sheets by X-ray and electron diffraction, J. Kuchár: Preparation and structural characterization of two carboxyle complexes, M. Vávra: Preparation and characterization of tetracyanoplatnatane complexes of copper with bidentate N-donor ligands

Organization: J. Černák

273rd Seminar

Centre of nanomaterials research, Faculty of Science, Palacky University, Olomouci
17. 10. 2007

Nanoparticles based on iron and iron oxides

Lectures:

M. Matíková Mařárová: Crystal structure $[\text{Co}(\text{en})_3][\text{Fe}(\text{CN})_6] \cdot 2\text{H}_2\text{O}$ and products of its dehydration, J. Tuček: Magnetism of nanoparticles of iron oxides, J. Filip: Environmental application of nanoparticles of iron and iron oxides, J. Cupalová: Magnetic nanoparticles produced by microorganisms, J. Frydrych: CEMS – method of study of nanolayers, K. Kluchová: Contrast compounds for MRI on the base of iron oxides, M. Heřmánek: Characterization of nanoparticles prepared by thermal decomposition of ferrous oxalate, L. Machala: Study of thermal decomposition of ferric sulphate by Mössbauer spectroscopy

Excursion in Center of nanomaterial research

Organization: M. Mašláň, D. Krausová

274th Seminar

Institute of inorganic chemistry, Slovak Academy of Sciences, 29. 11. 2007

to anniversary of František Hanic

Lectures:

F. Hanic: Influence of structural properties of water and and phase transitions of minerals on motion of continents in gravitation fields (supplement of principles of "global tectonics"), V. Petříček: Charms and hardships of structure analysis, J. Majling: Thermoanalytical measurements of optical transmissivity of materials - methodical application starting points, Z. Žák: Van der Waals radii, P. Baňacký: Basic electronic state of superconductors, M. Koman: Influence of X-ray analysis on some chemical ideas, J. Kameníček: Ni - complexes with selected S,S- and other N,P- ligands in coordination sphere, J. Hašek: Synchrotron radiation in X-ray structure analysis, J. Černák: Advances in research of kyanocomplexes – $\text{Cu}(\text{NH}_3)_2\text{Ag}_2(\text{CN})_4$, J. Fiala: Curved structures in carbon based materials.

Organization: L. Smrčok

275th Seminar

Institute of macromolecular chemistry, Academy of Sciences of the Czech Republic, 10. 12. 2007

History and future of structure analysis

Lectures:

V. Valvoda: History of structure analysis in Faculty of Mathematics and Physics, Charles University, Prague
J. Marek: X-ray diffraction equipment and methods - my experience since 1951, Production of X-ray tubes in Chirana-Modřany, M. Šlouf, D. Králová: Electron diffraction and microanalysis in Institute of Macromolecular Chemistry,

P. Mikulík: Central European Synchrotron Laboratory (CESLAB) in Brno, X-ray imaging, topography, J. Hašek: Use of synchrotron radiation for study of structure and dynamics of macromolecules, R. Kužel: Synchrotron radiation in structure analysis of polycrystals, beamline for powder diffraction and materials science, Petr Oberta: X-ray optical laboratory in CESLAB

Organization: J. Hašek, R. Kužel

Colloquium - Struktura 2006

Institute Laue-Langevin, ESRF, Grenoble
20. - 25. 6. 2006

Synchrotron radiation and neutron scattering

Bus trip in Villigen

Excursion in Paul Scherrer Institute, Villigen, 21. 6.

Main topics: powder diffraction, materials research, biocrystallography, X-ray imaging, thin films, neutron scattering

Lectures:

M. Brunelli: The High Resolution Powder Diffraction beamline ID31 at the ESRF, G. Vaughan: Time-resolved powder diffraction, D. Bourgeois: Kinetic protein crystallography, M. Budayová-Spano: Neutron biomacromolecular crystallography in Grenoble, J. Härtwig: X-ray imaging, P. Pernot: Synchrotron topography as an unique tool for investigation of various physical phenomena, M. Di Michiel: Fast microtomography, O. Caha: Evolution of the spontaneous lateral composition modulation in InAs/AlAs superlattices on InP, H. Metzger: X-ray scattering on surfaces and nanostructures, V. Holý: X-ray scattering from self-organized semiconductor nanostructures - our results and hopes for future, A. Wildes: Neutron reflectometry at the ILL, J. Rodríguez-Carvajal: Neutron powder diffraction, V. Honkimäki: High-energy X-ray diffraction, B. Janoušová: Neutron Laue diffraction - applications in magnetism and hard condensed matter, M. Kempa: Study of ferroelectrics by inelastic neutron scattering, M. Sládkovičová: Hydrogen Bonding in TRIS: INS Spectroscopy and Quantum Chemistry Methods, J. Hašek: Function of enzymes and their inhibition studied by X-ray crystal-



lography, M. Wimmerová: Protein-Carbohydrate interaction: Structural and thermodynamic characterization of high affinity binding between lectins from pathogens and host carbohydrates, J. Dohnálek: Structure of beta-galactosidase complexes, J. Ondráček: Multisolution refinement methods - closer to reality, J. Brynda: High precision protein crystallography, R. Černý: Complex intermetallic compounds and metal hydrides from powder diffraction, J. Maixner: Structural analysis of organic powders and microcrystals with synchrotron radiation, F. Laufek: Contribution to the crystallography of owoyheeite

WWW pages <http://www.xray.cz/xray/csca/kol2006/>

Participation: 80

Organization: J. Kulda, V. Holý, R. Kužel, J. Hašek, Z. Šourek

All abstracts published in *Materials Structure* v. 13, number 2 (<http://www.xray.cz/ms/>).

Colloquium - Struktura 2007

Penzion za vodou, Dvůr Králové
18. - 21. 6. 2007

Main topics: structure databases, diffraction under non-ambient conditions, phase transformations, surfaces and thin films, powder diffraction, course of protein crystallography, Panalytical users meeting, commercial presentation - Bruker, Panalytical, Rigaku, Pragolab

Main lectures:

R. Kužel, S. Daniš: Structure databases of inorganic structures ICSD, CRYSTMET, PDF4, Pearson's Crystal Data and other freely available structure oriented databases in Internetu, J. Hašek: Databases of organic structures CSD and related software, B. Schneider: Biostructural database PDB and NDB, F. Pavelčík: Automatic building of models of proteins and nucleon acids, V. Šíma: Phase transitions, phase diagrams, differential scanning calorimetry, V. Janovec: Databases of materials with structural phase transitions, D. Rafaja: Microstructure analysis of nanocrystalline materials and nanocomposites using the combination of X-ray diffraction and transmission electron microscopy, R. Kužel: Crystallography of surfaces, brief review of methods for study of structure of surfaces and thin films, I. Ošádal: Surface microscopies with atomic resolution, R. Kužel: Some commercial programs for structure visualization and simulation of diffraction patterns - Diamond, Crystallographica, Crystal Maker

7th 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. 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. One of the highest number of the presentations (25) in the history of the meeting was achieved. Main topics of presentations: re-

sidual stresses, thin films, structure solution, phase analysis, microdiffraction, protein crystallography, mineralogy.

The best presentations were evaluated and awarded - *Jan Filip* (Faculty of Science, Palacky University, Olomouc): Solid-state synthesis, characterization and applications of potassium ferrate(VI): A multi-analytical approach, *František Laufek* (Czech Geological Survey): Synthesis and structure of CoGeTe and CoSn_{1.5}Te_{1.5}, *Jan Krčmář* (Faculty of Science, Masaryk university i Brno): Standing-wave effects in grazing-incidence X-ray diffraction from polycrystalline multilayers, *Tatyana Prudnikova* (Institute of Physical Biology, University of South Bohemia, Nové Hradý): Structural and functional studies of higher plants photosystem II, *Daniela Králová* (Institute of macromolecular chemistry, Acad. Sci. Prague): Preparation and structure of titanate nanotubes

WWW pages: <http://www.xray.cz/xray/csca/kol2007/>

Number of participants: 79

5th Discussions of structural biologists

Institute of Physical Biology, Nové Hradý, 16. - 18. 3. 2006

Plenary lectures:

B. Schneider: Structural databases in biology, R. Ettrich: Molecular systems biology: Molecular simulations of proteins and their complexes, J. Šponer: Molecular simulations of RNA, J. Dohnálek: Structure elucidation by diffraction methods - contribution to structural biology,

Short contributions:

T. Obšil, K. Bezouška, J. Vlach, Z. Vokáčová, J. Florian, P. Macek, J. Šebek, P. Flecker, M. Hušák, P. Florek, M. Lexa, P. Palenčár, J. Brynda, V. Krejčířiková, D. Svozil, Z. Prokop, T. Mozga, R. Chaloupková, T. Chrobáková, M. Klvaňa

WWW <http://www.xray.czs/setkani/>

Number of participants: 84

Number of posters: 36

Organization: B. Schneider, I. Kutá Smatanová, R. Kužel, D. Štys, J. Hašek

Contributions in Materials Structure vol. 13 (2006), no. 1.

6th Discussions in Structural Molecular Biology and Bioinformatics

Institute of Physical Biology, Nové Hradý, 29. - 31. 3. 2007

Organized for the first time with bioinformatics

Plenary lectures:

F. Lankaš, T. Polívka,

Short contributions:

P. Plevka, P. Kolenko, M. Kolář, J. Brynda, T. Obšil, L. Židek, P. Srb, R. Štefl, V. Sychrovský, Z. Vokáčová, J. Burda, J. Mrázek, T. Zimmermann, J. Adam, R. Ettrich, O. Šulák, N. Mishra, B. Schneider, D. Nachtigallová,



D. Štys, P. Šebo, I. Kratochvílová, J. Pačes, E. Brumovská,
J. Dohnálek, J. Hašek, P. Řezáčová

WWW - <http://www.xray.czs/setkani/>

Number of participants: 109

Number of posters: 42

FEBS Course – FEBS PLC06-35

Advanced methods in macromolecular crystallization II

Nové Hradky, Czech Republic, October 06-13, 2006

The FEBS Practical and Lecture Course „Advanced methods in macromolecular crystallization II“ was organized as a second year-class of previous successful crystallization course FEBS AC04-13 held in October 2004. The course took place at the Academic and University Center (AUC) in Nové Hradky (near České Budějovice) during the first week of October (06. - 13. 10. 2006). The course was organized under auspices of the FEBS; ten other companies sponsored the course mainly by contribution of material and items for lab exercises. 14 notable lecturers/tutors have accepted invitation and thank them high level of the course was provided. 22 students from EU, one from Asia and one from Africa were attending the morning lecture sessions and afternoon laboratory exercises. Students (14F and 10M) were introduced to standard and advanced methods of protein isolation, purification and crystallization, using of seeding and cryo-cooling techniques and dynamic light scattering. They tested all from lectures gained experiences in the lab individually.

Most participants seemed to be very satisfied with scientific and social program of the course. In view of positive response from questionnaires, we are delighted to call the FEBS Practical and Lecture Course PLC06-35 a successful and very fruitful. We are looking forward to similar activities scheduled for the year 2008 (FEBS PLC08-002, October 3-10 2008).

No of students: 24

No of speakers/tutors: 14+3 organizers

Organizer: Ivana Kuta Smatanova

Co-organizers: Pavlína Řezáčová, Rolf Hilgenfeld

16th Regional powder diffraction conference

Tatranská Štrba, 19. - 21. 9., 2007

devoted to the anniversary of A. Buchala

Lectures:

A. Buchal: My life together with diffraction, V. Langer: Thermodiffraction of cerium sulfates, E. Smrčok: Neutron powder diffraction, quantum chemistry and β -cryolite, On inappropriate application of powder diffraction to structure determination of intercalates of dikite, V.

Jorík: Structure determination of $[\text{Cu}\{2,6-(\text{MeO})_2\text{nic}\}_2(\text{ron})_2]_n$ from powder - alternative way, V. Kavečanský: Structure and properties of $(\text{La}_{0.67}\text{Pb}_{0.33})(\text{Mn}_{1-x}\text{Co}_x)\text{O}_3$, E. Dobročk: Analysis of crystalline thin films by using of rotating anode and parallel beam optics, M. Jergel: Correlation of structure and magnetism in spin valves, R. Kužel: Structure investigations of deformed metals, J. Drahokoupil: Particle size distribution from the number of diffraction spots, D. Havlíček: Crystallochemistry of the design of phases with required properties - example - proton conductors, M. Čerňanský: Second moments of diffraction profiles, Z. Pala: Influence of cooling at polishing and milling on distribution of residual stresses in steels, J. Marek: Analysis of measurement errors of quantitative phase analysis of textured samples, F. Laufek: Investigations of new phases in systems Co-Sn-Te, Co-Ge-Te and Pd-Sn-Te, E. Čaplovič: Analysis of influence of deposition parameters on quantitative composition of hard coatings, M. Černík: Texture of steels sheets, M. Kusý: Phase analysis of boride layer of tool steel

Number of participants: 21

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

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

Autumn school of neutron scattering

Tatranská Štrba, 15. - 18. 9. 2007

Lecture blocks:

Scattering of thermal neutrons (J. Kulda)
Structures (powder diffraction - E. Smrčok, single crystals - J. Kulda)
Engineering applications of neutron diffraction (residual stresses, textures, mechanical properties - P. Lukáš)
Small-angle scattering, biology (SANS, reflectometry - J. Šaroun, P. Strunz; polymers - I. Krakovský, structural biology - M. Budayová-Spano)
Neutron spectroscopy (J. Kulda, M. Kempa, M. Sládkovičová), Experimental techniques (non-ambient conditions - K. Prokeš, Institute of Nuclear Physics, Řež near Prague - P. Lukáš, HMI Berlin - K. Prokeš, ILL Grenoble - J. Kulda)

Number of participants: 50

WWW page - <http://www.lm.uniza.sk/~jurecka/js/js.php>

Organization: J. Kulda, E. Smrčok, V. Jorík, V. Kavečanský, S. Jurečka



CSCA Scientific board

The scientific board was elected at the end of 2006.

Members

- Ing. Hana Brusová
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Zentiva, a.s.
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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

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J. Hašek, R. Kužel



16. - 19. 6. 2008

Valtice, Hotel Hubertus a Národní vinařské centrum

The colloquium is devoted to synchrotron radiation and its application in different scientific fields. Tutorials of Czech scientists will present physical and technological principles of synchrotron, origin and monochromatization of radiation in the range from infrared to hard X-rays and applications for diffraction, absorption, spectroscopic and imaging methods in materials science, physics, chemistry and biology. The colloquium is motivated by the Czech participation at existing synchrotrons (mainly ESRF and ELETTRA), preparation of the project CESLAB (Central European Synchrotron Laboratory) for construction of synchrotron radiation in the Czech Republic, and by the effort to spread the knowledge on the synchrotron and its application in a broad scientific community in a form of a short school. The colloquium is low-cost. In particular, the participation of students is welcome. The main languages are Czech and Slovak. English contributions are accepted as well.

XVII. Regional powder diffraction conference

Valtice, 18. 6. - 20. 6. 2008

