



CZECH AND SLOVAK CRYSTALLOGRAPHIC ASSOCIATION

The Czech and Slovak Crystallographic Association (CSCA) organized or co-organized several conferences and traditional one-day seminars in 2003.

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

258th Seminar

Institute of Chemical Technology,
Praha, 14. 5. 2003

Lectures:

B. Kratochvíl: Polymorphism of solid pharmaceutical substances, H. Petříčková: Molecular and crystal structure of semi-synthetic morphinan alkaloids, J. Čejka: Polymorphism ergot alkaloids, M. Hušák: Use of interactive visualization of electronic density map and similar functions for better interpretation of structural data, J. Had: X-ray phase analysis in Institute of Chemical Technology in Prague, J. Maixner: Data collection with X'Pert PRO program X'Pert Data Collector. Data evaluation with X'Pert HighScore, J. Maixner: X-ray fluorescence analysis – application of wave-dispersive spectrometer and quantitative element analysis using standardless software Uniquant 4, M. Hušák: Electron microscopy methods of structural studies of plant proteins.

Excursion:

- Laboratory of X-ray diffraction and spectrometry with the demonstration of measurement on spectrometer ARL 9400 and diffractometer X'Pert PRO (Dr. Maixner)
- Mineralogical collections in the Institute of Chemical Technology in Prague (Prof. Kratochvíl)

Organization: B. Kratochvíl

259th Seminar

Institute of Molecular Genetics, Academy of Sciences of the Czech Republic
Praha, 12. 11. 2003

Synchrotron radiation in structure analysis

Lectures

J. Hrdý: Refraction study at the Bragg and Laueho diffraction on perfect crystals, L. Palatinus: Advantages and drawbacks of the use of synchrotron radiation for precise

determination of intensities of Bragg reflections for crystal structure determination, J. Hašek: Protein structure determination in the Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic using synchrotron radiation at ELETTRA and ESRF, P. Řezáčová: Protein structure determination in the Institute of Molecular Genetics using synchrotron radiation at ESRF and DESY, L. Urbaníková: Mutants of RNase Sa - structure, stability, flexibility, J. Ševčík: Protein structure with atomic resolution, J. Brynda: Protein structure determination in the Institute of Molecular Genetics using laboratory protein diffractometer.

Excursion to protein diffractometer in the department of gene manipulation (rotation anode Nonius, area detector MarResearch, equipment for cooling of the crystal)

Organization: P. Řezáčová, J. Hrdý, J. Hašek

260th Seminar

Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic,
Praha, 21. 11.

X-ray scattering and synchrotron radiation in materials science

Lectures:

T. Ungár: The microstructure of crystalline materials determined by X-ray diffraction peak profile analysis, V. Holý: Use of synchrotron radiation for study of self-organized nanostructures, D. Rafaja: Structure-related changes in magnetoresistance of $\text{Co}_{90}\text{Fe}_{10}/\text{Cu}$ and $\text{Co}_{90}\text{Fe}_{10}/\text{Cu}_{85}\text{Ag}_{10}\text{Au}_5$ multilayers, R. Černý: Materials science at Swiss-Norwegian beamline in ESRF and at SLS, M. Rieder: Experience with diffraction of synchrotron radiation on mineral powders, M. Steinhart: Projects solved at small-angle scattering beamline in Elettra

Organization: R. Kužel, M. Steinhart, J. Hrdý

CSCA Colloquium - Computational Methods in X-ray and Neutron Structure Analysis

Nové Hradý, Academic and university center,
16. - 20. 6. 2003

Traditional colloquium organized as a course. State of art of some of the computational method in structure analysis, their use and possibilities for obtaining information on crystal structure in biology, chemistry, physics and mineralogy. It was a continuation of preceding colloquium Experimental methods which was held in Ostravice 2002.

Main topic: Fourier methods in diffraction, databases, structure visualization, Internet; powder diffraction - phase analysis, textures, stresses; structure solution and refinement from single crystal and powder diffraction, Rietveld analysis, protein structure determination, modelling of structures, deconvolution methods.

*Main lecturers:*

J. Komrská (FSI VUT Brno), K. Huml (ÚMCH AVČR, Praha), B. Schneider (Centrum pro komplexní molekulární systémy AVČR, Praha), J. Hašek (ÚMCH AVČR, Praha), R. Kužel (MFF UK, Praha), M. Hušák (VŠCHT Praha), J. Fiala (ZČU, Plzeň), P. Ondruš (Geologický ústav, Praha), V. Petříček (FzÚ AVČR, Praha), T. Obšil (PřF UK, Praha), J. Brynda (ÚMG AVČR Praha), R. Černý (University of Geneva, Ženeva), S. Daniš (MFF UK, Praha), J. Vévodová (PřF MU, Brno), P. Řezáčová (ÚMG AVČR, Praha), J. Ondráček (ÚMG AVČR, Praha), P. Čapková (MFF UK, Praha), B. Koudelka (MFF UK, Praha), T. Skálová (ÚMCH AVČR, Praha), J. Marek (FJFI ČVUT, Praha), M. Šlouf (ÚMCH AVČR, Praha), M. Černík (U. S. Steel, Košice), M. Čerňanský (FzÚ AVČR, Praha).

Small workshops in well-equipped computer room were included in the programme.

Workshops:

Databases, structure visualization (Schneider, Hašek, Hušák, Císařová), software for powder diffraction (Kužel), structure solution from single crystals (Dušek, Petříček, Brynda, Obšil), structure solution from powders (Černý, Daniš).

WWW pages <http://www.xray.cz/xray/csca/kol2003/> (including photos and video clips)

Number of participants: 71

Organization: R. Kužel, I. Kutá Smatanová, P. Řezáčová, J. Hašek, R. Černý, V. Petříček.

All abstract have been published in Materials Structure v. 10, number 1a (<http://www.xray.cz/ms/>).

5. review of student works in X-ray and neutron structure analysis in the Czech and Slovak republics

it was included in the colloquium This time only 12 students took part. They presented their results of diploma and PhD thesis. Three best works (or presentations) were awarded by diploms and financial sum -

B. Klepetářová (Institute of Chemical Technology, Praha): Solvatomorphism of ergot alkaloida, H. Petříčková (Institute of Chemical Technology, Praha): Structure analysis of morphinan alkaloids, V. Hlinková (Institute of Molecular Biology, Slovak Academy of Sciences, Bratislava): Complex of Ribonuclease Sa2 with 3'-GMP and 2', 3'-GCPT.

Report in Czech with photos in Materials Structure, 10 (2003), no. 2.

Structure Solution from Powder Diffraction data

Stará Lesná, 14. 9. - 19. 9. Congress Center of Slovak Academy of Sciences

see report below and with photos in Materials Structure 10 (2003) no. 2.

Development of Materials Science in Research and Education

15. - 19. 9.

Hotel of the Slovak University of Agriculture in Nitra, High Tatras

Report on the meeting in Materials Structure 10, (2003), no. 2 (in Czech).

2nd Meeting of Structural Biologists

Academic and University Center, Nové Hradý, 13. - 15. 3.

Lectures:

Plenary lecture:

Karel Ulbrich Dr.Sc. (Ústav makromolekulární chemie AVČR, Praha): Polymer carriers for targeted drug delivery and controlled drug release

Other lectures:

R. Dvorský, I. Barák, P. Flecker, R. Chaloupková, Z. Prokop, F. Vácha, K. Bezouška, J. Vondrášek, J. Damborský, R. Etrich, I. Bártová, R. Kužel, R. Hrabal, R. Fiala, B. Schneider, K. Réblová, V. Sychrovský, J. Dohnálek, J. Brynda, P. Řezáčová, R. Šouráčová, E. Urbaníková, J. Hašek, A. Lewit-Bentley, T. Obšil.

About 35 posters were presented.

The main aim of the meeting is information exchange between the groups working in the field of structural biology (NMR, XRD, IR spectroscopy, bioinformatics, computer experiments, quantum chemistry). Usually high number of students take part at the conference.

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

Number of participants: 90

Organization: B. Schneider, I. Kutá Smatanová, R. Kužel, D. Štys, V. Sklenář.

Abstracts in Materials Structure vol. 10 (2003), no. 1.

CSCA Scientific board

Election of a new scientific board was organized in 2003. Voting could be done by mail to the address of the chairman of the election committee or directly during the colloquium in Nové Hradý on June 16 and 17.

Election committee: chairman - Marian Čerňanský, members: Renata Štouráčová, Pavel Vojtíšek. There was 92 votes in total. The chairman announced the order of the first 13 candidates. None of candidates received less than 24 % of votes.

Results in alphabetical order (number of votes in parentheses):



- Dr. Antonín Buchal (57)
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- Dr. Ivana Císařová (67)
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Faculty of Natural Sciences, Charles University, Praha
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- Prof. Jaroslav Fiala (73)
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- Prof. Nikolaj Ganev (56)
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- Dr. Jindřich Hašek (76)
Institute of Macromolecular Chemistry,
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- Prof. Václav Holý (44)
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- Dr. Ivana Kutá Smatanová (47)
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- Prof. Radomír Kužel (90)
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- Prof. Zdeněk Weiss (52)
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The scientific board elected new CSCA officials (below) at its first meeting on June 17 in Nové Hradky

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

- Dr. Zbyněk Šourek (Chair person)
Institute of Physics, Academy of Sciences of the Czech Republic, Praha
- Prof. Marian Koman (Vice-chair persons)
Department of Inorganic Chemistry,
Faculty of Chemical Technology,
Slovak Technical University, Bratislava
- Dr. Ľubomír Čaplovič
Faculty of Materials and Technology
Slovak Technical University, Trnava
- Prof. Juraj Černák
Faculty of Nature, Safarik University, Košice
- Dr. Jaromír Hrdý
Institute of Physics, Academy of Sciences of the Czech Republic, Praha
- Prof. Jaromír Marek
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Faculty of Nature, Masaryk University
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- Prof. Pavol Šutta
Department of Physics,
Military Academy, Liptovský Mikuláš
- Prof. Zdeněk Trávníček
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Addresses of the CSCA officials

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J. Hašek, R. Kužel

Structure Solution from Powder Diffraction Data SSPD'03

held on 14-19 September 2003 in Stará Lesná, Slovakia

The international meeting Structure Solution from Powder Diffraction Data (SSPD'03) was a logical continuation of a long series of local conferences on powder diffraction, organized in Slovakia since 1992. At the origin of SSPD'03 was an idea to get together the best specialist in the structure determination from powder diffraction data with those working on the field of structure prediction. The purpose of this conference was to assess the progress made in the theory and techniques of structure solution based on powder diffraction data and to point to areas where further work is needed. Special attention was paid to structure prediction done by energy minimization, because its results are frequently checked by Rietveld refinement. It is believed that a combination of these two methods will in a near future become a standard tool. As a conference venue the beautiful environment of High Tatra mountains in Slovakia was chosen. The idea seemed first to be quite risky in the view of uncertain whether in this region in September and also in the view of the accumulation of meetings in this time period.

Following topics were covered by invited lectures:

- *indexing* by Armel Le Bail (Le Mans),
- *structure modeling and prediction of extended solids* by J. Christian Schön (Stuttgart) and of *molecular solids* by Alexander Dzyabchenko (Moscow),
- *intensity extraction* by Jonathan P. Wright (ESRF),
- *direct methods* by Jordi Rius (Barcelona),
- *global optimization* by Peter W. Stephens (Stony Brook) and Radovan Černý (Geneva),
- *total pattern analysis* by Robert L. Snyder (Atlanta),
- *applications to physics and chemistry* by Daniel Louër (Rennes), Robert Von Dreele (Argonne), James A. Kaduk (Naperville) and Paolo Radaelli (ISIS).

These topics and others, like structure determination from neutron powder diffraction, real structure, were covered also by 18 oral and 21 poster presentations. Altogether 69 participants from Croatia, Russia, United Kingdom, Italy, Denmark, USA, Turkey, Austria, Sweden, Slovenia, Spain, France, Norway, Israel, Germany, Algeria, Switzerland, The Netherlands, Czech Republic and Slovakia attended this meeting. Commercial lectures were delivered by A.Coelho (Bruker), C.Reiss and S.Prugovecki (Philips/PANalytical), commercial exhibitions were organized by Philips/PANalytical, Stoe and Oxford Cryosystems. The meeting was also supported by Seifert company. Owing to generous support from the IUCr the Organizers we are able to offer a financial support to a limited number of students and young scientists from several countries.

The basic idea of the program committee of the meeting was to create an atmosphere where the participants felt free to present and exchange their ideas, even the craziest ones. No proceedings from the meeting were planned, and despite of busy conference program there was time available for informal discussions. According to the majority of participants the objective was met. Especially the exchange between the people working on structure prediction by energy landscape investigation and those developing the method of structure solution by global optimization of the structural model was stimulating. SSPD'03 showed that such type of creative meetings is very much appreciated in the fields of science where the methodology is still under development, like is the case of powder diffraction.

Radovan Černý, Lubomír Smrčok





Crystallization Course CC2003

The second run of Protein Crystallization Course CC2003 held in the Academic and University Center (AUC) at Nove Hradky during the first week of October (3-8.10.2003).

In order to achieve its high level, qualified crystallographers from Germany (Prof. R. Hilgenfeld and Dr. J. Mesters of University of Luebeck and Dr. T. Klupsch of IHPT Jena), Spain (Prof. J.M. Garcia-Ruiz and Dr. J.A. Gavira Gallardo of Instituto Andaluz de Ciencias de la Tierra, Granada), Austria (Prof. R. Grandori of J. Kepler University, Linz and Dr. L. Janda of University of Vienna) and the Czech Republic (Dr. Jindrich Hasek from IMCH AS CR, Dr. Jiri Brynda from IMG AS CR) were invited to give the lectures as well as organize practices for 21 undergraduate and postgraduate students not only from the Czech Republic. The CC2003 was sponsored by Academic and University Center [CR] and CSCA [CR].

The official language of the course was English. During morning lectures students were acquainted with the theory of protein crystallography technique and latest methods of protein isolation, purification, crystallization and collection of diffraction data. Freshly obtained knowledge was trained during afternoon practices, which took place in the Laboratory of Crystallogenesi.

Using different crystallization methods such as hanging drop and sitting drop vapour diffusion methods, crystallization in a gel, etc., students grew their own crystals of model protein lysozyme.

Additional programme: excursion to Ceske Budejovice, poster session, round table discussion.

Considering the participants' answers gave in the questionnaire distributed at the end of the course, we are delighted to call the second year of crystallization course successful and very fruitful. We are looking forward to similar activities scheduled for 2004, when this crystallization course will be run as the FEBS Advanced Course called „Advanced Methods in Macromolecular Crystallization“.

More information will soon be available at <http://www.img.cas.cz/igm/cc2004>.

Ivana Kutá Smatanová, Pavlína Řezáčová

EPDIC-IX and Size-Strain IV

Prague, Czech Republic, August 31 - September 5, 2004

Traditional European Powder Diffraction Conference will be held at the Czech Technical University in Prague. The conference follows immediately the ECM in Budapest, Hungary. It begins with a Size-Strain workshop - the fourth continuation of the Size-Strain conferences, now planned as more focused to line profile analysis, crystallite size and lattice defects analysis. The EPDIC conference will start on Thursday, September 2 with a full-day software workshop organized by Lachlan Cranswick and concentrated to two topics - size/strain and phase analysis software. The programme schedule is similar to last EPDICs with plenary lectures, two parallel microsymbiosia and two poster sessions. Wide scope of powder diffraction should be presented with applications in physics, chemistry, materials science, pharmacy, mineralogy, and even in biology. Powder diffraction study of different materials will be presented: organic and inorganic materials, nanomaterials, thin films and multilayers, polymers, minerals, metals and alloys, magnetic and ferroelectric materials, ionic conductors, composites, ceramics, catalysts, intermetallic compounds, disordered structures, amorphous materials, glasses. Main topics: structure solution and refinement, stress, strain and texture, phase analysis, non-ambient conditions, phase transitions, fibre diffraction, software, databases, instrumentation, hard X-rays, diffraction of neutrons and electrons, reflectivity, small-angle scattering.

Relevant information is available on the Web site <http://www.xray.cz/epdic>, the conference E-mail address is epdic-9@post.cz. Preliminary registration is encouraged now as a help for organizers and also because the registered people can be quickly informed about any news and changes. The Web site includes a guestbook and discussion forum. There are different deadlines. The first important one is at the end of April, when all the applications for oral contributions and for financial support together with abstracts should arrive. The accommodation for reduced conference prices must be ordered till the end of May.