



# PROGRAMME

## LECTURES

### Monday, June 22

		17:00	
		SL3	k9
11:00	13:00	Registration	Jaroslav Maixner (VŠCHT Praha)
13:15		Struktura 2009 - Opening	Zkušenosti s provozem pozičně citlivého detektoru LynxEye
13:30	17:30	<b>Structure analysis, biocrystallography Advances in instrumentation</b> chair: <i>V. Petříček, J. Dohnálek</i>	Experience with PSD LynxEye
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13.20		L1	k5
		Pavel Vojtíšek (Přírodovědecká fakulta UK Praha)	
		Stereochemie komplexů lanthanoidů užívaných v medicíně: Vztahy mezi strukturou a funkcí	
		Stereochemistry of lanthanoid complexes used in medicine: Relations between structure and function	
14.00		SL1	k7
		František Laufek (Česká geologická služba, Praha)	
		Strukturální typy anorganických látek v databázi ICSD	
		Structure types of inorganic compounds in ICSD database	
14:20		L2	k7
		Pavčina Řezáčová (Ústav molekulární genetiky AV ČR, v. v. i., Praha)	
		Současné problémy v proteinové krystalografii	
		Current problems in protein crystallography	
15:10		SL2	k8
		Bohdan Schneider (Biotechnologický ústav AV ČR, v. v. i., Praha)	
		Nová skupina krystalografie proteinů na Biotechnologickém ústavu	
		A new group of protein crystallography in Biotechnological institute	
15:30		<i>Coffee break</i>	
16.00		CL1	k8
		Ladislav Pina (Rigaku Innovative Technologies Europe s.r.o., Prague)	
		Difrakční analyzátor s více jedinou krystalami pro vysokou rezoluci paralelního rentgenového záření	
		High resolution parallel-beam X-ray diffraction	
16.30		CL1	
		Boris Míč (Scientific Instruments, Brno)	
		Produkty firmy Bruker	
		17:00	
		SL4	k9
		Přemysl Beran (Ústav jaderné fyziky AV ČR, Řež u Prahy)	
		Prášková neutronová difrakce v Ústavu jaderné fyziky	
		Neutron powder diffraction in Institute of Nuclear Physics in Rez	
		<b>Introduction to courses</b>	
		C1	k69
		Jindřich Hašek (Ústav makromolekulární chemie AV ČR, v. v. i., Praha)	
		Úvod do kursu organické databáze CCDC	
		Introduction to the course on CCDC	
		C3	k71
		Radomír Kužel (Matematicko-fyzikální fakulta UK, Praha)	
		Úvod do kursu reálná struktura. Co to je reálná struktura?	
		Introduction to the course on real structure of polycrystalline materials	
		What is real structure?	
		19:00	Dinner
		C2	k70
		Michal Dušek (Fyzikální ústav AV ČR, v. v. i., Praha)	
		Úvod do kursu Jana2006, instalace programu	
		Introduction to the course Jana2006, program installation	
		Notation	
		L... main lectures	
		SL... short lectures	
		CL... commercial lectures	
		C...courses	

**Tuesday, June 23**

7:30 8:30 Breakfast

8:30 10:20 **Coherent diffraction, X-ray sources,**  
chair: *J. Hrdý, Z. Šourek*

8:30

L3

Stanislav Daniš

*(Matematicko-fyzikální fakulta UK, Praha)*

Koherentní difrakce

Coherent diffraction

k12

9:10

L4

Jan Dohnálek

*(Ústav makromolekulární chemie AV ČR, v. v. i., Praha)*

Laboratorní laditelné zdroje rentgenového záření

Laboratory tunable X-ray sources

k13

9:50

CL3

Till Samtleben

*(Incoatec, Geesthacht, Germany)*New Possibilities for X-ray Diffractometry: Bringing Light  
into Homelabs

k14

10:20 *Coffee break***Student session**chair: *N. Ganev, M. Čerňanský*

10:50

S1

Daniela Králová

*(Ústav makromolekulární chemie AV ČR, v. v. i., Praha)*

Tepelná stabilita titanátových nanotrubeček

Thermal stability of titanate nanotubes

k41

11:10

S2

Lea Nichtová

*(Matematicko-fyzikální fakulta Univerzita Karlova v Praze)*Rtg difrakční studium tloušťkové závislosti krystalizace a  
napětí ve vrstvách TiO<sub>2</sub>XRD study of thickness dependence of crystallization and stress in TiO<sub>2</sub>  
films

k43

11:30

S3

Jan Dolinár

*(Matematicko-fyzikální fakulta Univerzita Karlova v Praze)*

Párová distribuční funkce u nanoprášků

Pair distribution function in nanopowders

k44

11:50

S4

Václav Valeš

*(Matematicko-fyzikální fakulta Univerzita Karlova v Praze)*Study of the phase composition of Fe<sub>2</sub>O<sub>3</sub> nanoparticles

k46

12:10

S5

Zdeněk Pala

*(Fakulta jaderná a fyzikálně inženýrská, ČVUT Praha)*Residual stress determination by least square fitting  
method

k48

12:30 Lunch

chair: *P. Řezáčová, B. Schneider*

13:30

S6

Petr Kovář

*(Matematicko-fyzikální fakulta Univerzita Karlova v Praze)*Molekulární simulace Zn-Al podvojného vrstevnatého  
hydroxidu interkalovaného anionty porfyriuMolecular simulations of Zn-Al Layered Double Hydroxide intercalated  
with porphyrin anions

k50

13:50

S7

Petr Kolenko

*(Ústav makromolekulární chemie AV ČR, v. v. i., Praha)*High-resolution structure of extracellular domain of human  
CD69ubek

k51

14:10

S8

Tomáš Klumpler

*(Masarykova univerzita Brno)*

Struktura CKI1 receiver domeny z Arabidopsis

k52

14:30

S9

Petr Pachl

*(Ústav molekulární genetiky AV ČR, v. v. i., Praha)*

Design of selective inhibitors of 5'-nucleotidases

k53

14:50

S10

Andrea Štěpánková

*(Ústav makromolekulární chemie AV ČR, v. v. i., Praha)*The binding modes of ligands in the active site of  
-galactosidase

k54

15:10 *Coffee break*



15:30 S11 Ekaterina Sviridova (Ústav fyzikální biologie JČU, Nové Hradky) Crystallization study of the Iron-regulated outer membrane lipo-protein (FrpD) from Neisseria meningitidis	k54	18:30 S19 Silvie Bernátová (Přírodovědecká fakulta MU, Brno) Určení koncentrace precipitátů z Laueho difrakce Determination of precipitate concentration using Laue diffraction	k65
15:50 S12 Iryna Kishko (Ústav fyzikální biologie JČU, Nové Hradky) Investigation of biochemical structure and functions of the E. coli protein WrbA	k55	18:50 S16 Michael Barchuk (Matematicko-fyzikální fakulta Univerzita Karlova v Praze) X-ray scattering on GaN thin films, Monte Carlo simulation	k66
16:10 S13 Julie Wolfová (Ústav fyzikální biologie JČU, Nové Hradky) Structural changes of tetrameric flavoprotein WrbA upon flavin binding	k56	19.20 Dinner	
16:30 S14 Alena Stsiapanava (Ústav fyzikální biologie JČU, Nové Hradky) Structural characterization of three DhaA mutants from Rhodococcus rhodochrous	k58	20.00 Meeting of the scientific board of Czech and Slovak Crystallographic Association and IUCr Regional Committee of the Czech and Slovak Crystallographers	
16:50 <i>Coffee break</i> chair: P. Mikulík, Z. Šourek		<b>Wednesday, June 24</b> 7:30 8:30 Breakfast 8:30 10:30 <b>Surfaces, mapping of orientations</b> chair: R. Kužel, J. Hašek	
17:10 S15 Jan Endres (Matematicko-fyzikální fakulta Univerzita Karlova v Praze) Difuzní rozptyl z gradovaných vrstev SiGe Diffuse scattering from graded SiGe multilayers	k59	8:30 L5 Jaroslav Fiala (Západočeská univerzita Plzeň) Ivo Kraus (Fakulta jaderná a fyzikálně inženýrská, ČVUT Praha) Povrchy a rozhraní Surfaces and interfaces	k15
17:30 S16 Jan Jisa (Přírodovědecká fakulta MU, Brno) Limits of X-ray reflection	k60	9:20 L6 Milan Dopita (Bergakademie Freiberg, Germany) Electron backscattered diffraction - principles and applications	k16
17:50 S17 Lukáš Horák (Matematicko-fyzikální fakulta Univerzita Karlova v Praze) Determination of Mn and P concentration in Ga <sub>1-x</sub> Mn <sub>x</sub> As <sub>1-y</sub> P <sub>y</sub>	k62	9:55 L7 Petr Mikulík (Přírodovědecká fakulta MU, Brno) Mapování rozorientace krystalové mříže metodou rocking curve mapping Mapping of lattice misorientation by rocking curve mapping	k19
18:10 S18 Jan Krčmář (Přírodovědecká fakulta MU, Brno) Standing-wave-grazing-incidence x-ray diffraction from polycrystalline multilayers	k63	10:30 <i>Coffee break</i>	



11:00	13:00	<b>Instruments</b>		18:20	
			chair: <i>J. Hašek, R. Kužel</i>	SL8	k26
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11:00				Pavla Roupcová	
CL4				( <i>Ústav fyziky materiálů AVČR, v.v.i. Brno</i> )	
Uli Riedel		k20		Influence of protective gas on the phase composition of Mg-Ni-Fe-H based nanocomposite prepared by Spark synthesis	
( <i>Panalytical, Almelo, Netherlands</i> )					
New applications of the PIXcel detector				18:40	
				SL9	k27
11:20				Jaromír Kopeček	
CL5				( <i>Fyzikální ústav AV ČR, v. v. i., Praha</i> )	
Oliver Presly		k21		Feromagnetická slitina s tvarovou pamětí $\text{Co}_{38}\text{Ni}_{33}\text{Al}_{29}$ - příprava monokrystalů a jejich charakterizace	
( <i>Oxford Diffraction</i> )				Ferromagnetic alloy with shape memory $\text{Co}_{38}\text{Ni}_{33}\text{Al}_{29}$ single crystals and their characterization	
Cu vs Mo in Treatment of a Non-merohedral Twin using CrysAlisPro				<hr/>	
11:50				<b>Session B</b>	
SL5		k21		17:00 CCDC course	
Zbyněk Šourek				<b>Session B - Chemical crystallography</b>	
( <i>Fyzikální ústav AV ČR, v. v. i., Praha</i> )				chair: <i>J. Brynda</i>	
CENTRALSUNC, naše aktivity v ESRF				18:00	
12:10				SL10	k28
L8		k22		Pavel Vojtíšek	
Petr Mikulík				( <i>Přírodovědecká fakulta UK Praha</i> )	
( <i>Přírodovědecká fakulta MU, Brno</i> )				Užitečný disorder	
CESLAB				Useful disorder	
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13:00	Lunch			18:20	
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<b>Courses</b>				SL11	k29
14:00				Ján Moncol'	
Session A				( <i>Fakulta chemickej a potravinárskej technológie STU Bratislava</i> )	
Real structure				Polymorfia, izomorfia, distorzná izoméria a supramolekulová izoméria komplexov $[\text{Cu}(\text{RCOO})_2(\text{dena})_2(\text{H}_2\text{O})_2]$ (dena = N,N-dietylnikotinamid)	
Session B				18:40	
Jana 2006				SL12	k30
				Jindřich Hašek	
				( <i>Ústav makromolekulární chemie AV ČR, v.v.i. Praha</i> )	
				Struktura valinomycinu a jeho komplexů	
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<b>Session A - Real structure</b>			chair: <i>N. Ganev, V. Goliáš</i>	19:00	Assembly of the CSCA members
17:40				20:00	Dinner (Lovecká chata)
SL6		k23			
Jan Drahokoupil					
( <i>Fyzikální ústav AV ČR, v. v. i., Praha</i> )					
Výpočet instrumentální funkce					
Calculation of instrumental function					
18:00					
SL7		k24			
Marian Čerňanský					
( <i>Fyzikální ústav AV ČR, v. v. i., Praha</i> )					
Poznámky k momentům difrakčních profilů					
Notes to moments of diffraction profiles					

**Thursday, June 25**

7:30 8:30 Breakfast

8:30 12:30 **Nanomaterials, electron diffraction**chair: *J. Fiala, P. Bezdička*

8:30

L8

Marek Kotrlý

*(Kriminalistický ústav Praha)*

Mikro a nanomateriály ve forenzní oblasti

Micro and nanomaterials in forensic science

k32

9:05

L9

Miroslav Šlouf

*(Ústav makromolekulární chemie AV ČR, v.v.i. Praha)*

Elektronová difrakce, mikroprvková a obrazová analýza nanokrystalů

Electron diffraction, elemental and image analysis of nanocrystals

k33

9:40

L10

Mariana Klementová

*(Ústav anorganické chemie AV ČR, Řež u Prahy)*

Elektronová difrakce - SAED, CBED, NBED, PED

Electron diffraction – SAED, CBED, PED

k35

10:10

CL6

Stjepan Prugovecki

*(Panalytical, Almelo)*

Hard radiation, Pair Distribution Functions

k36

10:40 *Coffee break***Session A**11:10 12:30 **Nanometaterials**chair: *M. Šlouf, S. Daniš*

11:10

SL13

Viktor Goliáš

*(Přírodovědecká fakulta UK Praha)*

Zkušenosti s testováním RTG mikrodifrakčních technik pro použití ve forenzní oblasti

Experience with testing of X-ray microdiffraction techniques for the use in forensic science

k36

11:30

SL14

Pavel Kacerovský

*(Ústav fotoniky a elektroniky AV ČR)*

Mikroskopie nanočástic a vrstev s nanočásticemi

Microscopy of nanoparticles and layers with nanoparticles

k38

11:50

SL15

Pavel Klang

*(Přírodovědecká fakulta MU, Brno)*

X-ray characterization of GaAs nanowires on Si Nanowires

k39

**Session B**

11:00 12:30 CCDC course

12:30 Lunch

Courses

14.00

Session A

Real structure

Session B

Jana 2006



Major project prepared by the Academy of Sciences of the Czech Republic. Proposed project as a Centre of Excellence to the Operational Programme of Research and Development for Innovations.



## CENTRAL EUROPEAN SYNCHROTRON LABORATORY (CESLAB)



[WWW.CESLAB.EU](http://WWW.CESLAB.EU)  
[WWW.SYNCHROTRON.CZ](http://WWW.SYNCHROTRON.CZ)

Construction of the synchrotron facility has been proposed by the Academy of Sciences of the Czech Republic (ASCR) as one of the projects to be realized with the Structural Funds of the European Union. The CESLAB will be a modern third-generation electron synchrotron facility with energy of 3 GeV serving the Central Europe from the year 2015. Because of the favourable geographical location of Brno, the facility will serve not only to the needs of the Czech science, research and industry, but also to the Central European partners from Slovakia, Austria, Hungary, and others. It will be constructed in conjunction with other European and world synchrotrons; the accelerator complex itself is being realized in conjunction with the team of the Spanish synchrotron ALBA. The produced beamlines will be used in the fields of the structural biology, imaging techniques, biomedicine, structural chemistry, material sciences, nanotechnologies, and the environmental research.

As parts of the beamlines, scientific or industrial laboratories will be constructed, being distributed along the perimeter of the accelerator. In the laboratories, research and industrial activities will be conducted. The synchrotron will allow accommodate up to 33 beamlines.

In the future, CESLAB can become a natural centre of research and development in the Czech Republic. The scope of the beamlines will be still refined and most probably some of them will appear in the second stage. In the first stage, CESLAB will offer only seven beamlines, which will however cover the most important methods ranging from metrology and various diffraction methods, via the imaging and spectromicroscopy, to photoelectron spectroscopy, VUV ionization methods, and IR imaging.

The **Metrology beamline** (Peter Oberta) will operate a versatile end-station, which will permit metrology and optics testing studies as well as experiments in reflectometry, diffractometry and topography.

The **Imaging beamline** (Rajmund Mokso) aims in providing a state-of-art tool for tomography, laminography, nanoscale zoom-tomography and coherent imaging.

The **Diffraction beamline** (Petr Mikulík, Radomír Kužel) will cover various X-ray diffraction methods such as powder diffraction and high-resolution diffraction with key objectives on interface and bulk structure studies of crystalline materials.

The **Nuclear resonance scattering beamline** (Oldřich Schneeweiss) will be devoted to the exploration of static and dynamic, magnetic and electric properties of materials, which is an area of considerable interest for applied sciences (e.g. microelectronics and sensing).

The **Macromolecular Crystallography Beamline (MXB)** (Jindřich Hašek) focuses on complete structure determination of materials of any complexity in atomic resolution. Impacts of this technology are of basic importance in many branches of live sciences, medicine, and agriculture. Numerous applications are also in chemistry, mineralogy and high technology materials.

The **Spectromicroscopy beamline** (Vladimír Cháb, Luděk Frank) will offer several methods (ESCA, EXAFS, XANES, photoelectron diffraction, PEEM, LEEM) inherently necessary for modern research in surface science in both physics and chemistry.

In conjunction with a ground-breaking mass spectrometric end-station, the **VUV beamline** (Jana Roithová, Ján Žabka) will conduct innovative experiments on gaseous ions relevant for physics, chemistry, and biochemistry.

Finally, the **IR beamline** (Adam Dubroka) will be devoted to IR imaging microscopy and ellipsometry under high magnetic fields and will probe chemical composition of biological tissues and electronic structure of new materials.

