Section Chemistry

Chemistry Section is a unit of the Faculty of Science housed in three buildings at Kotlarska street and partly also outside at Kamenice street. Encompassing about one hundred academic staff, it offers a quality chemical education in bachelor’s program of chemistry, biochemistry and bachelor’s program for students of applied biochemistry. Besides graduate programme leading to a master degree in several areas of specialisation (analytical chemistry, biochemistry, environmental chemistry, inorganic chemistry, macromolecular chemistry, organic chemistry and physical chemistry) is available. In the same time bachelor’s program for teachers education as well as master degree program for them is offered. Graduate students may enter into the respective Ph.D. programmes.

Teaching activities are supported by a necessary research environment. A broad spectrum of modern chemical instruments enables thorough studies on chemical synthesis, molecular structure determination, trace element analysis and kinetics and mechanisms of chemical and biochemical processes, just to mention a few. There exists a significant cooperation with many universities and research institutes in Western Europe and U.S.A.

ORGANIZATIONAL STRUCTURE OF THE CHEMISTRY SECTION:

The Office

Head Milan Potáček (Prof., RNDr., CSc.)
Deputy Head Zdeněk Glatz (Associate Prof., RNDr., CSc.)
Secretary Milena Urbánková

The Departments

Analytical Chemistry
Biochemistry
Inorganic Chemistry
Organic Chemistry
Theoretical and Physical Chemistry

The Laboratories and Research Centers

Laboratory of Atomic Spectrochemistry
Computer Laboratory
NMR Laboratory
Research Center for Environmental Chemistry and Ecotoxicology
TEACHING AND RESEARCH ACTIVITIES

The department provides education in analytical chemistry including chemometrics: in bachelor studies for students of chemistry, biochemistry, biology and environmental science, in master studies for students of chemistry, biochemistry and environmental science, in postgraduate studies for specialists in analytical chemistry. External teaching activity also comprises basic, advanced and special lectures on analytical chemistry at the Faculty of Chemistry, Technical University, Brno.

The research involved the development of new analytical procedures and study of natural and newly synthesized substances (drugs, peptides, humic acids, etc.). Increasing accent was put on the development of new methods and instrumentation in the emerging field of bioanalytical chemistry. New analytical methods and approaches suitable for the determination of analytes in samples with complex matrix were developed. Chemometrical techniques such as Artificial Neural Networks combined with experimental design were routinely applied to optimize analyses. Attention was also paid to thermodynamic and kinetics study of complexation of transition metal ions (platinum group metal ions, copper(II), etc.) by various macrocyclic compounds, chemical model determination (equilibria, kinetics), chemical modelling (natural processes), chemistry of less common metals (f-elements, platinum metals, thallium, etc.), biocoordination chemistry (humic acids, macrocycles, drugs, etc.).

Capillary Electrophoresis (CE) was used for the study of humic substances of different origin (the study of oligomerisation, metal ion complexation, etc.). Also method for determination of some important analytes (sorbic acid, resveratrol, etc.) in wines was developed. Rapid screening methods for drug content of some drugs mentioned above in biological liquids were worked out and validated methods for determination of antiviral drugs like memantine and rimantadine were developed. CE instrumentation was also applied to determine chiral impurities. A CE instrument with laser-induced fluorescence detection was built in the department for both research and teaching purposes.

Matrix-assisted laser desorption/ionisation mass spectrometry (MALDI MS) played a key role in analysis and structural elucidation of biological compounds, such as peptides, peptide complexes and humic acids. In addition, it also served as a tool for analysis of small organic and inorganic compounds. Significant attention was paid to advanced sample preparation for an automated identification of proteins.

A chromatographic method for the analysis of adenine and cytosine as build-block molecules of DNA by reversed phase high performance chromatography (HPLC) was developed and compared with other techniques (CE, MALDI-TOF MS). In collaboration with industrial company, intensive study of reactive dyes by means of different experimental techniques was done.

Atomic absorption spectrometry (AAS) was used for the determination of metals, such as copper in biological samples. Dialysis and electrodeposition was applied for preconcentration of metals in flame AAS. Electrothermal atomic absorption spectrometry (ETAAS) was used for the determination of metals after electrodeposition on a graphite tube and graphite probe.

In Laboratory of atomic spectrochemistry, research activities are common with departmental. More details are given in a separate section.

DEPARTMENT STAFF

Head:
Josef Havel (Prof., RNDr., D.Sc.)

Professor:
Lumír Sommer (RNDr., D.Sc.), Professor Emeritus

Associate Professors:
Vratislav Chromý (Ing., CSc.), part time
Viktor Kanický (RNDr., CSc.)
Josef Komárek (RNDr., CSc.)
Vítězslav Otruba (RNDr., CSc.)

Assistant Professors:
Marta Farková (RNDr., CSc.)
Jan Havlíš (Mgr., Dr.)
Research Assistants:
Dagmar Gajdošová (Ing.)
Pavel Krásenský (Ing.)
Klára Novotná (Ing.), part time

Technical Assistants:
Helena Zavadilová (Ing.)
Jitka Nováková

Secretary:
Iva Šafaříková

Adjunct Lecturers:
Miloš Bartušek (Prof., RNDr., CSc.)
František Foret (Ing., CSc.), Institute of Analytical Chemistry, Academy of Sciences CR, Brno.
Ludmila Křivánková (Assoc. Prof. RNDr., CSc.), Institute of Analytical Chemistry, Academy of Sciences CR, Brno.
Miroslav Macka (RNDr., Ph.D.), University of Tasmania, Hobart, Australia.
Karel Šlais (Assoc. Prof., RNDr., D.Sc.), Institute of Analytical Chemistry, Academy of Sciences CR, Brno.

Ph. D. Students:
Full Time:
Vlastimil Dohnal (Mgr.)
Miloš Halúzka (Mgr.)
Aleš Hrdlička (Mgr.)
Radek Chalupa (Mgr.)
Alice Kotulánová (Mgr.)
Jiří Machát (Mgr.)
Jiří Maleček (Mgr.)
Sabina Malovaná (Mgr.)
Martin Muzikář (Mgr.)
Eva Niedobová (Mgr.)
Lenka Pokorná (Mgr.)
Pavla Polášková (Mgr.)
Lubomír Prokeš (Ing.)
Martin Semerád (Mgr.)
Jitka Studýnková (Mgr.)
Markéta Vašková (Mgr.)
Partial Time:
Klára Novotná (Ing.)
Marie Pištěková (RNDr.)
Michal Spěšný (Ing.)
Šárka Winklerová (RNDr.)

FOREIGN Ph.D. STUDENTS AT THE DEPARTMENT:
Gaston Bocaz Beneventi (Universidad de Concepcion, Concepcion, Chile)
Maria L. Pacheco Hernandéz (UAM, Mexico D. F., Mexico)
Julio A. Soto Guerrero (UNAM, Mexico D. F., Mexico)

THESES DEFENDED IN THE ACADEMIC YEAR 2001/2002
Diploma Theses
Tomáš Hottmar (J. Havel): Determination of Huperzin A using Capillary Electrophoresis
Pavlína Houserová (J. Komárek): Determination of Gold by Electrothermal Atomic Absorption Spectrometry
Soňa Humplíková (J. Havel): Separation and Determination of Monophosphatenucleotides, Markers of Hereditary Changes
Ilona Péterová (D. Gajdošová): Separation and Determination of Purine and Pyrimidine, Markers of Metabolic Disorders, using CE and MALDI TOF MS
Ivona Svobodová (P. Lubal): Complexation Study of Transition Metal Ions with Derivatized Macrocyclic Ligands of Cyclen/Cyclam Type
Jaroslav Šebela (K. Novotný): Optical Emission Spectrometry with Inductively Coupled Plasma and Laser Ablation in Analysis of Steels
Ondřej Šedo (J. Havel): Peptide Analysis Using MALDI-TOF Mass Spectrometry
Šenk Petr (V. Otruba): Optical Emission Spectrometry with Inductively-Coupled Plasma and Laser Ablation for Analysis of Glasses
Petr Táborský (P. Lubal): Protonation and Complexation Study of Rare Earth Elements with Bioligands and Macrocyclic Ligands Concerning Donor Atoms N, O, P
Vaculovič Tomáš (V. Kanicky) The Influence of Additional Gases on Optical Emission Spectrometry with Inductively Coupled Plasma and Laser Ablation in Analysis of Steels

PhD Thesis
Martin Muzikář (J. Havel): Development of New Methods for the Determination of Inorganic Ions and Metals by Capillary Electrophoresis and Inductively Coupled Plasma Spectrometry
Vlastimil Dohnal (J. Havel): Method Development in Capillary Electrophoresis and Applications
Sabina Malovaná (J. Havel): HPLC of Natural Polyphenolic Compounds and CZE of Pyridinium Aldoximes
Jiří Maleček (J. Havel): Electrophoretic Study of Cu(II) with Selected Ligands
Maria de Lourdes Pacheco (J. Havel): Capillary Electrophoresis and MALDI-TOF Mass Spectrometry of Humic Acids
Julio Soto-Guerrero (J. Havel): Uranyl Complexation with Some Dicarboxylic Acids and Uranium Determination with MALDI-TOF Mass Spectrometry
Gaston Bocaz-Beneventi (J. Havel): Capillary Electrophoresis, MALDI-TOF Mass Spectrometry and Artificial Neural Networks in Forensic and Legal Medicine

LIST OF PUBLICATIONS

Scientific papers


**Abstracts of conference papers and posters**


**Other professional publications**


KANICKÝ, V., LUBAL, P., HAEL, J. SPEKTROFOTOMETRICKÉ STUDIUM SOLVATAČNÍCH ROVNOVÁH URANU(VI) S N, N - DIMETHYLFORMAMIDEM. *CHEMICKÉ LISTY*, Praha : Česká


LUBAL, P., KOTEK, J., HERMANN, P., LUKEŠ, I. Complexes of 1,4,8,11-tetraazacyclotetradecane-1,8-bis(methylphosphonic acid) and similar ligands. In Book of Abstracts of International Conference on Coordination Chemistry ICC’35, 2002.


NIEDOBOVÁ, E., KANICKÝ, V., OTRUBA, V. Determination of iodine in biological samples by ICP-OES in VUV region. Praha (Czech Republic) : Česká společnost chemická, 96(S), Symposiap. 303-305, 2002.


**CONFERENCES (SYMPOSIA, SEMINARS) ORGANIZED BY THE DEPARTMENT STAFF MEMBERS:** 13


**GRANTS BESTOWED FOR PROJECTS**

**EU COST D18/0001/99**

Havel, J., Lubal, P.: Luminescent Lanthanide Complexes in Analytical and Diagnostic Applications. Collaboration. Responsible holder: Department of Inorganic Chemistry, Faculty of Natural Sciences, Charles University, Lukeš, I.

**GAČR 203/02/0493**

Havel, J., Lubal, P.: Bifunctional chelates. Synthesis and complexing properties. Responsible holder: Department of Inorganic Chemistry, Faculty of Natural Sciences, Charles University, Lukeš I.

**FRVŠ 793/2002**

Preisler, J., Havel, J., Vrábel, P.: Capillary Electrophoresis with Laser-Induced Fluorescence (LIF) Detection for Advanced Laboratory Practice.

**GAČR 203/02/P097**


**GAČR 203/02/1103**


**RAWRA, Prague, Czech Rep.; OECD Nuclear Energy Agency, Paris, France**

Havel, J., Lubal, P.: Thermodynamic database II.

**INDUSTRIAL COOPERATION**

Pliva-Lachema, Brno, Czech Republic.

**INVITED LECTURES AND WORKING STAYS OF STAFF MEMBERS ABROAD**

Havel, J., University Santiago del Compostela, Department of Inorganic Chemistry, Santiago del Compostela, Spain, 1 week.

Havel, J., Universidad Autonoma de Barcelona, Dept. Analytical Chemistry, Barcelona-Bellaterra, Spain, 1 week.
Havel, J., University of Girona, Department of Analytical Chemistry, Girona, Spain, 1 week.
Havel, J., Northwest University, Department of Chemistry, Xi’an, China, 1 week.
Havel, J., The use of Artificial Neural Networks in Analytical Chemistry, Charles University, Department of Analytical Chemistry, Faculty of Science, Prague, May 2002, invited lecture.
Havel, J., Artificial Neural Networks in Separation Science, University of Vienna, Department of Chemistry, 23.05.2002, invited lecture.
Havel, J., “Artificial Neural Networks in Separation Science” (for optimization and-or method Development), Universidad Autonoma de Barcelona, UAB, Barcelona, Department of Analytical Chemistry, 11.06.2002, invited lecture.
Havel, J., Artificial Neural Networks in Chemistry, Dept. of Chemistry, Northwest University, Xi’an, Peoples Republic of China, October 16, 2002, invited lecture.
Havel, J., Capillary Electrophoresis, Theory and Application, Northwest University, Department of Chemistry, Xi’an, Peoples Republic of China, October 21, 2002, invited lecture.
Kanický, V., May 2002, University of Cordoba, Department of Physics, (prof. M. Carmen Quintero) 1 week.
Kanický, V., June 2002, Utrecht, Netherlands, participation at the conference on laser ablation ICP mass spectrometry.
Lubal, P., 2002, April Adam Mickiewicz University, Poznan, Poland, 1 week.
Lubal, P., 2002, May - June - Universidad de Barcelona, Spain, 1 month.
Lubal, P., Eidgenossische Technische Hochschule (Department of Inorganic Chemistry), Zürich, Switzerland, (Prof. G. Anderegg), research stay.
Otruba, V., May 2002, University of Cordoba, Department of Physics, (prof. M. Carmen Quintero) 1 week.
Otruba, V., April 2002, Université Claude Bernard, (dr. Jean-Michel Mermet) 1 week.
Preisler, J., November 2002, Barnett Institute/NEU, Boston, USA, 1 week.

OTHER INTERNATIONAL CONTACTS AND CO-OPERATIONS OF STAFF MEMBERS

Cooperation
Université Louis Pasteur, Ecole Européenne des Hautes Études des Industries Chimiques de Strasbourg, Department of Bioinorganic Chemistry, Strasbourg, France (Prof. A.-M. Albrecht-Gary; J. Havel).
Université Paris 7, France (Prof. J. P. Doucet; J. Havel).
Free University Brussels, Farmaceutical Institute, Belgium (Prof. D. L. Massart; J. Havel, J. Pazourek)
University of Tasmania, School of Chemistry, Australia (Prof. P. R. Haddad; J. Havel)
Ecole d’Ingénieurs en Génie des Systèmes Industriels, EIGSI, La Rochelle, France (Prof. J. A. Videau; J. Havel).
Universidad Autónoma de Barcelona, Bellaterra, Spain (Prof. M. Valiente; J. Havel).
Universidad de Barcelona, Barcelona, Spain (Prof. R. Tauler; J. Havel, P. Lubal).
Universidad National Autónoma de Mexico, UNAM, Mexico (Prof. A. Rojas-Hernández; J. Havel).
Universidad Autónoma de Mexico, UAM, Cuatitlán, Mexico (Prof. G. Pérez-Caballero; J. Havel).
Universidad Nacional de Cordoba, Facultad de Ciencias Químicas, Departamento de Fisicoquímica, Córdoba, Argentina (Prof. Carlos de Pauli; J. Havel).
Universidad de Salamanca, Department of Physical Chemistry, Salamanca, Spain (Prof. J. L. González; J. Havel, P. Lubal).
San José State University, California, U.S.A. (Prof. L. Yengoyan; J. Havel).
The Royal Institute of Technology, Department of Inorganic Chemistry, Stockholm, Sweden (Prof. I. Grenthe, Prof. M. Muhammed; J. Havel).
The R.W. Johnson Pharmaceutical Research Institute, Raritan, New Jersey, USA, (Dr. N. A. Guzman; J. Havel).
Dionex, Inc. U.S.A. (Dr. P. Jandik; J. Havel).
Eidgenossische Technische Hochschule, Department of Inorganic Chemistry, Zürich, Switzerland, (Prof. G. Anderegg; J. Havel; P. Lubal).
Universidad de Barcelona, Barcelona, Spain (Prof. R. Tauler; J. Havel, P. Lubal).
Barnett Institute, Northeastern University, Boston, USA (Prof. B. Karger, Prof. G. Davies; J. Preisler; J. Havel).
University of Ljubljana, Faculty of Chemistry and Chemical Technology, Ljubljana, Slovenia (Prof. Veber, M.; Komárek, J.).
Veterinary and Agrochemical Research Centre, Section of Ecochemistry and Spectroscopy, Tervuren, Belgium (Dr. Hoenig, M., Otruba, V.).
Technical University Košice, Faculty of Metallurgy, Department of Chemistry, Košice, Slovak Republic (Prof. Krakovská, E., Otruba, V.).
Institut für Analytische Chemie, Abteilung Atomspektroskopie, Fakultät für Naturwissenschaften und Mathematik, Universität Wien, Österreich, Univ. (Prof. Dr. Steffan, I., Otruba, V.).
Adam Mickiewicz University, Department of Water and Soil Analysis, Poznan, Poland. (Prof. Dr. Siepak, Hab. J., Otruba, V.).
Departamento de Fisica, Universidad de Cordoba (Prof. Dr. Carmen Quintero Ortega, M., Otruba, V.).
Departamento de Química Analítica, Facultad de Estudios Superiores Cuautitlán, Universidad Autonoma de Mexico (Dr. Revilla Vazquez. A. L., Havel, J., Otruba, V.).
Lina Spark Applications, S.a., Cully, Switzerland (Dipl. Ing. Vogel, W., Otruba, V.).
Ben Gurion University of Negev, Israel (Dr. Brenner, I. (Joe), Otruba, V.).

Foreign visitors
Peña-Méndez, E. M., (Prof., Dr.), Universidad de La Laguna, Tenerife, Spain, visiting professor.

STUDENTS STUDYING ABROAD

Dohnal, V.: University of La Laguna, La Laguna, Tenerife, Spain, 5 months.
Muzikář, M.: University of Girona, Girona, Spain, 4 months.
Pišný, R.: Universidad de Barcelona, Spain, 4 months.
Hrdlička, A., Universidad de Córdoba, Spain, 3 months.
Studýnková, J.: Université Claude Bernard, France, 3 months.
Halúzka, M.: Université Claude Bernard, France, 3 months.
Vaculovič, T.: Université Claude Bernard, France, 3 months.
AWARDS
Šedo, O., Competition for the best student scientific work in analytical chemistry (MERCK), VŠCHT Prague, February 5-6, 2002, the first prize.
Táborský, P.: Competition for the best student scientific work in analytical chemistry (MERCK), VŠCHT Prague, February 5-6, 2002, the first prize.

OTHER PROFESSIONAL ACTIVITIES
Havel, J.: Head of the Department of Analytical Chemistry, Masaryk University; Member of the Editorial Board of Folia Fac. Sci. Nat. Masaryk. Univ.; Member of the International Society for Chemometrics; Member of the Working Party for Chemometrics of the Czech Chemical Society; Member of the Committee of the Regional Branch of the Czech Chemical Society; Member of the Spectroscopic Soc. of J. M. Marci, Prague; Member of the New York Academy of Sciences, Chairman of the Council for Doctorate Studies in Analytical Chemistry, the Masaryk University; Member of the Council for Doctorate Studies in Analytical Chemistry at Charles University in Prague, Member of the Council for Doctorate Studies in Analytical Chemistry at the College of Chemical Technology, Prague; Member of the Scientific Council of the Faculty of Sciences of the Masaryk University; Member of the Council for Doctorate Studies in Analytical Chemistry at Slovak Academy of Sciences, Bratislava, Slovak Republic, Member of International Geographic Society, Member of Americal Association for the Advancement of Science(AAAS).
Kanický, V.: Member of the Committee of the Spectroscopic Soc. of J. M. Marci, Prague; Vice-Chairman of the Working Party of Analytical Chemistry of the Czech Chemical Society; Member of the Committee of the Regional Branch of the Czech Chemical Society; Member of the Academic Senate of the Faculty of Sciences, Masaryk University; Member of the habilitation commission in analytical chemistry of the Faculty of Chemistry of the Technical University Brno; Deputy Head of the Laboratory of Plasma Sources for Chemical Analysis of the Faculty of Science, the Masaryk University Brno.
Komárek, J.: Deputy Head of the Department of Analytical Chemistry; Member of the Council for the Doctorate Study in Analytical Chemistry and Environmental Chemistry at the Masaryk University Brno.
Otruba, V.: Head of the Laboratory of Plasma Sources for Chemical Analysis.
Preisler, J.: Deputy Head of the Department of Analytical Chemistry.
Sommer, L.: Professor Emeritus, Member of the Working Party for Chemistry of the Commission for Accreditation of the Czech Government; Emeritus Member of the Commission for Analytical Reactions, Reagents and Separations, IUPAC; Member of the Council for Postgraduate Studies in Analytical Chemistry, the Masaryk University; Member of the Scientific Council of the College of Chem. Technology, Prague; Member of the Councils for Postgraduate Studies in Analytical Chemistry: Technical Univ. Prague and Palacký Univ. Olomouc; Member of the Working Party of Analytical Chemistry of the Czech Chemical Society; Member of the Spectroscopic Soc. of J. M. Marci, Prague; teaching at the Faculty of Chemistry of the Technical University Brno.
Department of Biochemistry

TEACHING AND RESEARCH ACTIVITIES

Department of Biochemistry arranged for teaching of the basic biochemical disciplines at the bachelor and master levels for students of chemistry, biology, and future high school teachers of our Faculty. In addition, specialized education of graduate students of biochemistry and some branches of biology (e.g., molecular biology) was carried out.

New students were accepted for graduate study. We guaranteed the teaching of 28 students in 4th and 5th year and 24 graduate students. The staff of the department participated in many national and international congresses. The department organized International Net Conference of Diploma Theses with participation of several Czech and Slovak Universities. Research activities are oriented to the topics studied in the following laboratories:

- Laboratory of biochemistry of plant-pathogen interactions (V. Mikeš, J. Mazoch, V. Kratochvílová)
- Laboratory of biosensors (P. Skládal)
- Laboratory of environmental biotechnology (M. Mandl, O. Janiczek, H. Říčánková)
- Laboratory of microbial bioenergetics (I. Kučera, P. Boublíková, Rotrekl, V., M. Kuňák, J. Neužilová)
- Laboratory of separation of biomolecules (Z. Glatz, P. Zbořil, M. Wimmerová, L. Poláková)
- Laboratory of proteom research (P. Bouchal, cooperation with the permanent staff)

Our research was supported almost exclusively by external sources: Grant Agency of the Czech Republic, Fund of the Development of Universities, research projects sponsored by foreign institutions, including the 5th Frame Program of the European Union and bilateral programs. The most of the research workers participated in Research Program of the Ministry of Education. Some research activities were carried out in cooperation with the Ministry of Health of the Czech Republic (animal biochemistry - S. Pavelka) and National Centre for Biomolecular Research (M. Wimmerová).

DEPARTMENT STAFF

**Head:**
Vladimír Mikeš (Assoc. Prof., RNDr., CSc.)

**Professor:**
Igor Kučera (RNDr., D.Sc.)

**Associate Professors:**
- Zdeněk Glatz (RNDr., CSc.)
- Martin Mandl (Ing., CSc.)
- Petr Skládal (RNDr., CSc.)
- Petr Zbořil (RNDr., CSc.)

**Assistant Professors:**
- Pavla Boublíková (RNDr., CSc.)
- Oldřich Janiczek (RNDr., CSc.)
- Stanislav Pavelka (RNDr., CSc.), part time
- Vladimir Rotrekl (Mgr, Ph.D.)
- Michaela Wimmerová (RNDr., Ph.D.)

**Research Assistants:**
- Pavel Bouchal (Mgr.)
- Šárka Helánová (Mgr.)
- Michal Kuňák (Mgr.)
- Jiří Mazoch (Mgr.)
- Ivo Pluháček (RNDr.)

**Technicians:**
- Věra Kratochvílová
- Hedvika Říčánková
- Jitka Neužilová
- Ludmila Poláková

**Secretary:**
Stanislava Fousová

**Adjunct Lecturers:**
Ph.D. Students:

Full time
- Pavel Bouchal (Mgr.)
- Lenka Drábková (Mgr.)
- Gabriela Fanfrdlová (Mgr.)
- Jan Halánek (Mgr.)
- Šárka Helánová (Mgr.)
- Jan Lochamn (Mgr.)
- Andrea Kašná (Mgr.)
- Jitka Kašparovská (Mgr.)
- Tomáš Kašparovský (Mgr.)
- Michal Kuhák (Mgr.)
- Iva Navrátilová (Mgr.)
- Soňa Nováková (Mgr.)
- Petra Ševčíková (Mgr.)
- Renáta Solná (Mgr.)
- Jan Přibyl (Mgr.)
- Marta Zeisbergrová (Mgr.)
- Jiří Žeravík (Mgr.)

Part time
- Iva Bartáková (Mgr.)
- Martina Budová (Mgr.)
- Ivana Huvarová (Mgr.)
- Nikola Kostlánová (Mgr.)
- Jiří Mazoch (Mgr.)
- Jana Sýkorová (Mgr.)
- Radek Tesařík (Mgr.)

THESES DEFENDED IN THE ACADEMIC YEAR 2001/2002

Diploma theses:

Böhmová, G.: Isolation of haem O and a study of its conversion to haem A by the enzymatic system of Paracoccus denitrificans (supervisor I. Kučera).


Faltýsková, E.: Electrochemical studies on mitomicines and their interaction with DNA (supervisor L. Trnková).


Gavlasová, P.: Inhibition of elemental sulfur oxidation by arsenic in Acidithiobacillus ferrooxidans (supervisor M. Mandl).

Koutská, K.O.: Tumour suppressor protein p53 binding to DNA (supervisor J. Paleček).

Lochman, J.: Identification of Armillaria by molecular biological methods and isoenzyme analysis (supervisor V. Mikes).

Měcháčková, V.: Reactive oxygen compounds (supervisor P. Zbořil).


Novák, P.: Immunosensors for glycohemoglobin determination (supervisor P. Skládal).

Očadlíková, D.: The purification of glyoxalase I from bacterium P. denitrificans and yeast S. cerevisiae (supervisor P. Zbořil).


Přibyl, J.: Studies on interactions of saccharides and glycoproteins with boric acid using piezoelectric biosensors (supervisor P. Skládal).

Šnajdrová, L.: Application of capillary electrophoresis for separation of bacterial cells (supervisor Z. Glatz).
LIST OF PUBLICATIONS

Books, book chapters and review articles


Scientific papers


MITCHELL, E., HOULES, C., SUDAKEVITZ, D., WIMMEROVÁ, M., GAUTIER, C., PÉREZ, S., WU, A. M. - Gilboa-Garber, Nechama - Imberty, Anne. Structural basis for oligosaccharide-mediated adhesion of


Abstracts of conference papers and posters


BUHOT, N., MIKEŠ, V., PONCHET, M., DOULIEZ, J. Des élicitines de Phytophthora aux LTPs végétales (Elicitins of Phytophthora in vegetal LTPs). In Book of Abstracts of Quatriemes rencontres de Mycologie - Phytopathologie. p. 120-120, 2002.


**Other professional publications**


KUŇÁK, M., KUČERA, I. Využití rekombinantního pseudoazurinu jako donoru elektronů nitritreduktasy s následným měřením dvouenzymové kinetiky (Utilization of recombinant pseudoazurin as an electron donor of nitrite reductase and follow-up measuring of dual enzymatic kinetics.), 2002.


SKLÁDAL, P. *Biosensores de armas biologicas são destaque de hoje* (Biosensors for detection of biological weapons), 2002.


CONFERENCES (SYMPOSIA, SEMINARS) ORGANIZED BY THE DEPARTMENT MEMBERS

Boublíková, P., Zbořil, P.: Member of the Organizing Committee, 6th Workshop of Biochemists and Molecular Biologists, Masaryk University, Brno, February 2002.


PROJECT GRANTS RECEIVED

Grant Agency of the Czech Republic

203/02/1447
Kahle, V., Gaš B. Glatz Z.: Capillary electrochromatography in monolytic polymer columns

203/01/1589
Kučera, I.: Mechanisms involved in regulation of respiratory systems in denitrification bacteria by environmental factors.

525/00/0785

GA522/02/0925
Mikeš, V. Modeling of the structure and interactions of Phytophthora elicitors

203/00/P097
Rotrekl, V.: Identification of genes involved in nitrate transport in P. denitrificans and basic characterisation of their products.

Fund of the Development of Universities

740/2002

734/2002
Drábková, L., Janiczek, O: Oxidation of tetraionate by Acidithiobacillus ferrooxidans.

725/2002
Janiczek, O.: A new manuals, instructions and lectures for biochemistry students.
753/2002
Kašparovský T., Mikeš, V. Role of calcium in defense reaction of plants.
756/2002
Kuňák, M., Kučera, I.: Utilization of recombinant pseudoazurin as an electron donor of nitrite reductase.
759/2002
Mazoch, J.: Interaction of elicitors from cell walls of Armillaria and their interaction with plant cells.
F 804/2002
Mikeš, V.: Innovation of practical course of Biochemistry.
766/2002
Nováková S.: Application of electrophoretically mediated microanalysis for the study of enzymes.
762/2002
Ševčíková P.: Development of new methods for the determination of homocysteine in human plasma.

Foreign grants

QLK3-2000-01481

QLK3-CT-2000-00244

IHP-ARI-2002

MENRT No. 3

Other grants

ME 598, Kontakt
Mikeš, V.: Role of lipids in the elicitation of plant defense reaction (Czech Ministry of Education).
2002-042-1 Barrande
Mikeš, V.: Structural and functional genomics of plant defense proteins (Czech Ministry of Education).

NJ/6109-3
Pavelka, S.: Interference of bromide from the environment with the metabolism of iodine in the thyroid and other tissues (Grant Agency of the Ministry of Health of the Czech Republic).

INVITED LECTURES AND RESEARCH STAYS OF STAFF ABROAD

Mikeš, V.: Laboratory of Plant Pathogen Interactions, INRA Antibes, France, 2 weeks.
Rotrekl, V.: Department of Molecular Medicine, Institute of Biotechnology, The University of Texas Health Science Center, San Antonio, USA, one year.


Wimmerová, M.: Centre de Recherches sur les Macromolécules Végétales (CERMAV), Molecular Glycobiology Group, Grenoble, France, two stays, 9 months and 3 weeks.

Wimmerová, M.: Invited lecture and FP5 project, LMC, The Royal Veterinary and Agricultural University, Food Technology, Copenhagen, Denmark, 1 week.
OTHER INTERNATIONAL CONTACTS AND CO-OPERATION OF THE STAFF

Cooperations

Department of Analytical Chemistry, Lund University, Lund, Sweden; Amperometric biosensors, flow-injection analysis, portable detectors (T. Ruzgas, J. Emnéus, P. Skládal).

Department of Bioanalytical Chemistry, University of Potsdam, Potsdam, Germany; Piezoelectric biosensors, cholinesterase-based affinity sensors (A. Makower, F. Scheller, P. Skládal).

Department of Biotechnology, Lund University, Lund, Sweden; Cell-based microelectrodes, multichannel amperometric detectors (E. Csöregi, P. Skládal).

Department of Chemistry, State University of New York, Potsdam College, Potsdam, USA; Piezoelectric biosensors (M. Hepel, P. Skládal).

Catholic University Leuven, Pharmaceutical Faculty Laboratory of Pharmaceutical Chemistry Leuven, Belgium; Electrophoretically mediated microanalysis (A. Van Schapdael, Z. Glatz).

Centre de Recherches sur les Macromolécules Végétales (CERMAV), Molecular Glycobiology group, Grenoble, France; Proteins in carbohydrate synthesis and specific recognition (A. Imberty, N. Kostlánová, M. Wimmerová).

Department of Molecular Cell Physiology, Free University, Amsterdam, The Netherlands; Regulation of bacterial denitrification (R. van Spanning, I. Kučera).

Institut für Chemie, Universität für Bodenkultur, Wien, Austria; Eucaryotic fucosyltransferases (I.B.H. Wilson, M. Wimmerová).

Institute of Chemistry, Universidade Estadual Paulista, Araraquara, Brazil; Piezoelectric biosensors for nucleic acids (H. Yamanaka, P. Skládal).

LMC, The Royal Veterinary and Agricultural University, Food Technology, Copenhagen, Denmark; Bioinformatics and chemometric approaches in genome analysis (S.B.Engelsen, M. Wimmerová).

UMR INRA/Université de Bourgogne, France, Project Barrande; Plant elicitors (J.-P. Blein, V. Mikeš).

School of Biological Sciences, University of Wales, Bangor, UK; Iodinin in sulfur-oxidizing bacteria (D.B. Johnson, M. Mandl).

Foreign visitors

Prof. P. Coutos, University of Poitiers, France, a visit to V. Mikeš, December 2002; Plant elicitors.

Dr. J.-P. Blein, UMR INRA/Université de Bourgogne, France, a visit to V. Mikeš, December 2002; Plant elicitors.

Dr. E. Gomes, University of Poitiers, France, a visit to V. Mikeš, December 2002; Lecture: nsLTPs in plant defense mechanisms: facts and hypothesis.

Dr. K. Knösche, Department of Bioanalytical Chemistry, University of Potsdam, Potsdam, Germany, a visit to P. Skládal, November 2002; Piezoelectric biosensors.

Dr. I.B.H. Wilson, Institut für Chemie, Universität für Bodenkultur, Wien, Austria, a visit to M. Wimmerová, December 2002; Eucaryotic fucosyltransferase.

STUDENTS STUDYING ABROAD

J. Halámek: Research stay at the University of Potsdam, Department of Analytical Biochemistry, Potsdam, Germany, 3 months.

J. Friml: Research stay at the University of Tuebingen, Germany, 6 months.

N. Kostlánová: Centre de Recherches sur les Macromolécules Végétales (CERMAV), 2 month (Fellowship of French Embassy).
I. Navrátilová: Research stay at the National University of Ireland in Galway, Department of Physical Chemistry, Galway, Ireland, 1 month.

P. Novák: Research stay at the University of Potsdam, Department of Analytical Biochemistry, Potsdam, Germany, 1 month.

Nováková S.: Research stay at the Catholic University Leuven, Pharmaceutical Faculty P Laboratory of Pharmaceutical Chemistry Louvain, Belgium, 10 months.

R. Solná: Research stay at the Lund University, Department of Analytical Chemistry, Lund, Sweden, 6 month.

FOREIGN STUDENTS STUDYING AT THE DEPARTMENT

Kana Ito: Department of Chemistry, State University of New York, Potsdam College, Potsdam, USA (a visit to P. Skládal).

AWARDED STUDENTS AND STAFF

Pavelka, S.: Excess bromide in the lactating rat is transferred through mother’s milk to the suckling; Awarded as the best poster presented at the international symposium “Macro and Trace Elements/Mengen- und Spurenelemente”; held in Jena (Germany) on October 18-19, 2002.

OTHER PROFESSIONAL ACTIVITIES

Glatz Z.: Member of the Committee of Chromatography and electrophoresis group of the Czech Chemical Society, vice head of the Chemistry Section.

Janiczek. O.: Member of the Committee of the Agency of Fund for Development of Ministry of Education.

Mandl, M.: Member of the Committee of the Czech Biotechnological Society; Lectures on biotechnology, Faculty of Chemistry, University of Technology, Brno.

Mikeš, V.: Member of the Committee of the Czech Society for Biochemistry and Molecular Biology; Member of the Committee of the Agency of Fund for Development of Ministry of Education.

Wimmerová, M.: Member of the Brno Branch Committee of the Czech Chemical Society; Member of the Regional Committee of the Czech Chemistry Olympiad.

Zbořil, P.: Member of the Committee of the Agency of Fund for Development of Ministry of Education.
Department of Inorganic Chemistry

TEACHING AND RESEARCH ACTIVITIES

Teaching activities

The Department of Inorganic Chemistry provides education in the basic chemical disciplines, i.e. general and inorganic chemistry for students at the bachelor level, who major in chemistry, biology, geology and physics, as well as for chemistry teachers. Advanced inorganic chemistry lectures and courses at the master level are offered for students who major in inorganic chemistry. The Department also provides a basic course of nuclear chemistry and offers an advanced course in radioecology. A specialized laboratory course of inorganic chemistry students is offered to the students who major in inorganic chemistry. A new study program of Materials Chemistry was accredited by the Ministry of Education. It offers a two-year program leading to master degree in a modern and progressive chemical discipline. The curriculum involves courses in inorganic materials synthesis and characterization, material science of metals and alloys, and polymer chemistry. Courses “Multimedia in chemistry education” were introduced.

Instrumentation

The Department has an up-to-date X-ray structure laboratory. The four circle -axis diffractometer KUMA KM-4 which is equipped with Oxford Cryosystem low-temperature device and CCD camera has been upgraded by installing a new X-ray source, 3kW X-ray tube + layered collimators, with enhanced brilliance. The low-temperature device enables a routine low temperature data collection and growing single crystals from liquids or liquefied gases and thus determine their solid state structure. A new P1-C40P Phoenix refrigerated circulator has been purchased for X-ray structure laboratory. Temperature of its large 12 l bath can be controlled to 0.01°C in the wide range from -40°C to 150°C.

An inert atmosphere glove box MBraun UNILAB allows handling of highly moisture and air sensitive materials. The moisture and O2 analyzers show that the inner nitrogen atmosphere of the box contains less than 1 ppm of water and oxygen. A new solvent trap was added to the system to remove organic vapors.

A programmable horizontal tube furnace allows heat treatment of samples up to 1250 °C under controlled atmosphere.

A laboratory of multimedia technologies was established.

Research activities

The systematic study of the chemical reactivity of phosphorus(V) halogenide-oxides and their derivatives provided the following interesting results. The POCl3 in its reaction with 4-dimethylaminopyridine (DMAP) undergoes a base catalysed dismutation to PCl5 and DMAP.PO2Cl which in a successive reaction with DMAP yields [(DMAP)2PO2Cl]. It is a salt of a donor-stabilized cation [PO2]+, a hitherto unknown analogue of the nitronium ion, [NO2]+. A 31P NMR spectroscopic study of the reaction course enabled to suggest a likely reaction mechanism involving all observed species. The cation [DMAP.POCl2]+, a proposed product of the first reaction step, was also successfully synthesized by a treatment of POCl3 with silylated DMAP.

An intensive work continued on the study of reactions of chlorodithiophosphoric acid pyridiniumbetaine, PyPS2Cl, with polyfunctional nucleophile reagents. Reactions of PyPS2Cl with thiosemicarbazide derivatives, phosphazenes and other nucleophiles were studied. A series of new heterocyclic compounds was prepared and characterized. In the research area of inorganic materials chemistry, we prepared a series of cage aluminophosphonates and titanosilicates as organic-soluble molecular precursors. The reactions of these molecular building units with various reagents were studied with the aim of establishing reactivity patterns of their functional groups. The functionalized molecules will be assembled via non-aqueous sol-gel routes to form three-dimensional ordered networks. Resulting materials find applications as molecular sieves, adsorbents, and selective catalysts. A new non-aqueous sol-gel route to mixed oxide materials has been developed. It allows mixing of the components at a molecular level and provides materials with a high degree of homogeneity. These products are useful refractory, optical, and electronic materials. Mesoporous metallophosphate materials based on Al, Zr, La, Co, Cu, Cr, and Ni were prepared by a supramolecular templating route. Two gemini type surfactants were employed. Reactivity of alumazene was studied in reactions with phosphoric acid triesters, phosphonate diesters, sulphonic acid esters, nitriles, carbodiimides, and metal alkoxides. A novel aluminium amide-phosphate, amide-sulphonate, and nitrile adducts were isolated and spectroscopically and structurally characterized.

Selenium trioxide forms adducts with organic oxygen donors under suitable conditions. The donor-acceptor
complexes $\text{Et}_2\text{OSeO}_3$ and $(\text{Me}_2\text{O})_2\text{SeO}_3$ can be obtained as primary products in the reaction of selenium trioxide with dimethyl ether $(\text{Me}_2\text{O})$ or diethyl ether $(\text{Et}_2\text{O})$. The crystal and molecular structures of both complexes, that are stable only below their melting points, were determined by X-ray structure analysis. Conversion of these adducts to dialkylesters of diselenic and selenic acid in the liquid phase was monitored by Raman, $^1\text{H}$- and $^{77}\text{Se}$-NMR spectroscopy.

Two cyclic esters of selenic acid - $\text{C}_2\text{H}_4\text{O}_4\text{Se}$ and $\text{C}_2\text{H}_4\text{O}_8\text{Se}_2\text{C}_4\text{H}_8\text{O}_2$- were isolated from the dioxane/selenium trioxide system without using an inert solvent The donor-acceptor complex $\text{C}_4\text{H}_8\text{O}_2\text{SeO}_3$ can be prepared in liquid sulfur dioxide only. If tetrachloromethane is used as an inert solvent, the solvates of triselenium heptoxide $\text{Se}_3\text{O}_7\cdot 2\text{C}_4\text{H}_8\text{O}_2$ and $\text{Se}_3\text{O}_7\cdot 3\text{C}_4\text{H}_8\text{O}_2$ were formed. All mentioned compounds were characterized by X-ray analysis and Raman spectroscopy.

The synthesis and spectroscopic characterisation of chalcogenophosphoryl ligands derived from pyridine have been introduced in our research activities. The synthesis was based on the oxidation of $\text{C}_5\text{H}_3\text{N}(\text{PPh}_2\text{)}_2$ by elementary sulfur and selenium, and hydrogen peroxide, respectively. The organic ligands act as tridentate, with both chalcogens and nitrogen involved in chelation. To extend the knowledge of the co-ordination chemistry of ligands (including structural investigations), a series of new compounds were isolated and structurally characterized.

Halogenides of imido-bis(sulfuric) acid and their salts have recently attracted an attention as perspective solutes in lithium batteries. The reactions of $\text{Cl}_3\text{PNSO}_2\text{Cl}$ and its derivatives with various nucleophilic and electrophilic reagents lead to derivatives of imido-bis(sulfuric) acid and various polyheteroatomic cyclic molecules. Thus, we have prepared and structurally characterized several P-N-S-As and P-N-S-B heterocycles.

The study of cyclic halogenotriphosphazenes chemistry was concentrated on reactions of $\text{P}_3\text{N}_3\text{Cl}_6$ and $\text{P}_3\text{N}_3\text{F}_6$ with silyl amines, e.g. heptamethyldisilazane, and cyclic amines, e.g. pyriferidine, pyrrolidine. New, till now not published, compounds were detected by physicochemical methods.

Research activities of the radiochemical section of the Department focus on the use of radioactive tracers in the study of complex equilibria in solutions and in elucidation of the chemistry of solvent extraction of selected metal ions. Recent topics included the study of solvent extraction of Eu(III) and Am(III) from aqueous-organic media, and complexation of selected metals with humic acids. The radiochemical laboratory is also engaged in the determination of radon in the environment.

**DEPARTMENT STAFF**

**Head:**
Josef Novosad (RNDr., CSc., Associate Professor, since June 2002)

**Professors:**
Jiří Hála (RNDr., CSc.)
Zdirad Žák, (RNDr., CSc.)

**Associate Professors:**
Jiří Pinkas (RNDr., Ph.D.)
Jiří Přihoda (RNDr., CSc.)
Jiří Toužín (RNDr., CSc.)

**Assistant Professors:**
Milan Alberti (RNDr., CSc.)
Miloš Černík (RNDr., CSc.)
Dalibor Dastych (RNDr., Dr.)
Jiří Křivohlávek (Mgr., since June 2002)
Aleš Mareček (RNDr., CSc.)
Marek Nečas (Mgr., Ph.D.)

**Technicians:**
Světlana Filipková
Helena Hřibová
Aleš Mareček, Jr. - part time
Zdena Michaličková
Jiří Smola
Alena Ševčíková
Jiří Verner (ing.) – part time

**Secretary:**
Vladimíra Veselská

**Ph.D. Students:**
Full time
THESES DEFENDED PER ACADEMIC YEAR 2001/2002

Diploma theses:


PhD theses:


LIST OF PUBLICATIONS

Scientific papers


JANICKIS, V., NEČAS, M., NOVOSAD, J., DUŠEK, M., PETŘIČEK, V. Commensurate and incommensurate structures of the hexabromotellurate(IV) bis {dibromodiselenenate(1)} ion - [{\(\text{C}_2\text{H}_5\text{H}_5\)}(4-n)\(\text{TeBr}_6\text{Se}_2\text{Br}_2\)(2)], \(n=0,1\). *Acta Crystallographica Section B-Structural Science*, Denmark : BLACKWELL MUNKSGAARD, 58, 6, p. 977-985, 2002.


**Abstracts of conference papers and posters**

BERAN, M., PŘÍHODA, J. Studium reakcí halogenosírových kyselin s močovinou, kyselinou amidosírovou a látkami podobnou typu (Reactions of halogenosulfuric acid with urea, amidosulfuric acid, and similar compounds). In *Sborník příspěvků IV. semináře "Pokroky v anorganické chemii"*, Vranov u Brna, September 2002, pp. 18-19


KRATOCHVÍL, J., PINKAS, J. Příprava molekulárních a vrstvenatých hlinitosfosfonátů (Preparation of Molecular and Layer Aluminophosphonates). In *Sborník příspěvků IV. seminář „Pokroky v anorganické chemii”*, Vranov u Brna, September 2002, pp. 43-44


**Scientific lectures**


**Other professional publications**


**GRANTS BESTOWED FOR PROJECTS**

**Research Project**

MSS 143100011

Žák, Z.: Structure, Bonding, Properties, and Analysis of Synthetic and Natural Molecular Ensembles.

**Grant Agency of the Czech Republic**

203/01/1533

Pinkas, J.: New Nonaqueous Routes to Phosphate, Silicate, Hybrid, and Oxide Materials.

**Ministry of Education, Youth, and Sports of the Czech Republic**

Project No. 46 (Faculty of Science MU Brno)

Přihoda J.: Integrated study of the specialization Conservator-restorator in the cooperation of study program Chemistry with social sciences

Project No. 45 (Faculty of Science MU Brno)

Mareček, A.: Development of distance education in the Faculty of Science MU – the laboratory for multimedia and network support of education

**INVITED LECTURES AND WORKING STAYS OF STAFF MEMBERS ABROAD**


Přihoda, J.: School of Technology and Economics Dresden, Germany, 1 week (August 2002).

Alberti, M.: School of Technology and Economics Dresden, Germany, 1 week (August 2002).

Žák, Z.: University of Ljubljana, Slovenia, 2 weeks (May 2002)

Přihoda, J.: Humboldt University Berlin, Germany, 3 days (June 2002)

Přihoda, J.: School of Technology and Economics Dresden, Germany, Socrates Program, lecture series on
Methods in Chemical Laboratory (May 2002)
Novosad, J.: Department of Chemistry, University of Bergen, Norway, invited lecture „Coordination chemistry of P-X-P ligands“ (July 2002).

OTHER INTERNATIONAL CONTACTS AND CO-OPERATIONS OF STAFF MEMBERS

Foreign visitors
Prof. Herrmann, E., School of Technology and Economics, Dresden, Germany, 6 days (July 2002).
Klose, J., School of Technology and Economics, Dresden, Germany, Socrates, 5 months, (March-July 2002).
Prof. Mori, H., Chubu University, Kasugai, Japan, 3 days (September 2002).

Cooperations
Department of Inorganic Chemistry, University of Göttingen, Germany, (Professor H. W. Roesky), Molecular Alumino- and Gallophosphates as Models of Zeolite Building Units and New Non-Aqueous Sol-Gel Routes to Oxide Materials (J. Pinkas).
Institute of Inorganic and Analytical Chemistry, Justus-Liebig-University of Giessen, Germany, (Professor M. Fröba), New Mesoporous Aluminophosphate Materials (J. Pinkas).
Department of Chemistry, University Jena, Germany, (Professor W. Plass), Synthesis, Structure, and Properties of Vanadosilicate and -phosphate Materials (J. Pinkas).
Department of Physical Engineering, Faculty of Mechanical Eng., Brno Technical University, Doc. RNDr. T. Šikola, CSc., „Formation of Nanostructures by Scanning Probe Microscope“ (J. Pinkas).
School of Technology and Economics, Dresden, Germany (Professor E. Herrmann) „Organophosphorus compounds and their complexes“ (Z. Žák, J. Přihoda).
University of Wroclaw, Institute of Chemistry, Poland (Professor T.Glowiak), „Low temperature diffractometry“ (Z. Žák).
University of Vienna, Institute of Inorganic Chemistry (Dr. P. Unfried) and Institute of Mineralogy and Crystallography (Dr. G. Giester), „Structures of rare earth metal compounds“ (Z. Žák).
University of St Andrews, Department of Chemistry, St Andrews, UK (Prof. J.D. Woollins), „Coordination Chemistry of P-N Ligands“ (J. Novosad, M. Nečas).
University of Bergen, Department of Chemistry, Bergen, Norway (Prof. S. Husebye), „Studies of Structure, Coordination and Bonding in Tellurium Compounds“ (J. Novosad, M. Nečas).
Chubu University, Department of Applied Chemistry, Kasugai, Japan (Prof. M. Watanabe), „Chemistry of Polyphosphates“ (J. Novosad).
Kaunas University of Technology, Department of Chemical Technology, Kaunas, Lithuania (Prof. V. Janickis), „Chemistry of Polychalcogen Compounds“ (J. Novosad, M. Nečas).
Department of Chemistry and Biochemistry, Faculty of Science, University of Lisbon, Portugal (Prof. M.J. Calhorda), „New heterobimetallic and bifunctional molecular architectures“ (J. Novosad).

STUDENTS STUDYING ABROAD
Jablonská, L.: School of Technology and Economics, Dresden, Germany, 2 months, (January-February 2002).
Kratochvíl, J.: Institute of Inorganic Chemistry, University of Göttingen, Germany, 3 months (February-April 2002).
Löbl, J.: Institute of Inorganic Chemistry, University of Göttingen, Germany, 3 months (October-December 2002).

OTHER PROFESSIONAL ACTIVITIES
Černík, M.: Member of Inorganic Chemistry Committee, Czech Chemical Society, Prague. Member of the Inorganic Chemistry Board of Examiners for Ph.D. study, Masaryk University, Brno.
Hála, J.: Associate member of the Commission V.8 (Solubility) of IUPAC. Member of the Inorganic Chemistry
Board of Examiners for Ph.D. study, Masaryk University, Brno. Member of the Nuclear Chemistry Board of Examiners for Ph.D. study, School of Nuclear Engineering, Technical University, Prague.

Novosad, J.: Member of Inorganic Chemistry Committee, Czech Chemical Society, Prague. Member of the Inorganic Chemistry Board of Examiners for Ph.D. study, Masaryk University, Brno.

Pinkas, J.: Member of the American Chemical Society. Member of the Chemistry Board, Grant Agency of the Czech Republic. Coordinator of the Socrates/Erasmus Program. Member of the Inorganic Chemistry Board of Examiners for Ph.D. study, Masaryk University, Brno.

Přihoda, J.: Member of the Inorganic Chemistry Board of Examiners for Ph.D. study, Masaryk University, Brno. Member of the Inorganic Chemistry Board of Examiners for Ph.D. study, Charles University, Prague. Coordinator of the Socrates/Erasmus Program, Head of the organizing Committee: 4th Meeting: ”Progress in Inorganic Chemistry”, Vranov near Brno, September 2002

Toužín, J.: Member of the Inorganic Chemistry Board of Examiners for Ph.D. study, Masaryk University, Brno.

Žák, Z.: Member of the Inorganic Chemistry Board of Examiners for Ph.D. study, Masaryk University, Brno. Member of the Scientific Board of the Faculty of Sciences, MU Brno. Member of the Scientific Board of the Faculty of Chemistry, Technical University, Brno
TEACHING AND RESEARCH ACTIVITIES

The fundamental part of the education as well as research in the field of Organic chemistry is concentrated at the Department of Organic Chemistry with its Division of Macromolecular Chemistry.

TEACHING ACTIVITIES

The Department is responsible for teaching the organic chemistry, macromolecular chemistry, chemical technology, and related subjects. These disciplines are taught to students seeking a bachelor’s degree in chemistry (3 years Bc), master’s degree (5 years Mgr), as well as to students involved in the chemical education. Education is provided also for non-major students of biology and environmental science. The department makes a substantial contribution to the education of all specialists in organic, inorganic, physical and analytical chemistry, and biochemistry.

Undergraduate study

The primary focus of the Department is the education of the students having their major in organic and macromolecular chemistry. The usual study length is five years and it is completed with the student’s diploma thesis. The Master’s (Magister “Mgr.”) degree is conferred after a successful completion of this program. The students are gaining knowledge and experience in all the theoretical and experimental chemistry disciplines including: synthesis, isolation, identification, and structural studies on chemical compounds using modern methods of analysis as well as knowledge in the application of computer assisted chemistry. Diploma thesis, its defense, and the state examination complete the program.

Graduate study

The department offers a program leading to the Ph.D. degree. The program usually takes three years. The students within this program, besides studying some new chemical disciplines, are teaching undergraduate programs in the laboratories and seminars and they are active members of the research groups having an access to all the research facilities available at the department, including NMR, UV - VIS and IR spectrometer instruments, GC, GC/MS and HPLC chromatography, microwave and ultrasound reactors, X-ray analysis and advanced computer technology. The study is completed following the successful defense of the doctoral thesis, and the final rigorous examination.

RESEARCH ORIENTATION

There are three basic orientations in research at the department: (1) synthetic organic chemistry focused on heterocyclic compounds, (2) physical organic chemistry, and (3) computer assisted organic chemistry in research of the structure and dynamic of biomolecules.

Synthetic Organic Chemistry

Heterocyclic Organic Chemistry

New methods of synthesis, cyclization reactions, and reaction mechanisms, reactivity of the new heterocyclic systems as well as their structure are studied. There are several research groups working in this area. One of the groups is concentrated on cyclization reactions leading to heterocyclic systems. Pericyclic reactions, their regio- and stereochemistry, especially 1,3- dipolar cycloadditions of ylides derived from quaternary isoquinoline derivatives, are investigated. The research efforts include special types of cycloadditions, so-called the “criss-cross” cycloadditions, and very interesting transformations of this way prepared heterocycles. Some of the reactions, especially intramolecular varieties, are carried out under microwave initiation. Besides, the center of the interest are naturally occurring quaternary isoquinoline alkaloids in reactions with the nucleophiles and their other transformations. An application of organonmetals on the preparation of new adamantane derivatives is upon investigation as well (M. Potáček, J. Dostál, M. Trávníček, J. Verner, R. Vicha, S. Man, J. Pospíšil).

The synthesis of substituted cyclic -methylene lactones and their reactivity in nucleophilic vinylic substitution and 1,3-dipolar cycloaddition with respect of stereo and regioselectivity of these reactions are the fields of interest of the second research group (J. Jonas, C. Mazal, P. Melša, P. Bouzek). The chemistry of substituted bicyclo[1.1.1]pentanes aimed at the development of new synthetical methods for construction of rod-like molecules with various substitutional patterns (terminal and/or lateral) useful in the construction of larger molecular or supramolecular objects is a second area of interest of this group (C. Mazal, P. Bartoš, O. Škarka).

Another group (P. Pazdera, R. Čmelík, D. Fajkusová, J. Záletovalová and M. W. Fathalla) is interested in
synthesis, structure elucidation and reactivity studies on fused five, six, seven and eight membered heterocycles containing nitrogen atom and/or the sixth group elements. Heterocyclic skeletons are prepared by an application of aromatic or heterocyclic carboxylic and carbonic acid functional derivatives. This research group is concentrated also on the preparation of new heterocyclic compounds containing chalcogene-chalcogene bond by oxidative heterocyclization reactions. In some cases, the syntheses are carried out as the domino-processes. Other research interests lie on “green chemistry” techniques (such as applications of the phase transfer catalysis, ultrasound; one-pot, multi-component and domino-reactions, and search of new simple reagents for synthesis).

General multicomponent reactions are major interest of the Benovsky’s group, especially four component Ugi reaction and its stereoselective variations. The same group is also working on the project of stereoselective aza-annulation reactions as a synthetic tool for the fast and efficient construction of heterocycles.

The spectroscopy (FTIR, UV-VIS, NMR, MS) and X-ray analysis methods are used for the identification and structure elucidation. In some cases, applications of chemical \textit{ab initio} (HF, DFT) calculations are done in a cooperation with the National Centre for Biomolecular Research.

Physical Organic Chemistry

Organic Photochemistry

The research activities of the group are concentrated in several areas. One is the study of photoinduced hydrogen and energy transfer in various systems. The reactions are studied by standard photokinetics as well as laser flash spectroscopy. The second area involves the study of various photochemical transformations, such as hydrogen abstraction or di- -methane rearrangement, with a special interest in photochemical reactivity of organic compounds in aqueous solutions, ice, as well as in the solid state. The group is also involved in developing a completely new photochemical field – photochemistry in the microwave field. (P. Klán, M. Zahadal, D. Heger, J. Literák, R. Růžička)

NMR Spectroscopy

NMR spectroscopy of organic and bioorganic molecules is the field of interest of the NMR research group (R.Marek, P. Sečkářová, J. Toušek, O.Humpa). The research is focused on the study of alkaloids, purine analogues, and other nitrogen containing heterocycles. The tautomerism, protonation, and hydrogen bonding of purine analogues are investigated by using $^{15}$N NMR spectroscopy (solution and solid-state) and \textit{ab initio} (DFT) approach. The research group is collaborating on these projects with several research groups (Antwerp, Jyväskylä, Olomouc, Prague, Szeged).

Computer assisted organic chemistry and molecular modeling

The research effort of the computer assisted organic chemistry group (J. Koča, M. Kratochvíl) is concentrated in three areas. The first is computer assisted organic synthesis using both topological and quantum chemistry methodology. Current attention is paid to reaction paths and transition states elucidation. The second field involves conformational studies on flexible molecules of a biological interest (pheromones, peptides, carbohydrates, nucleic acids). The third direction is focused on computer study of interactions and reactions of large biological polymers, especially proteins, with small substrates. This group has made an important contribution to information technology applications in chemistry.

Macromolecular chemistry

An integral part of the Department of Organic Chemistry is the Division of Macromolecular Chemistry (J. Sedlář, J. Petrů, M. Potáček and Z. Salajka, L. Pospíšil). It seems to be a significant bridge for collaboration with the Polymer Institute of Brno and Faculty of Chemistry of the Technical University of Brno. The scientific interest of the Division is focused on olefin polymerization, polymer stability studies, and development of photostabilizers and composite materials.
**Associate Professors:**
Petr Klán (RNDr., Ph.D.)
Pavel Pazdera (RNDr., CSc.)
Jaroslav Petrů (RNDr., CSc.)

**Assistant Professors:**
Petr Beňovský (RNDr., Ph.D.)
Slávka Janků (RNDr., Ph.D.) – maternity leave
Ctibor Mazal (RNDr., CSc.)
Jiří Sedlář (Ing., CSc) - part time
Richard Čmelik (Mgr.) – part time
Petr Kulhánek (Mgr.) - part time
Stanislav Man (Mgr.) - part time
Ondřej Škarka (Mgr.) – part time
Martin Trávníček (RNDr., Mgr.) – part time
Jiří Verner (Ing.) - part time
Robert Vicha (Mgr) - part time
Miroslav Zabádal (Mgr.) - part time

**Teaching Assistant:**
Jitka Halová (Ing.)

**Research Assistants:**
Raděk Marek (RNDr., Ph.D.)
Radovan Karel (Mgr.)
Hana Navrátilová (RNDr.)

**Technicians:**
Jiří Mikulášek
Marek Poděl
Česlav Ulreich
Ing. Milan Bečka – from September 2002

**Secretary:**
Milena Urbánková

**Librarian:**
Jana Foltýnová

**Adjunct Lecturers:**
Vladimír Kysilka (RNDr., CSc.) – Pliva - Lachema, a.s., Brno
Jiří Matoušek (Prof., Ing., D.Sc.) Chemical Faculty, Technical University, Brno
Karel Picka (RNDr.) Chemical Faculty, Technical University, Brno
Jiří Pichler (Ing., CSc.)
Antonín Sikora (Ing., CSc.) – Institute of Macromolecular Chemistry, Academy of Sciences, Czech Republic
Tomáš Veselý (Ing., CSc.) – Chemical Faculty, Technical University, Brno

**Ph.D. Students:**
Full time
Kamil Antoš (Mgr.)
Petr Bartoš (Mgr.)
Luzuriaga Sharbel Eduardo (Mgr.)
Michal Čajan (RNDr.)
Richard Čmelik (Mgr.)
Dagmar Fajkusová (Mgr.)
Petr Kulhánek (RNDr.)
Stanislav Man (RNDr.)
Petr Melša (Mgr.)
Martin Prokop (Mgr.)
Pavlína Sečkárová (Mgr.)
Robert Skeřil (Mgr.)
Ondřej Škarka (Mgr.)
Zdeněk Vytiska (Mgr.)
Martin Trávníček (RNDr.)
Jiří Verner (Ing.)
Zdeněk Vytiska (Mgr.)
Robert Vícha (Mgr)
Mohamed Walid Fathalla (M.Sc.)
Miroslav Zabadal (Mgr.)
Dominik Heger (Mgr.)
Jaromír Literák (Mgr.)
Jiří Pospíšil (Mgr.)
Radovan Růžička (Mgr.)

Part time
Hana Navrátilová (RNDr.)
Michal Kovář (Ing.)

THESES DEFENDED IN THE ACADEMIC YEAR 2001/2002

Diploma theses

Heger, D.: Photoinduced Triplet Energy Transfer in Flexible Bichromophores with Oligoester Tether. (Supervisor: P. Klán.)

Literák, J.: Microwave Photochemistry. (Supervisor: P. Klán.)


Pospíšil, J.: Intramolecular 1,3-dipolar cycloadditions of azomethine ylides initiated by microwaves. (Supervisor: M. Potáček.)

Růžička, R.: PCT in photochemistry. (Supervisor: P. Klán.)

Švarc, J.: Contribution to multimedial education of organic chemistry. (Supervisor: M. Potáček.)

Ph.D. theses

Fathala, W. M., M.Sc.: The Regioselectivity in Reactions of Thioamides. (Supervisor: P. Pazdera.)

Trávníček, M., RNDr.: Selectivity in 1,3-Dipolar Cycloaddition Reactions of Azomethine Ylides. (Supervisor: M. Potáček.)

Navrátilová, H., RNDr.: trans – 4-(4-Fluorophenyl)-3-substituted-1-methylpiperidines. (Supervisor: M. Potáček.)

Čajan, M.: Some Anionic Complexes and Their Building Blocks (Supervisor: J. Koča)

RNDr. Theses

Kulhánek, P.: Intra-intermolekulární criss-cross cykloadiční reakce. (Supervisor: M. Potáček.)

Man, S.: Reaction of berberine and coptisine with nucleophiles. (Supervisor: M. Potáček.)

Pospíšil, J.: Influence of N-substitution in carbamoyl stabilized azomethine ylides upon the stereoselectivity of 1,3-dipolar cycloaddition reactions. (Supervisor: M. Potáček.)

Habilitation


LIST OF PUBLICATIONS
Books, book chapters and review articles


Scientific papers


TRÁVNÍČEK, M., POTÁČEK, M. Pyrrolidine and 1,3-oxazolidine formation from azomethine ylides influenced by change from classical conditions to microwave irradiation. ARKIVOC, Florida : ARKAT-USA, 2001, (V)p. 156-163, 2002.

VERNER, J., POTÁČEK, M. Criss-cross cykloadice HNCO a HNCS na 1,4-diaza-1,3-butadienech - metoda přípravy substituovaných perhydroimidazo[4,5-d]imidazolů (Criss-cross cycloaddition of HNCO and HNCS to 1,4-diaza-1,3-butadienes - method to preparation of substituted perhydroimidazo[4,5-d]imidazoles). Chemické listy, Praha : Česká společnost chemická, 96, 3, p. 394-394, 2002.


Abstracts of conference papers and posters


KŘÍŽ, Z., OTYEPKA, M., KOČA, J. Hydration of the CDK2 active site. Molecular dynamics study.


OTYEPKA, M., STRNAD, M., DAMBORSKÝ, J., KŘÍŽ, Z., KOČA, J. Proteins and Their Interactions With Small Molecules Studied by Computer Simulations.


Other professional publications


Major popularisations and other professional publications


GRANTS BESTOWED FOR PROJECTS

Grant Agency of Ministry of Education

COST D 10.20 / 2002

Fund of International Co-operation

KONTAKT ME 571

Fund of the Development of Universities

758/2002

761/2002
MELŠA, P.: 1,3-Dipolární cykloadice alfa-methylenlaktonů.
**Grant Agency of the Czech Republic**

203/02/0879
Klán, P. - Vliv mikrovlnného záření na fotochemické reakce

205/02/0896
Klán, P., Holoubek, I. - Fotochemie persistentních organických látek v ledu a na povrchu ledu a půd za různých klimatických podmínek

203/00/1011

203/01/1333
Pazdera, P.- Chalkogenorganic compounds – synthesis, structure and reactivity study

**AWARDS**


**CONFERENCES (SYMPOSIUMS, SEMINARS) ORGANIZED BY THE DEPARTMENT STAFF MEMBERS**


Marek, R.: Member of the Organizing Committee – Meeting of the Central European NMR Discussion Groups, April, 2002. Valtice. Czech Republic


**INVITED LECTURES AND WORKING STAYS OF STAFF MEMBERS ABROAD**

**Stays**

Klán P.: Norwegian Institute for Air Research; Ny-Ålesund, Svalbard, Norway (10 days)

Koča J.: CERMAV, Grenoble, France (visiting professor, 3 months)

Marek, R.: University of Antwerp, Belgium (1 months)

Marek, R.: University of Szeged, Hungary (4 days)

Mazal, C.: University of Colorado at Boulder, USA (3 months)

Pazdera, P.: University of Innsbruck, Austria (visiting professor, 4 days)

**Invited Lectures**


Beňovský, P.: Stereoselective aza-annulation reactions. Institut für Organische Chemie, Universität Regensburg, Germany.


OTHER INTERNATIONAL CONTACTS AND CO-OPERATIONS OF STAFF MEMBERS

Lectures

Prof. Dr. Josef Michl, University of Colorado, Boulder, USA, lecture: The Chemistry of Carborane Anions and Radicals.


Prof. Dr. Joachim G. Schantl, Institut für Organische Chemie, Universität Innsbruck, Austria lecture: Diazene – Derived Azomethine Imines.

Ing. Daniel Horák, CSc., Institute of Macromolecular Chemistry, Academy of Science, Prague, lecture: Synthetic and Natural Hydrogels as Carriers of Biologically Active Compounds for Medicine and Biology.

Prof. Dr. Jacek Mlochowski, Institute of Organic Chemistry, Biochemistry and Biotechnology, Wrocław University of Technology, Poland, lecture: Recent Development in the Synthesis of new Bioactive Selenium Containing Heterocycles.

Prof. Dr. Fernando Langa, Faculty of Science, Universidad de Castilla-La Mancha, Toledo, Spain: lecture: Synthesis and Profoperties of Electroactive Fulleren Derivatives.

Prof. Dr. Uroš Urleb, University of Ljubljana, Slovenia, lecture: Design, Synthesis and Biological Activity of Thrombin Inhibitors with an Azaphenylalanine Scaffold.

Prof. Dr. Chris Strauss, Centre for Green Chemistry, School of Chemistry, Monash University, Victoria, Australia, lecture: Green, Thermal Organic Chemistry

Prof. Jakob Wirz, Institut für Physikalische Chemie, Universität Basel, Switzerland, lecture: Bringing light to dark reactions, lecture course: A crash course on laser flash photolysis.

Dr. Lajos Kovács, Department of Medicinal Chemistry, University of Szeged, Hungary, lecture: Regioselective substitution of guanine.

Cooperation

Prof. Dr. Albrecht Mannschreck, Institut für Organische Chemie, Universität Regensburg, Germany, Enantiomeric separations. (M. Potáček,).

Dr. André Loupy, Université Paris – Sud, Institut de Chimie Moléculaire d’Orsay, Laboratoire des Réactions sur Supports, France. Microwave Assisted Organic Synthesis (M. Potáček, P.Klán).

Dr. Lajos Kovács, University of Szeged, Hungary, N7/N9 – Guanine Derivatives (R. Marek).

Prof. Erkki Kolehmainen, University of Jyväskylä, Finland, NMR of Purine Analogues (R. Marek).
Prof. Roger Domnisse, Prof. Luc Pieters, University of Antwerp, Belgium, Structural Studies of Alkaloids (R. Marek)

Prof. Dr. Wolf-Diethard Pfeiffer, Institut für Chemie, Universität Greifswald, Germany, Synthesis of Organic Selenium Compounds (P. Pazdera).

Prof. Dr. Peter Kutschy, Prof. Dr. Milan Dzurilla, Department of Organic Chemistry, P. J. Šafárik University, Košice, Slovak Republic, Synthesis of phytoalexin analogues (P. Pazdera).

Prof. Dr. Jackie Mlochowski, Institute of Organic Chemistry, Biochemistry and Biotechnology, Wroclaw University of Technology, Poland, Synthesis of 2-Aminoselenophenolation and its Synthetic Applications (P. Pazdera).

Prof. Dr. Joachim Schantl, Institute of Organic Chemistry, Innsbruck University, Austria, One-pot synthesis of some thiazoles and imidazole derivatives.

Dr. Walid Fathalla Mohamed, Suez Canal University, Faculty of Engineering, Port Said, Egypt. Synthesis of quinazoline derivatives by domino-reactions.


Prof. Jakob Wirz, Institut für Physikalische Chemie, Switzerland: Laser flash photolysis of phenacyl chromophores (P. Klán).

Dr. Anne Imberty, CERMAV Grenoble, France: Structural studies in carbohydrate chemistry (J. Koča).

STUDENTS STUDYING ABROAD
Hana Zachová, Universität Regensburg, Institut für Organische Chemie, Germany – 4 months.
Martina Rozypalová, Universität Regensburg, Institut für Organische Chemie, Germany – 4 months.
Luboš Vrbka, University of Missouri, USA- 2 months.
Tomáš Pospíšil, University of Missouri, USA- 2 months.
Veronika Trávníčková, Universita Degli Studi di Palermo, Italy – 3 months.
Lenka Baráková, University of Antwerp, Belgium – 4 months.
Pavlina Sečkárová, Mgr., University of Jyväskylä, Finland – 4 months.
Radovan Růžička, Mgr., University of Jyväskylä, Finland – 4 months.
Dagmar Fajkusová, Mgr., Universität Innsbruck, Institut für Organische Chemie, Germany – 3 months.
Jiří Pospíšil Mgr., Université Catolique, Louvain-la-Neuve, Belgium – 3 months
Miroslav Zabadal, Mgr., Universität Regensburg, Institut für Organische Chemie, Germany – 3 months.
Kamil Antoš, Mgr., Universität Regensburg, Institut für Organische Chemie, Germany – 4 months.
Petr Bartoš, Mgr., University of Colorado, Boulder, USA – 6 months.

STAYS OF FOREIGN STUDENTS AT DEPARTMENT
Mgr. Jana Záletová, Department of Organic Chemistry, P. J. Šafárik University, Košice, Slovak Republic, Syntheses of Compounds with Indol-3-yl Benzothiazole Skeleton – 5 months (Supervisor: P. Pazdera).
Luisanna Antonina Caradona, Universita Degli Studi di Palermo, Italy – 3 months (Supervisor: M.Potáček, S.Man).
Dr. Walid Fathalla Mohamed, Suez Canal University, Faculty of Engineering, Port Said, Egypt. Synthesis of Quinazoline Derivatives by Domino-reactions. Post-doc-stay – 2 months (Supervisor: P. Pazdera).

STUDENT AWARDS
OTHER PROFESSIONAL ACTIVITIES

Potáček M.: Chairman: Chemical Section, Chemical Section Scientific Board and Organic Chemistry Scientific Board at Masaryk University, Member of Organic Chemistry Scientific Board at Charles University of Prague, Prague Institute of Technology and Palacky University of Olomouc, Member of the State Examination Committee at Prague Institute of Technology, Palacky University Olomouc, University of Pardubice and Technical University of Brno, Faculty of Chemistry.

Pazdera, P.: Vice-chairman of Faculty Senate. Member of Czech Universities Council. Member of Commission for Defences of Ph.D. Thesis, Department of Organic Chemistry, Prague Institute of Technology, University of Pardubice and Slovak Technical University, Bratislava, Member of Habilitation Commision, Faculty of Chemistry, University of Pardubice.

Beňovský, P.: Member of the Group for Organic, Bioorganic and Pharmaceutical Chemistry, the Czech Chemical Society.

Koča, J.: member of the scientific board of Faculty of informatics, chairman of the Brno branch of the Czech chemical society, member of the American chemical society, member of the government accredit board in chemistry, doctoral study board (organic chemistry, physical chemistry, environmental chemistry, biomolecular chemistry, biophysics).
Department of Theoretical and Physical Chemistry

TEACHING AND RESEARCH ACTIVITIES

The Department of Theoretical and Physical Chemistry at the Faculty of Science continued to contribute substantially to the education of future chemists in the field of physical chemistry (about 60 students per year), future teachers of chemistry (about 30 students per year), future biologists and ecologists (about 60 students per year) as well as to research activity in the fields of theoretical and physical chemistry.

Pedagogical efforts involved fundamental lectures on physical chemistry, including quantum chemistry and chemical constitution and specialized courses in electrochemistry, chemical kinetics, quantum chemistry, spectroscopy (NMR, EPR, MS), phase equilibria, statistical thermodynamics and irreversible processes including extensive laboratory courses at undergraduate and postgraduate levels.

The research activity of the department concerned the study of the chemical and electrochemical reactivity of chemical substances and the relation to their structure through the use of different experimental and theoretical methods of physical chemistry. Reactions provided by electron transfer have been studied by means of electrochemical methods. New method of electrochemical signal processing and electrochemical methods with simultaneous membrane introduction mass spectrometry and with simultaneous electron paramagnetic resonance have been designed. Phase equilibrium and diffusion studies in metallic systems have been performed in collaboration with the Institute of Physics of Materials, Academy of Sciences of the Czech Republic, electrochemistry of nucleic acids and proteins are performed in collaboration with the Institute of Biophysics, Academy of Sciences of the Czech Republic. The spatial structure of biological macromolecules and biomacromolecular dynamics is studied by means of high field NMR in solutions. In addition this department studies other physico-chemical properties of molecules (surface tension, viscosity, conductivity, etc.) in relation to their molecular structure using computer simulations and molecular modeling.

DEPARTMENT STAFF

Head:
Jan Vřešťál (Prof., RNDr., D.Sc.)

Professors:
Miroslav Holík (RNDr., CSc.)
Vladimír Sklenár (RNDr., D.Sc.)

Associate Professors:
Pavel Janderka (RNDr., CSc.)
Pavel Kubáček (RNDr., CSc.)
Marie Studničková (RNDr., CSc.) – till September 2002
Libuše Trnková (RNDr., CSc.)

Assistant Professors:
Pavel Brož (RNDr., Ph.D.)
Jiří Sopoušek (RNDr., CSc.)
Jaromír Toušek (RNDr., Ph.D.)

Technicians:
František Macourek
Dana Tesařová

Secretary:
Marta Holíková

Adjunct Lecturers:
Jiří Čermák (RNDr., CSc.) Inst. of Physics of Materials Acad.Sci. CR Brno

Ph.D. Students:
Full time
Iveta Bártová (Mgr.)
Eva Drbálková (Mgr.)
Miroslava Filgasová (Ing.)
Klára Hladečková (Mgr.)
Jana Houserová (Mgr.)
Radka Chaloupková (Mgr.)
Josef Chmelík (Mgr.)
Květuše Chvátalová (Ing.)
Libor Kapička (Mgr.)
Jan Kmuniček (Mgr.)
Hana Krčíková (Mgr.)
Karel Kubiček (Mgr.)
Barbora Láňová (Mgr.)
Eva Lichnerová (Ing.)
Michaela Matějková (Mgr.)
Natália Musilová-Sedláčková (Mgr.)
Radim Picha (Mgr.)
Filip Rážga (Ing.)
Radka Vařková (Mgr.)
Martin Zeman (Mgr.)

Part time
Petr Kovařík (Mgr.)
Lukáš Králík (Ing.)
Petr Padrt (Mgr.)
Vladimir Proks (Mgr.)
Věra Rothová (RNDr.)

THESES DEFENDED IN THE ACADEMIC YEAR 2001/2002

Diploma theses:
Chmelík, J.: NMR and Molecular Dynamics: Tools for Structural Studies of Proteins (supervisor: V. Sklenář) (in English)

Ph.D. theses:
Houserová, J.: First principles studies of ordered structures in systems of transition metals (supervisor: J. Vřešťál) (in English)
Padrta, P.: Analysis of NMR Data for Structure Elucidation of Nucleic Acids (supervisor: V. Sklenář) (in English)

LIST OF PUBLICATIONS

Books, book chapters and review articles

Scientific papers


Abstracts of conference papers and posters


KAPÍČKA, L. Vlastnosti a využití softwaru gNMR (Advantage of gNMR program). In IV. seminář POKROKY V ANORGANICKÉ CHEMIÍ. p. 42-42, 2002.


TRNKOVÁ, L., SOUKENÍKOVÁ, N., ADAM, V., MAZAL, C. Elektrochemické chování azidových sloučenin na rtuťových elektrodech (Electrochemical behaviour of azide compounds on mercury electrodes). In Sborník přednášek z XXII. celostátního semináře Moderní elektrochemické metody. p. 31-33, 2002.


Major popularisations and other professional publications:


TRNKOVÁ, L.: Two Workshops in the Faculty of Science, Masaryk University, Brno, MU and Foundation Universitas Masarykiana, No.4, p. 24-29, 2002, Brno, ISSN 1211-6866.

GRANTS BESTOWED FOR PROJECTS

Grant Agency of the Czech Republic

106/02/0876
Brož, P. (co-ordinator Buršík, J., IPM AS CR Brno): Theoretical and experimental study of Ni-based model systems and thermodynamic description of phase equilibria

203/00/0511
Sklenář, V.: Dynamics and Thermodynamics of Mouse Pheromone - Protein Complexes.

106/00/0855
Sopoušek, J. (co-ordinator Foret, R., FSI VUT Brno): Kinetics of Carbide Precipitation in Cr-Mo Steels

203/02/0422

106/00/0174

106/02/0877
Vřešíč, J.: Experimental and theoretical studies of stability of intermetallic phases on the base of transition metals

Grant Agency of the Academy of Sciences of the Czech Republic

A 1163201 (G0396)
Trnková, L.: Application of adsorptive transfer and elimination techniques in oligonucleotides and nucleic acids analysis.

Grant Agency of the Ministry of Education, Youth and Sports

F0808/2002 (G0382)
Janderka, P.: Advanced Kinetics Methods

F4812/2002 (G0385)
Kubáček, P.: EPR-spectroscopy in examples.

F 0794/2002 (G0380)
Trnková, L.: Multimedial learning texts for seminar on physical chemistry.

COST OC. 531.001 (G0336)
Vřešíč, J: Theoretical modelling of phase diagrams of alloys with low melting points.

KONTAKT TSR-004-99

KONTAKT ME 428 (G0332)
CONFERENCES (SYMPOSIA, SEMINARS) ORGANIZED BY THE DEPARTMENT STAFF MEMBERS

17th NMR Valtice, Meeting of the Central European NMR Discussion Groups. 8.-10.4. 2002, Valtice, CR, Holík M. - Chairman of the Organizing Committee.

54th Congress of Chemical Societies of Czechia and Slovakia, Brno, 1.- 4.7.2002, Holík M. – Member of the Organizing Committee.

Chemometrics VI, International Chemometric Conference, Brno, 1.-5.9.2002, Holík M. - Member of the Organizing Committee.

3rd Workshop of Physical Chemists and Electrochemists. 6.2.2002, Brno, CR, Janderka P. - Member of the Organizing Committee.

3rd Workshop of Physical Chemists and Electrochemists. 6.2.2002, Brno, CR, Trnková L. - Chairman of the organizing committee.

6th Workshop of Biochemists and Molecular Biologists. 7.2.2002, Brno, CR, Trnková L. - Member of the organizing committee.

Chemometrics VI., Brno, CR, Trnková L. - Member of the organizing committee.


34.IOC on Minning and Metallurgy, 30.9.-3.10.2002, Bor, Yugoslavia, Vřeštál, J. - Member of the Scientific Committee

INVITED LECTURES AND WORKING STAYS OF STAFF MEMBERS ABROAD


Janderka, P.: Dechlorination of Chlorobenzene – a DEMS study, University Bonn, Bonn, Germany, 27.5.-7.6.2002.


Trnková, L.: Department of Analytical Chemmistry, University of Barcelona, Spain, 16.-22.12.2002

Vřeštál, J.: Modelling of Thermodynamic Properties of Phases and CALPHAD Method. 25.11.2002, Bor, Yugoslavia

OTHER INTERNATIONAL CONTACTS AND CO-OPERATIONS OF STAFF MEMBERS

Foreign visitors

Thomas Loeffler, University Bonn, Bonn, Germany, 2 weeks, study stay, lecture.

Cooperations

Collaboration with the Institut of Theoretical and Physical Chemistry, University Bonn, Germany, prof.H.Baltruschat (P.Janderka, J.Vřeštál).

Collaboration with Nankai University Tianjin, China, prof. Lin, Shao-fan (P.Brož, P.Janderka).
Collaboration with the Department of Physical Chemistry, Davis, University of California, USA, prof. R.W. Fawcett (L.Trnková).

Collaboration with the Institute of Biophysics AS CR, Brno, Czech Republic (L. Trnková).

Collaboration with the J. Heyrovský Institute of Physical Chemistry, Praha, Czech Republic (L. Trnková).

Collaboration with the Institute of Physics of Materials AS CR Brno, Czech Republic (J.Vřešťál, P.Brož, J.Sopoušek).

STUDENTS STUDYING ABROAD

Láňová, B.: University Bonn, Bonn, Germany, 1 year.
Lichnerová, E.: TU München, Germany, 1 year.
Picha, R.: University of Vienna, Vienna, Austria, 6 months

OTHER PROFESSIONAL ACTIVITIES

Holík, M.: Member of the Czech Committee for Chemistry-national associate organization to IUPAC, Chairman of the Discussion Group Magnetic Resonance Spectroscopy, Secretary of the Brno Branch of the Czech Chemical Society, Member of the German Chemical Society, Member of the Physical Chemistry Board for Ph.D.studies, Palacký University, Olomouc, Member of the Physical Chemistry Board for Ph.D.studies, Faculty of Chemistry, Technical University, Brno, Member of the Physical Chemistry Board for Ph.D.studies, Masaryk University, Brno., Member of the Organic Chemistry Board for Ph.D.studies, Masaryk University, Brno.

Janderka, P.: Member of the Physical Chemistry Board for Ph.D.studies, Masaryk University, Brno.

Kubáček, P.: Member of the Physical Chemistry Board for Ph.D.studies, Masaryk University, Brno.

Sklenář, V.: Member of the Editorial Board of the Journal of Magnetic Resonance Academic Press San Diego, USA, Member of the New York Academy of Sciences, Member of the Council of the Society International Society of Magnetic Resonance, Member Groupement Ampere, Member of the Physical Chemistry Board for Ph.D.studies, Masaryk University, Brno, Member of the Scientific Council, Faculty of Science, Masaryk University, Brno, Member of the Scientific Council, Masaryk University, Brno, Member of the Scientific Council, Charles University, Prague.


Studničková, M.: Member of the Physical Chemistry Board for Ph.D.studies, Masaryk University, Brno.

Vřešťál, J.: Member of Scientific Board of Institute of Physics of Materials Academy of Sciences of the Czech Republic, Brno, Member of Scientific Board Faculty of Science Palacký University Olomouc and Chemical Faculty of Technical University, Brno, Member of the Physical Chemistry Board for Ph.D.studies, Masaryk University, Brno, Member of the Physical Chemistry Board for Ph.D.studies, Palacký University, Olomouc, Member of the Physical Chemistry Board for Ph.D.studies, Technical University, Brno.

AWARDS GIVEN TO STAFF MEMBERS AND STUDENTS

Holík, M.: Hanuš- Medal Czech Chemical Society

Vřešťál, J.: Medal-10. Years Chemical Faculty Technical University Brno

Houserová, J.: Prize of Dean of Faculty of Science

Picha, R.: Prize of Dean of Faculty of Science
TEACHING AND RESEARCH ACTIVITIES

RECETOX (Research Centre for Environmental Chemistry and EcoTOXicology) was established in July 7, 1994. The Centre was a research unit of the Department of Environmental Chemistry and Ecotoxicology. In 2001, RECETOX merged with the Department of Environmental Chemistry and Ecotoxicology and, since, provides master and postgraduate studies in the fields of environmental protection, ecotoxicology and environmental chemistry. In 2002, RECETOX was honoured by European Commission and currently is supported by European Union as "The Center of Excellence for Environmental Chemistry and Ecotoxicology". At present, RECETOX is an interdisciplinary, inter-institutional research and teaching centre working in the field of fundamental research in the environmental chemistry, ecotoxicology and risk analysis, as well as with the training of bachelor, master and postgraduate students in the fields of environmental chemistry and ecotoxicology.

Centre is not setting a goal to be a large research workplace or institute but it is based on the philosophy of relatively smaller groups of co-workers and ad hoc research teams. The fundamental goal of RECETOX is to participate in joint research projects with European institutes and to establish creative scientific teams from various countries for the solution of environmental problems, grants, and orders from industry etc. External co-workers of the Centre take significant part on education in both master and doctoral studies.

Structure of RECETOX is as follows: Division of Environmental Chemistry (Head: Ivan Holoubek), Ecotoxicology Division (Head: Luděk Bláha), Environmental Analytical Chemistry Division (Head: Jana Klánová), Risk Analysis and Data Evaluation (Head: Ladislav Dušek). RECETOX staff consists of members of the Faculty of Science and outside co-workers from the Czech Republic and other countries. Research activities of RECETOX are based on the basic philosophy of Project TOCOEN (TOxic COmpounds in the ENvironment) and are focused on the following research topics: environmental fate and long-range transport of persistent organic pollutants, research and development of new ecotoxicological tests and methods, methodology of environmental and ecological risk assessment, mathematical modelling of the fate of pollutants, regionally-specific ecological risk assessment activities based on available multivariate environmental data, development of effective biomonitoring of stressed soils in Czech Republic, development of a novel type of software for environmental science based on expert-system built over interactive database.

The original objective of TOCOEN Project was extended to cover heavy metals, natural toxins and Persistent, Bioaccumulative and Toxic pollutants (PBTs). The acronym TOCOEN is now interpreted as "TOxic COmpounds in the ENvironment" and running projects are concerned with persistent toxic substances (PTS). Currently, the main goal are the studies of relations between the concentration levels of pollutants in the environment and their potential effects to living organisms. Additionally, risk assessment and the fate of selected organic pollutants in the environment is studied in details. This includes inputs of PTS to various parts of environment (through emissions), their transport in compartments and between them, their transformations (photochemical, chemical, thermal, biochemical), their biological effects (dose / concentration - exposure analysis), modelling of the processes, and risk assessment, management and prognosis of contamination development.

Certain groups of PTS such as polycyclic aromatic hydrocarbons (PAHs), chlorinated pesticides (OCPs), polychlorinated biphenyls (PCBs), dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs) were selected as model compounds at the beginning of the project. Currently, other groups of organics such as chlorinated benzenes, phenols, certain other types of pesticides, chlorinated aliphatic hydrocarbons and other chlorinated aromatic compounds are also being intensively studied. Model compounds are studied in all environmental compartments. New research topics are also focused on the environmental photochemistry of PBT compounds in ice and environmental surfaces (in co-operation with research group of dr. Petr Klan, Dept. of Organic Chemistry, Faculty of Science, Masaryk University), assessment of toxicity and ecotoxicity of environmental photoreaction products, studies of effects of new types of PBTs, such as chlorinated paraffins or brominated compounds.

From 1997, cooperating research groups of the RECETOX team, TOCOEN, Ltd., and several other Czech and international institutions use for their common presentations the acronym RECETOX - TOCOEN & Associates (R - T & A). Present activities of R - T & A group are focused on the establishment a Scientific Network on Persistent, Bioaccumulative and Toxic Chemicals (PBTs). The main goal of this Network is to bring together scientists working in this field and to explore the potential of an organised and coordinated research programme.
on persistent, bioaccumulative and toxic chemicals at a European level. This scientific network aims to provide a platform for scientists working in the field of environmental chemistry, environmental toxicology, ecotoxicology and risk analysis.

The basic scientific topic of the newly established Center of Excellence "RECETOX" is the study of relationships between environmental occurrence and levels of various types of pollutants (mainly persistent, bioaccumulative and toxic - PBTs). The activities of the Centre of Excellence cover: (1) establishment of the European scientific network on persistent, bioaccumulative and toxic substances based on the previous activities in this field; (2) the Central and Eastern European Countries PBTs Network with special attention to the PBT environmental contamination in the region; (3) Czech National Network in Environmental Chemistry and Ecotoxicology. These networks organize under the auspice of the Centre every year special workshops and thematic conferences as a base for exchange of scientific results and information and common preparation of various projects and programmes. Educational activities are focused on the exchange of scientists, PhD students and postdoctoral students and also on the preparation of specifically oriented Summer school. As a part of common networks activities, the special study concerning to PBTs in Central and Eastern European Countries and special environmental database will be developed.

RECETOX have participated on the Global Inventory of Persistent Toxic Substances as a part of activities which are connected with implementation of Stockholm Convention. RECETOX coordinated this inventory for European region and was responsible for preparation of European Regional Report, which was prepared as a part of project "Regionally Based Assessment of Persistent Toxic Substances Covered by UNEP Chemicals and GEF.

DEPARTMENT STAFF

Head:
Ivan Holoubek (Prof., RNDr., CSc.)

Professor:
Jiří Matoušek (Prof., Ing., DrSc.) - part time

Associate Professors:
Aleš Hrdlička (Doc., RNDr., CSc.) - till August 2002
Blahoslav Maršálek (Doc., Ing., CSc.) - part time
Zdeněk Šimek (Doc., RNDr., CSc.) - part time

Assistant Professors:
Ladislav Dušek (RNDr., Dr.)
Luděk Bláha (Mgr., Ph.D.)
Pavel Čupr (Mgr., Ph.D.) - part time

Research Assistants:
Jakub Hofman (Mgr.)
Alena Ansorgová (RNDr.) - till August 2002
Jana Klánová (RNDr.) - part time
Irena Holoubková (RNDr.) - part time

Technicians:
Romana Kostrhoumová (Ing.)
Eva Krejčí - from July 2002
Iva Poláková (Mgr.) - on maternity leave

Secretary:
Hana Kordačová

Adjunct Lecturers:
Petr Anděl (RNDr., CSc.) - Evernia Ltd., Liberec
Jiřina Hofmanová (Doc., RNDr., CSc.) - Institute of Biophysics, Academy of Sciences CR, Brno
Anton Kočan (Ing., CSc.) - Institute of Preventive and Clinical Medicine, Bratislava, Slovakia
Alois Kozubík (Doc., RNDr., CSc.) - Institute of Biophysics, Academy of Sciences CR, Brno
Miroslav Machala (RNDr., CSc.) - Veterinary Research Institute, Brno

Ph.D. Students:
Full time
Michal Boháč (Mgr.)
Pavel Babica (Mgr.)
Jindřiška Dolinová (Mgr.)
Michaela Drábková (Mgr.)
THESES DEFENDED IN THE ACADEMIC YEAR 2001/2002

Diploma theses:

Bezchlebová, J.: Validation of qCO2 coefficient (supervisor: J. Hofman) (in Czech)
Štejnarová, P.: PBT compounds in wet atmospheric deposition (supervisor: A. Ansorgová) (in Czech)
Šváchová, L.: PBT compounds in wet atmospheric deposition (supervisor: A. Ansorgová) (in Czech)
Ph.D. theses:
Jesenská, A.: Detoxication of halogenated aliphatic compounds by Mycobacteria
Malý S.: Analysis biotic and abiotic factors affecting microbial indicators

Master of Science Theses
Dušek, L.: Ecological Risk Assessment Studies Based on Biomonitoring Data - Biostatistical Modelling Approach
Hodovský J.: Assessment of Quality of Surface Waters - Application of Data from Biomonitoring Studies
Prokop Z.: Bioavailability of Soil and Sediment Contaminants

LIST OF PUBLICATIONS

Books, book chapters and review articles
SVOBODNÍK, A., DUŠEK, L., MUŽÍK, J., PECEN, L., NOVOTNÝ, J. Projekt CARMEN - výsledky epidemiologické studie karcinomu prsu u žen v ČR (CARMEN project - results of the epidemiological study of breast cancer in women from Czech Republic). In J. Abramámová (Ed) Vybrané otázky onkologie VI. p. 97-100, 2002

Scientific papers


Abstracts of conference papers and posters


PROJECT GRANTS RECEIVED

UNEP Chemicals/GEF
Holoubek, I. (Regional co-ordinator for Europe): UNEP Chemicals/GEF Project Regionally Based Assessment of Persistent Toxic Substances

UNIDO/GEF
Holoubek, I.: Enabling activities to facilitate early action in the implementation of the Stockholm Convention on Persistent Organic Pollutants (POPs Convention) in Czech Republic

5th Framework Programme of EU
Holoubek, I. - "RECETOX" - Center of Excellence for Environmental Chemistry and Ecotoxicology (kontrakt No. EVK1-2002-00519)
Holoubek, I. - "APOPSBAL" - Assessment of the selected POPs (PCBs, PCDD/Fs, OCPs) in the atmosphere and water ecosystems from the waste materials generated by warfare in former Yugoslavia (kontrakt No. ICA2-CT-2002-10007)
Holoubek, I. - Dioxins and PCBs - Environmental Levels and Human Exposure in Candidate Countries (kontrakt No. ENV.C.2/SER/2002/0085)

Polar Programme of Norway
I. Holoubek, P. Klán: Polar Programme, Expedition Svalbarg - The Photochemistry of PBT Compounds in Ice

Grant Agency of the Czech Republic
525/00/D101
Bláha, L.: In vitro methods for studies of epigenetic toxicity of xenobiotics
205/02/0896
Holoubek, I.: Photochemistry of persistent organic compounds in water ice and on its surface

Grant Agency of the Ministry of Education, Youth and Sport
MŠMT:FRVŠ 786/2002
Hofman, J.: Adaptation of soil microbial biomass on positive and negative changes
MŠMT:FRVŠ 745/2002
Holoubek, I.: Laboratory for Studies of Environmental Processes
MŠMT:FRVŠ 755/2002
Kosubová, P. Optimalization of toxaphen analyses in environmental matrices. (supervisor: J. Klánová)

Governmental Council for Science and Research CR / Ministry of the Environment CR
CEZJ 0714 0003
Holoubek, I.: Environment, Carcinogenesis, Oncology

VaV/340/1/00
Holoubek, I.: Region specific approaches in the analysis of ecological risks – methodology of assessment in the relationships to the natural catastrophes

VaV/340/1/01
Holoubek, I.: Effects of environmental pollution to the contamination and quality of biotic components of ecosystems. Subproject: Photochemistry of organic pollutants in wax layer from the needles surfaces

VaV/740/2/01
Holoubek, I.: Transformations of atmospheric pollutants in the relationships to the negative anthropogenic processes, their effects on human population, landscape receptors and modelling of atmospheric transport
Holoubek, I.: Evaluation of ecosystem and health risks of heavy metals and persistent organic pollutants in the relationships to the obligations of CR from Convention CLRTAP

Holoubek, I.: The investigation of measures effectiveness concerning to the limitation of air pollution based on reduction of negative effects of pollutants to the environmental compartments and human health

CONFERENCES (SYMPOSIA, SEMINARS) ORGANIZED BY THE DEPARTMENT MEMBERS

The 2nd Technical Workshop on effects and transboundary movement of persistent toxic substances (Project UNEP/GEF Regionally-Based Assessment of Persistent Toxic Substances) 19-23/2/2002, Göteborg, Sweden (Holoubek I. - Chair of Organizing Committee, other staff of RECETOX - organizers)

The Second PCB Workshop - Recent Advances in the Environmental Toxicology and Health Effects of PCBs. 7-11/5/2002, Brno, Czech Republic (Holoubek I. - Chair of Organizing Committee, other staff of RECETOX - organizers)

Regional Priority Setting Meeting - Europe (Project UNEP/GEF Regionally-Based Assessment of Persistent Toxic Substances), 28/5-1/6/2002, Průhonice, Czech Republic (Holoubek I. - Chair of Organizing Committee, other staff of RECETOX - organizers)

7th Regional Meeting of the Central and Eastern European Section "SECOTOX 2002" - Trends and Advances in Environmental Chemistry and Ecotoxicology. 14-16/10/2002, Brno, Czech Republic (Holoubek I. - Chair of Organizing Committee, other staff of RECETOX - organizers)

NATIONAL AND INTERNATIONAL AWARDS OF THE STAFF MEMBERS

Holoubek, I. Silver medal of Faculty of Chemistry, Technical University, Brno (10th anniversary of the faculty establishment)

Matoušek, J. Gold medal of Faculty of Chemistry, Technical University, Brno (10th anniversary of the faculty establishment); Diploma and selection for publication in "Great Minds of the 21st Century", American Biographical Institute, U.S.A.; Diploma and selection for publication in "2000 Outstanding Europeans of the 21st Century", International Biographical Centre, Cambridge, U.K.

INVITED LECTURES AND RESEARCH STAYS OF STAFF ABROAD


Holoubek I. Persistent, bioaccumulative and toxic substances – sources, environmental levels and risks. Conference Hazardous Chemicals and Environmental Safety. Moscow, Russia, 6.-8.3.2002 (invited lecture).


Maršálek, B. Early warning and prediction of cyanobacterial water blooms. Porto University, Portugal, 28.2-1.3.2002 (invited lecture)


Maršálek, B. Cyanobacterial toxins. District Hygiene Institute, Michalovce, Slovakia, 23.5. 2002 (invited lecture)


Matoušek, J., Assistance and Protection – One of the main pillars of the Chemical Weapons Convention: Access of the Czech Republic to the Article X of the Convention. NATO-RTA-SAS Panel Symposium on Defensive Aspects of Chemical and Biological Warfare, Delft, Netherlands, 5.6.2002 (invited lecture)


Matoušek, J.: Banning chemical weapons – forever. NGO Committee for Peace, UNO Vienna, 19.3.2002 (invited lecture)

Matoušek, J.: Personal decontamination within the rescue measures following terrorist chemical, biological and radiological attacks. NATO-ARW: Technology for Combating WMD Terrorism, Baltimore - Hunt Valley, USA, 19.-22.11.2002 (invited lecture)

OTHER INTERNATIONAL CONTACTS AND CO-OPERATION OF STAFF

Based on the previous activities of EERO (European Environmental Research Organization), ESF (European Scientific Foundation) and the 5th Framework Programme of European Union (RECETOX - Center of Excellence, kontrakt EVK1-2002-00519) Network on Persistent, Bioaccumulative and Toxic chemicals (ESF Network on PBTs Chemicals) was established with the following scientific and research topics:

♦ the fate of PBTs in the European region - source inventories, emission/deposition processes, long-range transport, transformation processes and bioavailability of PBTs in terrestrial ecosystems, modeling of chemical fate in the environment at the local, regional and global scale with special attention to new types of chemicals and those for which inadequate monitoring data exist;

♦ the developing of new sampling and analytical methods for PBTs;

♦ the study of effects on various types and levels of biota with special attention to study of effects of environmental mixtures and study of ”unknown” effects – study of phytotoxic effects, effects on soil microbial populations and soil fauna, effects on aquatic biota, the developing of mechanism-based biomarkers of effect, study of non-genotoxic carcinogenesis;

♦ ecological risk assessment – reliable monitoring data are needed for risk assessment and model calibrations.

Research centre RECETOX is the co-ordination centre of this network. ESF Network on PBTs compounds includes 15 European and US universities and research institutes. Research activities of RECETOX cover the Czech participation on EMEP Programme of UN ECE Convention CLRTAP and completely performed the regional background monitoring of persistent, toxic substances in the area of Košetice observatory of Czech Hydrometeorological Institute.

At present, RECETOX as a part of R-T&A is the implementation agency of Stockholm Convention in the Czech Republic (GEF/UNIDO project Enabling activities to facilitate early action in the implementation of the Stockholm Convention on Persistent Organic Pollutants (POPs Convention) in Czech Republic). Also RECETOX participates on the UNEP/GEF Project Regionally Based Assessment of Persistent Toxic Substances (co-ordination of region III - Europe).
OTHER PROFESSIONAL ACTIVITIES

Holoubek, I.: member of UNEP/IFCS – POPs Protocol – regional experts group – Regional Co-ordinator of GEF Regionall Based Assessment on Persistent Toxic Substances; member of UN/ECE – Task Force for Measurements and Modelling, Task Force on Emission Inventories; member of SETAC - Society of Environmental Chemistry and Toxicology; member of SECOTOX - Society of Ecotoxicology and Chemical Safety - member of Central and Eastern Europen Regional Committee; member of Society for Risk Analysis; chairman of the Czech Society for Environmental Chemistry and Ecotoxicology, member of Scientific Council of Masaryk Oncological Institute; person responsible for Environmental Risk Assessment (Ministry of the Environment); member of Working group Biology and Ecology, Commission for Accreditation, Ministry of Education, Youth and Sport; member of sub-commission for Chemistry, Grant Agency, CR; chairman of the council of Ph.D. study Environmental Chemistry MU Brno, member of the council of Ph.D. study Environmental Chemistry VUT Brno, member of the council of Ph.D. study Ecology MU Brno, member of the council of Ph.D. study Food chemistry and analysis VŠCHT Praha, Ecology and Applied Ecology Charles University, Praha; member of editorial board Air Protection (CR), member of editorial board Environmental Science and Pollution Research, Acta Hydrobiologica et Hydrochimica, and Fresenius Environmental Bulletin.

Dušek, L.: Chief manager of the Center of Biostatistics and Analyses, Faculty of Medicine and Faculty of Science, Masaryk University, Brno; member of the Pedagogical and Accreditation Advisory boards, Faculty of Science, Masaryk University, Brno; member of the Czech Society for Environmental Chemistry and Ecotoxicology, member of the Czech Society for Analytical Cytometry

Maršálek, B.: vice-chairman of the Czech Algological Society, member of the council of MSc. studies Ecotoxicology, Masaryk University, member of the council of PhD study of Environmental Chemistry, Masaryk University, Brno, member of the Ph.D. council of Hydrobiology, Masaryk University, Brno

Laboratory of Atomic Spectrochemistry

TEACHING AND RESEARCH ACTIVITIES

The Laboratory provides research possibilities to students of doctoral study programmes Chemistry and Physics. The Laboratory staff participates also in teaching of students of chemistry and physics of bachelor’s and master’s study programmes. Educational activities comprise the semestrial lecture and seminar on analytical chemistry for students involved in teaching career in chemistry, semestrial lectures on analytical molecular spectrometry, spectrophotometry, analytical atomic spectrometry, spectrometry with inductively coupled plasma, plasma spectrometry, lasers in analytical chemistry, and measurement and automation. The personnel of the Laboratory is involved in laboratory exercise of analytical chemistry for students of biology, laboratory exercise concerning the methods of chemical research, and spectrometric methods for special exercise in analytical chemistry. Diploma and bachelor’s theses are focused on development of atomic emission spectrometry methods of elemental analysis using atomic spectrometry instruments i.e. two ICP spectrometers, a flame-emission high-resolution spectrometer, a pulsed laser for vaporization of solid samples, and plasma-jet excitation source. Laboratory cooperates with the Department of Analytical Chemistry and with the Plasmachemical Laboratory of the Section Physics and the Department of Physical Electronics of the Section Physics.

In the year 2002, research activities were focused on fundamental aspects of laser ablation inductively coupled plasma atomic emission spectrometry (LA-ICP-AES), on the LA-ICP-AES analysis of tungsten carbide ceramics, steels, glass, agricultural soils, scoria and milk powder. Energy distribution in the crossection of the laser beam was studied. Equipment for laser induced breakdown spectrometry, ICP atomic fluorescence spectrometry and RTG fluorescence spectrometry was installed in the laboratory. Development of hydride generation technique was carried out using ICP-AES for the determination of trace concentrations of selenium. Non-spectral interferences and mechanism of excitation of selenium atoms in ICP were studied. Development of device for UV-photolysis of samples with organic matrix, such as biological materials, animal or human tissues, whole blood, blood serum, plants or foodstuff was continued. Research and development of the high-frequency plasma jet and the microwave plasma torch were continued in co-operation with Plasmachemical laboratory. Development and application of method for the analysis of human bones from ancient skeletal residues were carried out for the Department of Anthropology of the Faculty of Science. Solution analysis with ICP-AES was concentrated on the determination of elements in samples of agricultural soils monitoring in co-operation with the State Agricultural Institute for Supervising and Testing. Vacuum UV spectral region was investigated with the aim of spectrochemical determination of sulphur, phosphorus, and iodine. ICP-AES methods for determination of iodine and sulfur with generation of volatile compounds were investigated.

LABORATORY STAFF

Head:
Vítězslav Otruba (Associate Prof., RNDr., CSc.)

Scientific Workers:
Vladimír Aubrecht (Associate Prof., RNDr., CSc.), Technical University Brno,
Masaryk University Brno
Viktor Kanický (Associate Prof., RNDr., D.Sc.)
Vratislav Kapička (Prof., RNDr., D.Sc.)

Research Workers:
Karel Novotný (Mgr., Ph.D.)
Jiří Machát (Mgr., Ph.D.)

Technical Assistants:
Pavel Krásenský (Ing.)
Jan Mikoláš (Mgr.) – till February 2002
Věra Stuchlíková (Ing.) – till March 2002
Iveta Lekešová (Ing)
Eva Niedobová (Mgr.) – part time
Jan Piše – part time

Secretary:
Iva Šafaříková

Ph.D. Students:
Full time:
Jiří Machát (Mgr.)
Martin Semerád (Mgr.)
Markéta Vašková (Mgr.)
THESIS DEFENDED IN THE ACADEMIC YEAR 2001/2002

Diploma Theses:
Jaroslav Šebela – Inductively coupled plasma – optical emission spectrometry with laser ablation in analysis of glass (supervisor: K. Novotný)

Petr Šenk – Inductively coupled plasma – optical emission spectrometry with laser ablation in analysis of steels (supervisor: V. Otruba)

Tomáš Vaculovič – The influence of additional gases in inductively coupled plasma – optical emission spectrometry and laser ablation in analysis of steels (supervisor: V. Kanický)

PhD Thesis
Jiří Machát – Interferences in ICP spectrometry of biological materials and sample preparation (supervisor: V. Otruba)

LIST OF PUBLICATIONS

Scientific papers


Abstracts of conference papers and posters


Other professional publications


NIEDOBOVÁ, E., KANICKÝ, V., OTRUBA, V. Determination of iodine in biological samples by ICP-OES in VUV region. Praha (Czech Republic) : Česká společnost chemická, 96(S), Symposia. 303-305, 2002.


PROJECT GRANTS RECEIVED

Grant Agency of the Czech Republic
203/00/0415
Responsible holder: Masaryk University Brno, Laboratory of Plasma Sources for Chemical Analysis of the faculty of Sciences. Kanický, V., Otruba, V., Novotný, K., Mikoláš, J.: The study of interaction of laser radiation with pressed powdered materials for laser ablation inductively coupled plasma atomic emission spectrometry. Special materials, ceramic powders, agricultural soils, geological samples, solid wastes are studied with methods of atomic emission, electron and laser spectroscopy.

Ministry of Education, Youth and Sports of the Czech Republic
CEZ: J07/98: 143100003
Otruba, V., and co.: Laboratory of Atomic Spectrochemistry. A project of research of plasma discharges as excitation sources for spectral analysis. Programme of doctoral studies in analytical chemistry.

Grant Agency of the Czech Republic
203/02/P097
Novotný K.: The study of interaction of laser radiation with solid materials by plasma spectrometry methods

INVITED LECTURES AND RESEARCH STAYS OF STAFF ABROAD

Kanický V.: invited lecture, University of Cordoba, Department of Physics, May, 2002.


Kanický, V.: research stay (3 weeks) at Laboratoire des Sciences Analytiques, Université Claude Bernard - Lyon I, Villeurbanne, France.

Kanický, V.: research stay (1 week) at Departamento de Fisica, Universidad de Cordoba, Cordoba Spain.

Otruba, V.: research stay (3 weeks) at Laboratoire des Sciences Analytiques, Université Claude Bernard - Lyon I, Villeurbanne, France.

Otruba, V.: research stay (1 week) at Departamento de Fisica, Universidad de Cordoba, Cordoba Spain.

Kanický V.: research stay (2+2 weeks) at Swiss Federal Institute of Technology, Zurich, Swiss.

OTHER INTERNATIONAL CONTACTS AND CO-OPERATION

Cooperation
University of Beograd, Yugoslavia, (Prof. N. Konjevic, Kapička)
Université Claude Bernard - Lyon I, Laboratoire des Sciences Analytiques, Lyon, France (J.-M. Mermet; V. Kanický, V. Otruba).
Veterinary and Agrochemical Research Centre, Section of Ecochemistry and Spectroscopy, Tervuren, Belgium (M. Hoenig, V. Otruba, V. Kanický)
Technical University Košice, Faculty of Metallurgy, Department of Chemistry, Košice, Slovak republic (Prof. E. Krakovská, Otruba, Kanický)
University of Vienna, Dept. of Analytical Chemistry, Division of Atomic Spectroscopy, Vienna, Austria (Prof. I. Steffan, Kanický, Otruba)
Lina Spark Applications, S.a., Cully, Switzerland (Dipl. Ing. Wilfried Vogel, Kanický, Otruba)
Departamento de Fisica, Universidad de Cordoba. (Prof. Dr. M. Carmen Quintero Ortega, Otruba, Kanický).
Institut für Analytische Chemie, Abteilung Atomspektroskopie, Fakultät für Naturwissenschaften und Mathematik, Universität Wien. Spolupráce v oblasti atomové spektrochemie prvků (Univ. Prof. Dr. Ilse Steffan).
Departamento de Química Analítica, Facultad de Estudios Superiores Cuautitlán, Universidad Autonoma de Mexico, (Dr. A. L. Revilla Vazquez, Kanický, Otruba).
Adam Mickiewicz University, Department of Water and Soil Analysis, Poznan, Poland (Prof. J. Siepak; V. Kanický, K. Novotný).
Eidgenossische Technische Hochschule, Department of Inorganic Chemistry, Zürich, Switzerland, (Prof. D. Guenther; V. Kanický).

Foreign visitors
Alma Luisa Revilla Vazquez, Departamento de Química Analítica, Facultad de Estudios Superiores Cuautitlán, Universidad Autonoma de Mexico, two-week stay

STUDENTS STUDYING ABROAD
Miloslav Halázk (Mgr.), Laboratoire des Sciences Analytiques, Université Claude Bernard - Lyon I, Villeurbanne, France, 3 months, granted by SOCRATES/ERASMUS project, PhD.
Aleš Hrdlička (Mgr.), Departamento de Fisica, Universidad de Cordoba, Spain, 3 months, granted by SOCRATES/ERASMUS project, PhD.
Jitka Studýnková (Mgr.), Laboratoire des Sciences Analytiques, Université Claude Bernard - Lyon I, Villeurbanne, France, 3 months, granted by SOCRATES/ERASMUS project, PhD.
Tomáš Vaculovič (Mgr.), Laboratoire des Sciences Analytiques, Université Claude Bernard - Lyon I, Villeurbanne, France, 3 months, granted by SOCRATES/ERASMUS project, PhD.

OTHER PROFESSIONAL ACTIVITIES

Aubrecht, V.: Teaching at the Faculty of Science, Masaryk University and the Faculty of Electrical Engineering, Technical University, Brno: Electrical Discharges.
Kanický, V.: Member of the Council for Postgraduate Students (Analytical Chemistry); Head (alternating) of the Analytical Chemistry Board of Examiners for Ph.D. study; Member of the Committee of the Spectroscopic Soc. of J. M. Marci, Prague; Vice-chairman of the Working Party of Analytical Chemistry of the Czech Chemical Society; Vice-dean of the Faculty of Science.
Kapička, V.: Member of the Scientific Council of the University Ostrava and South Bohemia, České Budějovice and Biophysical Institute, Academy of Sciences of Czech Republic, Brno. Member of working group of Grant Agency, Academy of Science and Grant Agency of Czech Republic. Member of the Council for the Postgraduate Study in Plasma Physics at the Faculty of Applied Physics, the University Plzeň, the Faculty of Mathematics and Physics, Charles University, Prague, and the Faculty of Sciences, Masaryk University, Brno. Member of the Council for the postgraduate study in applied physics, the Faculty of Science, Palacký University, Olomouc.
Otruba, V.: Member of the Council for Postgraduate Students (Analytical Chemistry); Member of the Spectroscopic Society of J. M. Marci, Prague.