

Academy of Sciences of the Czech Republic
J. Heyrovský Institute of Physical Chemistry

Annual Report 2003

Director:

Prof. RNDr. Petr Čásky, DrSc.

Vice-director:

Prof. Ing. Vladimír Mareček, DrSc.

Scientific Secretary:

RNDr. Slavoj Černý, CSc.

Scientific Council Chairman:

Doc. RNDr. Petr Nachtigall, Ph.D.

Economic Manager:

Ing. Vladimír Levit

Technical Manager:

Ludvík Hoffmann

Address: Dolejškova 3, 182 23 Prague 8, Czech Republic
Telephone (secretariat): (+420) 2 8658 3014; (+420) 2 6605 2011; (+420) 2 6605 3265
Fax: (+420) 2 8658 2307
E-mail: director@jh-inst.cas.cz
Internet address: <http://www.jh-inst.cas.cz>

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1. BASIC INFORMATION

1.1. Scope of Activities

During 2003, the Institute continued to carry out fundamental research in a range of branches of physical chemistry, electrochemistry and chemical physics. Fundamental research was the Institute's main objective, but some applied aspects were also pursued. Within the framework of the Institute the Research Centre for structure and dynamics of complex molecular systems and biomolecules was developing its activity.

Furthermore, the Institute continued to be deeply involved in training of both undergraduate and graduate students, in supervision of their Ph.D. and Diploma theses, and in teaching at universities. The Institute also functioned as Marie Curie Training Site of EC in quantum chemical methods and quantum molecular dynamics and as a member of two IHP Research Training Networks of EC concerned with generation, stability and reaction dynamics of multiply charged ions, and with electron and positron induced chemistry.

1.2. Staff and Structure

The average number of employees throughout the year 2003 equalled 150.77 full-time positions.

The staff of the Institute was organized into four sections: Research; Secretariat and library; Administration; Technical and supporting services. The number of positions in the Research section amounted to 112.0, i.e. 74.0 per cent of the total. 22 working stays from 30 days upwards of guest scientists from institutions abroad were realized besides (see paragraph 6.1.).

1.3. Research Section

Table 1.1. The number of positions in the Research Section (recalculated to full-time contracts) as of December 29, 2003

Category	Number of positions	Per cent
Graduates with Ph.D. degree or its equivalent	85.2	76.1
All graduates	104.5	93.3
Technical assistants	7.5	6.7

The Institute had on its staff 10 and 3 full professors at Czech and foreign universities, respectively; 8 associated professors; and 13 scientists with the DrSc. Degree.

The staff of the Research Section was organized into 4 departments: Department of Chemical Physics, Department of Complex Molecular Systems, Department of Catalysis, and Department of Electrochemistry (see paragraph 1.6.).

In 2003, the Center for Structural and Dynamical Studies of Complex Molecular Systems and Biomolecules continued to work in the Institute within a project of the Ministry of Education, Youth and Sports for focusing research in the country on several selected problems. The Center was formed in 2000 for a five-year period in cooperation with Institute of Physics ASCR, Institute of Organic Chemistry and Biochemistry ASCR, and Institute of Chemical Technology, Prague. Close contacts were further developed with the corresponding departments of Charles University, University of Pardubice, Masaryk University in Brno, and University of Ostrava. Staff of the Center in the Heyrovský Institute essentially coincided with the staff of the Department of Complex Molecular Systems.

1.4. Management

The management of the Institute consisted of the director, the vice-director, the scientific secretary, heads of the four research departments, and heads of the administration and technical sections. In their regular sessions participated the Scientific Council chairman.

1.5. Scientific Council

The Scientific Council elected for a two-year period (2002-2003) had the following make-up:

Internal members

Doc. RNDr. Petr Nachtigall, Ph.D. (chairman)
Doc. RNDr. Lubomír Pospíšil, CSc. (vice-chairman)
Mgr. Jiří Dědeček, CSc.
Michael Heyrovský, Ph.D.
Doc. Dr.rer.nat. Martin Hof
Prof. RNDr. Ladislav Kavan, CSc.
RNDr. Jiří Ludvík, CSc.
Ing. Vladimír Špirko, DrSc.

External members

Doc. RNDr. Bohuslav Gaš, CSc.
(*Faculty of Science, Charles University*)
Prof. Ing. František Liška, CSc.
(*Faculty of Chemical Technology, Institute of Chemical Technology Prague*)
Prof. RNDr. Karel Procházka, DrSc.
(*Faculty of Science, Charles University*)
Prof. Ing. K. Štulík, DrSc.
(*Faculty of Science, Charles University*).

In January 2003 Doc. Nachtigall resigned from the position of chairman. The Scientific Council was afterwards directed by vice-chairman Doc. Pospíšil.

1.6. International Advisory Board

Prof.Dr.C.Amatore (*Ecole Normale Supérieure,Paris*),
Prof.Dr.B.Brutschy (*Universität Frankfurt/Main*),
Prof.Dr.F.A.Gianturco (*Università di Roma*),
Prof.Dr.P.Jacobs (*Katholieke Universiteit Leuven*),
Prof.Dr.W.Plieth (*Technische Universität Dresden*),
Prof.Dr.H.Schwarz (*Technische Universität Berlin*).

The first session of the Board was held on February 28 and March 1, 2002.

1.7. List of the Personnel (as of December 29, 2003)

A. Research Section

DEPARTMENT OF CHEMICAL PHYSICS

Head: Prof. RNDr. Zdeněk HERMAN, DrSc.
Telephone (+420) 26605 3485
E-mail herman@jh-inst.cas.cz

Deputy Head: RNDr. Jan Hrušák, CSc.
Telephone (+420) 26605 3436
E-mail hrusak@jh-inst.cas.cz

Scientific staff (36.05 full-time contracts):

Z.Bastl, S.Civiš, P.Čársky, S.Černý, R.Čurík, Z.Dolejšek, V.Hanuš, Z.Herman, L.Hládek, M.Hof, J.Hrušák, I.Jirka, Z.Knor, M. Kovačič, P.Kubát, J.Kubišta, K. Nikiforov, I.Paidarová, Š.Pick, J.Pittner, J. Pišek, R.Polák, M.Polášek, P.Pracna, J.Roithová, I.Spirovová, M.Šimečková, J.Šmydke, P.Španěl, L.Šroubková, Š.Urban, O.Votava, M.Werner, R.Zahradník, Z.Zelinger.

Technical assistants:

K.Bastl, M.Dušek, M.Knapová, R.Žohová.

Ph.D. students (imbursed by the Institute):

D.Babánková, A.Benda, M.Beneš, O.Demel, K. Dryahina, V.Horká, P. Hrubý, J.Humpolíčková, P.Kania, L. Stříteská, J.Sýkora.

DEPARTMENT OF COMPLEX MOLECULAR SYSTEMS

Head: **Prof. Ing. Pavel HOBZA, DrSc.**

Telephone (+420) 26605 2056

E-mail hobza@jh-inst.cas.cz

Deputy Head: **Doc. Pavel Jungwirth, CSc.**

Telephone (+420) 26605 3265

E-mail jungwirt@jh-inst.cas.cz

Scientific staff (16.021 full-time contracts):

O.Bludský, M.Hanus, P.Hobza, J.Chocholoušová, P.Jungwirth, P.Jurečka, M.Kabeláč, F.Lankaš, P.Nachtigall, D.Nachtigallová, A.Prokop, M.Roeselová, F.Ryjáček, D.Řeha, B.Schneider, P.Slavíček, V.Sychrovský, M. Šilhan, M.Šindelka, V.Špirko, J.Šponer, J.Vacek, W. Zierkewicz, P. Žďárská.

Ph.D. students (imbursed by the Institute):

J.Černý, P.Dobeš, T.Kubař, J.Kučera, B. Minofar, E. Mrázková, M.Mucha, J.Rejnek, T. Šedivcová, M.Šilhan, L. Vrbka, L. Zendlová.

Technical assistant:

E.Týleová

The Department is the essential constituent of the Research Center for Structural and Dynamical Studies of Complex Molecular Systems and Biomolecules (see Sect. 1.2.).

DEPARTMENT OF CATALYSIS

Head: **Ing. Blanka WICHTERLOVÁ, DrSc.**

Telephone (+420) 26605 3595
E-mail wichterl@jh-inst.cas.cz

Deputy Head: **Doc. Ing. Jiří Čejka, CSc.**

Telephone (+420) 26605 3795
E-mail cejka@jh-inst.cas.cz

Scientific staff (27.165 full-time contracts):

H.Balcar, V.Bosáček, L.Brabec, Z.Brož, L.Čapek, J.Čejka, J.Dědeček, H. Drobná, , R.Gyepes, M.Horáček, P.Hrabánek, D.Kaucký, M.Kočířík, J.Kotrla, V. Kreibich, M.Křivánek, P.Kubánek, K.Mach, P.Novák, J.Nováková, J. Pinkas, L.Petrusová, O.Prokopová, J.Rathouský, Z.Sobalík, L.Šabo, J. Šponer-Molnár, P.Štěpnička, Z.Tvarůžková, L.Veselá, A.Vondrová, B.Wichterlová, A.Zikánová, A.Zukal, M.Zukalová, N.Žilková.

Technical assistants:

H.Havlíková, I.Holá, J.Kudová.

Ph.D. students (imbursed by the Institute):

M.Boldiš, M.Fryčová, V.Gábová, R.Hamtil, P.Hrabánek, H.Jirglová, K.Juristová, J.Klisáková, G.Košová, V.Kreibich, L.Lukešová, P.Mokrejš, I. Nekomsová, K.Novoveská, J.Pinkas, P.Prokešová, P.Sazama, M.Schwarze, M.Staňková, P. Štěpánek, P.Topka.

DEPARTMENT OF ELECTROCHEMISTRY

Head: **Prof. RNDr. Zdeněk SAMEC, DrSc.**

Telephone (+420) 26605 2017
E-mail samec@jh-inst.cas.cz

Deputy Head: **RNDr. Jiří Ludvík, CSc.**

Telephone (+420) 26605 3975
E-mail ludvik@jh-inst.cas.cz

Scientific staff (26,624 full-time contracts):

F.Dousek, J.Fiedler, R.Heyrovská, M.Heyrovský, J.Hlavatý,
K.Holub, M.Hromadová, P.Janda, H.Jänchenová, J.Jirkovský,
M.Kalbáč, R.Kalvoda, L.Kavan, J.Klíma, P.Krtil, H.Krýsová,
J.Langmaier, A.Lhotský, J.Ludvík, K. Macounová, V.Mareček,
K.Micka, T.Navrátil, L.Novotný, H.Pelouchová, L.Pospíšil,
Z.Samec, K.Stejskalová, I.Šestáková, A.Trojánek, J.Urban,
A.Vlček, J.Volke, J.Weber, S.Záliš.

Technical assistants:

V.Kailová.

Ph.D. students (imbursed by the Institute):

P. Čížková, V.Dorčák, R.Fadrná, H.Hoffmannová, J.Jirkovský,
M. Kolář, T.Kostlánová, H.Měšťánková, P. Mořkovská, D.Rozbroj,
J. Šebera, S.Šebková.

B. Secretariat and Library

V.Bergerová, J.Javůrková, M.Kovářová, M.Moučková,
M.Vojtíšková.

C. Administration

Head: **Ing. Vladimír LEVIT**
Telephone (+420) 26605 3215
(+420) 28658 3022
E-mail levit@jh-inst.cas.cz

Deputy Head: **Ing. Jitka Ondráčková**
Telephone (+420) 26605 3467
(+420) 28658 4708
E-mail ondracko@jh-inst.cas.cz

Staff: J.Beranová, J.Donáth, V.Králová, V.Levit, B.Molová,
J.Ondráčková, M.Orlová, V.Poesová, M.Řezanková,
J.Svobodová.

D. Technical and Supporting Services

Head: **Ludvík HOFFMANN**
Telephone (+420) 26605 2101
(+420) 28658 5339
E-mail hoffmann@jh-inst.cas.cz

Deputy Head: **Alois Kulhánek**
Telephone (+420) 26605 2016
(+420) 26605 3295
E-mail kulhanek@jh-inst.cas.cz

Staff: L.Hoffmann, A.Kulhánek, B.Kolář, L.Kopka, B.Pšenička, K.Štys, J.Tomšů;
J.Bečvář, M.Hanzlík;
J.Řezník, R.Žibřid;
J.Bendová, A.Brotánek, M. Čápová, H.Heřmanová, V.Král, F.Pokorný;
A.Bečvářová, J.Černá, J.Elstnerová, J.Klinderová, J.Křivanec, M. Pěchočová, E.Polaninová, M. Procházková.

1.8. Most Important Events in 2003

- Prof. RNDr. L. Kavan, DrSc. and Ing. Z. Sobalík, CSc. resigned from the position of vice-directors effective 1 January 2003, and Prof. Ing. V. Mareček, DrSc. was appointed to the vacated function.
- 13th Brdička Memorial Lecture was delivered on 2 June by Professor Helmut Schwarz.
- Institutional research plan for the period of 2005 through 2010 including its personnel, financial, material and technical provision was worked out and submitted to the Evaluation Board of the Academy.
- In pursuance of an agreement between the institutes, the Department of Complex Molecular Systems changed from the Heyrovský Institute to the Institute of Organic Chemistry and Biochemistry AS CR at the turn of the years 2003 and 2004.

2. FINANCES

2.1. Non-investment Means

Non-investment financial resources of the Institute in 2003 amounted to 113.158 million CZK (Table 2.1.)

Table 2.1. Breakdown of the non-investment funds of the Institute in 2003 (in thousand CZK; 1 USD ~ 26 CZK)

Source	Income	
	thousand CZK	per cent
State budget	71 582	63.3
Domestic research grants	28 125	24.8
Foreign research grants	9 592	8.5
Contracts	550	0.5
Licences	143	0.1
Others	3 166	2.8
Total	113 158	100.0

2.2. Investment Means

Besides 0.871 million CZK for building maintenance, 17.676 million CZK were available in 2003 from the budget and research grants for purchase of major instrumentation and computer technique. These means were spent for acquisition of equipment including the following major items:

- Computer upgrade of Bruker Spectrometer FT120 (Aero Laser)
- Chemoluminescence analyzer CLA-355 (Horiba)
- Parallel Micro Reactor (In-situ Research Instruments)
- Potentiostat AUT 30 V (Ecochemie)
- Nicolet Nexus Interface (Thermo Electron Corporation)
- NOx Analyzer - model 200AH (MVL Ltd.)
- Titrator Titrilat 856/25 (Scanlab Systems)
- High Sensitivity Schottky Detector (Radiometer Physics)
- Amplifier AHP (Richardson Electronics)
- Intel/Itanium clusters
- PC Dual Xeon

3. RESEARCH

Activities of the Institute were focused primarily on basic research. To a limited extent the Institute was also engaged in contracts with industry and applied research establishments both in the Czech Republic and abroad. The contracts concerned in particular development of adsorbents with specific properties; development and testing of new materials for use in batteries and other electrochemical technologies; synthesis, characterization and activity testing of microporous and mesoporous catalysts; synthesis of special organometallic complexes and their catalytic application; and analysis of solid materials by ESCA method.

The research was carried out within the framework of four departments (Chemical Physics; Complex Molecular Systems; Catalysis; Electrochemistry) pursuing the following research topics:

DEPARTMENT OF CHEMICAL PHYSICS

1. Development and Application of Quantum Chemical Methods.
2. Dynamics and Kinetics of Ion-Molecule Collisions.
Organic Mass Spectrometry.
3. Surface Interactions on Metals.
4. Chemistry of Surfaces, Interfaces and Thin Films (Photoelectron Spectroscopy).
5. Molecular Spectroscopy and Photochemistry.
6. Phospholipids in Biological Systems (Fluorescence Spectroscopy).

DEPARTMENT OF COMPLEX MOLECULAR SYSTEMS

1. Structure and Dynamics of Atomic and Molecular Systems.
2. Structure and Dynamics of Molecules and Molecular Clusters with Biological Relevance.
3. Quantum Chemical Studies of Zeolites and Their Chemistry.

DEPARTMENT OF CATALYSIS

1. Synthesis and Reactivity of Catalytic Materials.
2. Interactions and Mobility of Molecules in Microporous Systems.
3. Sol – Gel Microstructured Materials.
4. Organometallic Catalysis.

DEPARTMENT OF ELECTROCHEMISTRY

1. Electrochemistry of Liquid Interfaces and Membranes.
2. Electrocatalysis.
3. Organic and Organometallic Electrochemistry.
4. Electroanalytical Chemistry.

The particular topics were subject of the following projects supported by grants both from domestic and foreign sources.

Acronyms used:

(a):	associated contractor (project leader is affiliated with another institution)
AS CR:	Academy of Sciences of the Czech Republic
CZ - A:	Bilateral Czech-Austrian scientific and technological cooperation
CZ - DE:	Bilateral Czech-German scientific and technological cooperation
CZ-PL:	Bilateral Czech-Polish scientific and technological cooperation
DFG:	German Research Association
EC:	European Commission
GA ASCR:	Grant Agency of the Academy of Sciences of the Czech Republic
GA CR:	Grant Agency of the Czech Republic
HI:	Heyrovský Institute (internal grant)
IAEA:	International Atomic Energy Agency
IPP ASCR:	Institute of Plasma Physics, Academy of Sciences of the Czech Republic
MEYS:	Ministry of Education, Youth and Sports of the Czech Republic
NATO:	NATO Science Programme
NSF:	National Science Foundation (US)
VW:	Volkswagen Foundation
P&G:	Procter & Gamble Inc.

DEPARTMENT OF CHEMICAL PHYSICS

TOPIC 1. Development and Application of Quantum Chemical Methods

Grant projects

1. Multireference “coupled clusters” method, its development and chemical applications.
P. Čársky, GA ASCR, 2001-2003.
2. European Laboratory for Multireference Quantum Chemical Methods.
P. Čársky, EC/COST (MEYS), 2001-2004.
3. Marie Curie Host Fellowship: Quantum chemical methods and quantum molecular dynamics. Development and applications.
P. Čársky, EC, 2001-2004.
4. International Academy of Quantum Molecular Sciences.
P. Čársky, MEYS (INGO), 2002-2005.

5. Research Training Network: Electron and positron induced chemistry (EPIC).
P. Čársky (a), EC (IHRP, 5th Programme Training Network), 2002-2005.
6. Structure and thermodynamic properties of small clusters of rare gases.
I. Paidarová (a), GA CR, 2002-2004.
7. Dynamics and spectroscopy of metastable molecules: semiclassical simulations and quantum studies.
I. Paidarová, Barrande/MEYS, 2003-2004.

Main results in 2003

- a) Implementation of the state-specific multireference Brillouin-Wigner CCSD method for on principle any number of reference configurations with closed and open shells, covering the whole model space. This code is a part of the program for coupled cluster calculations ACES II. An interactive correction of size extensivity was also developed for this method (J. Pittner, P. Čársky).
- b) Calculation of the energetics, structure, heat of evaporation, charge localization and spectra of Kr_n^+ ion clusters using the DIM semiempirical method
(I. Paidarová).
- c) Elucidation of the effect of geometry relaxation on the cobalt adatom or cluster on Cu(001) surface by means of combined *ab initio* and semiempirical tight bonding methods (Š. Pick).
- d) Utilization of the calculated electrical field gradient on atoms of N_2 , N_2^+ and NO
 - i)* for determination of the bonding changes induced by transitions between different electronic states of the same system and between molecular systems differing in the number of electrons; *ii)* for elucidation of the dependence of nuclear quadrupole interaction on electronic and vibrational states (R. Polák).

TOPIC 2. Dynamics and Kinetics of Ion-Molecule Collisions. Organic Mass Spectrometry

Grant projects

1. Generation, stability and reaction dynamics of multiply charged ions.
Z. Herman, EC (IRHP, 5th Programme Training Network), 2000-2003.

2. Data for molecular processes in edge plasmas.
Z. Herman, IAEA Co-ordination Project, 2001-2003.
3. Theoretical and experimental investigation of dynamics of elementary processes.
Z. Herman, EC/KONTAKT (MEYS), 2002-2004.
4. Kinetics and dynamics of elementary reactions of cations and dications.
Z. Herman, EC/BARRANDE (MEYS), 2002-2003.
5. Atomic physics, data for edge plasmas & plasma-wall interactions.
Z. Herman, EURATOM, 2000-2003.
6. Characterization of unstable molecules by mass spectrometric and theoretical methods.
J. Hrušák, GA CR, 2002-2004.
7. Modeling of metallocene catalysts in the gas phase.
M. Polášek, GA ASCR, 2002-2005.
8. Reaction of molecular dications CHX^{++} ($\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{OH}, \text{SH}, \text{NH}_2$): theoretical and experimental investigation.
J. Roithová, GA ASCR, 2003-2005.
9. Study of elementary processes in low-temperature and technologically oriented plasma and development of relevant diagnostic methods.
P. Španěl (a), GA CR, 2003-2005.

Main results in 2003

- a) Successful application of the SIFT-MS (Selected Ion Flow Tube Mass Spectrometry) method to clinical research including rapid determination of water transport across the peritoneal membrane and of trace metabolites in a single breath exhaled by patients suffering from different diseases. Sensitivity of the method is at the level of parts per billion (ppb) and its accuracy amounts to +/-10 per cent (P. Španěl).
- b) Determination of the effect of the projectile inner energy on dissociation of hydrocarbons in their collision with surfaces. Simple hydrocarbon ions (CH_3^+ , CH_4^+ , CH_5^+ , C_2H_4^+ , C_2H_5^+) use their initial inner energy completely in dissociation processes induced by collision with a surface (Z. Herman).
- c) A complete experimental and theoretical treatment of the dynamics of chemical reactions and charge transfer for the system dication $\text{CHCl}^{2+} + \text{D}_2, \text{Ar}, \text{Kr}, \text{Xe}$. Comparison of theoretical calculations with experiments resulted in determination of the mechanisms of the occurring elementary processes, of the reactions between the quantum states and of the role of isomers of the HCCl^{2+} and CClH^{2+} dications, and in the first description of the dynamics of proton transfer from a dication (Z. Herman, J. Hrušák).

- d) Mass spectrometric determination of the product of synthesis of α -aminoacids by a new method using alkylation of achiral nickel complexes (M. Polášek).

TOPIC 3. Surface Interactions on Metals

Grant projects

1. A measuring unit for material research using synchrotron radiation.
Z. Knor (a), GA CR, 1998-2003.
2. Reactivity of bimetallic systems s,p - (Al, Sn) and transition metals (Pd, Rh): study of volume alloys and interfaces between bimetallic layers and oxides.
Z. Knor (a), GA CR, 2002-2004.

Main result in 2003

Identification of how the dissipation of energy of an impinging atom and thereby its mobility are influenced by a removable interlayer of xenon adsorbed on a metal surface. The work was performed within the framework of a study of factors influencing the morphology of metal layers on supports (catalysts, microelectronic elements) (Z. Knor, J. Pišek).

TOPIC 4. Chemistry of Surfaces, Interfaces and Thin Films (Photoelectron Spectroscopy)

Grant projects

1. Laser photolysis and laser pyrolysis of organic and organometallic compounds for preparation of metal nanoparticles in polymer matrices.
Z. Bastl, GA ASCR, 2001-2003.
2. Platinum modified conducting polymers as an alternative anode material for low temperature fuel cells.
Z. Bastl (a), GA CR, 2002-2004.

Main results in 2003

- a) Experimental determination of angle resolved photoemission from inner levels of atoms in the surface nanostructures of Au/Pt, Re, Pd/Nb, Au/NbO_x/Nb and Au/Nb₂O₅ systems. A detailed description of the electron structure, thermal stability and interdiffusion of the metal/metal and

metal/oxide interphases. The results are of importance for catalysis, electrochemical sensors and microelectronics (Z. Bastl).

- b) Application of angle resolved photoelectron spectroscopy to determination of the chemical composition and population of the particular oxidation states in a platinum catalyst, and identification of their depth distribution in the surface layers of polypyrrole films deposited on glassy carbon. These materials represent alternative anodes for fuel cells operating at low temperatures and having enhanced tolerance of CO poisoning (Z. Bastl).
- c) Determination of changes in the surface composition of Mg_4Mn_2 , Co_4Mn_2 and Ni_4Al_2 catalysts for $deNO_x$ reactions. The observed deactivation does not result from the changed population of oxidation states of the active components of the given catalysts (Z. Bastl).
- d) Elucidation of the mechanism of photolysis of CS_2 induced by 193 nm radiation leading to polymeric $(CS)_n$, and determination of population of sulphur bond configurations in the polymer in dependence on the conditions of photolysis (Z. Bastl).
- e) Realization of targeted surface modifications of selected polymers (cyclic polyolefins, high molecular polyethylene and their mixtures) using accelerated nitrogen ions and nitrogen plasma, determination of the dependence of surface nitrogen on the implantation procedure, and identification of the formed surface groups for controlling bioadhesion of the binding tissue in joint implants (Z. Bastl).

TOPIC 5. Molecular Spectroscopy and Photochemistry

Grant projects

1. Urban air pollution control: Model and *in situ* measurements.
S. Civiš, EC/COST (MEYS), 1999-2003.
2. Dynamics and structure of small ion clusters studied by high resolution spectroscopy.
S. Civiš, GA CR, 2001-2003.
3. Interaction of new porphyrins with biopolymers: complex formation and photoinduced processes.
P. Kubát, GA CR, 2001-2003.
4. Tetrapyrrole metallocomplexes: modification of nucleic acid triplex structures.
P. Kubát (a), GA CR, 2002-2004.

5. Physical and chemical modeling of secondary pollutants production and propagation in the urban and rural areas. Z. Zelinger, GA ASCR, 2001-2004.
6. New laser-based hybride technologies for thin layer deposition. Z. Zelinger, GA ASCR, 2001-2005.
7. Fast tunable MID-IR and IR laser diode spectrometer based on non-linear optical effects. S. Civiš, GA ASCR, 2001-2005.
8. The role of the upper troposphere and lower stratosphere in global change. Z. Zelinger, COST/MEYS, 2003-2006.
9. High resolution molecular spectroscopy (with aspects to molecular physics, energy transfer, distant detection of atmospheric molecules and metrology). Š. Urban, GA CR, 2001-2003.
10. Sub-Doppler hyperfine spectroscopy: experiment and theoretical Interpretation. Š. Urban, EC/KONTAKT (MEYS) and CZ-DE, 2001-2003.
11. Spectroscopy and photochemistry of organic peroxy-radicals in the near infrared region. O. Votava, GA ASCR, 2001-2003.
12. Recombination of H_3^+ , D_3^+ and H_2D^+ ions with electrons in hydrogen plasma. O. Votava (a), GA CR, 2002-2004.

Main results in 2003

- a) Characterization of the plasma arising in ablation of a superconductor by means of Langmuir probe and description of the processes occurring in plasma ablation of graphite in nitrogen atmosphere (S. Civiš).
- b) Development of a new method to determine recombination of H_3^+ with electrons using the highly sensitive "cavity ring-down" spectroscopy. Realization of pilot experiments providing recombination coefficients for exactly defined ion quantum states which are unavailable by other methods (O. Votava).
- c) Calculation of the structure of vibration-rotation levels of $^{13}CH_3F$ molecule from high resolution IR and MMW spectroscopies. Utilization of the results for a quantitative interpretation of ortho-para conversion in electrical field (P. Pracna).
- d) A quantitative description of anionic photosensibilizer complexation with cyclodextrines. Spectroscopic measurements showed that anionic porphyrins form with cyclodextrines 1:1 and 2:1 inclusion complexes. The

calculated bond constants and physical parameters of those complexes depend primarily on the cyclodextrine cavity size and on the extent of the photosensibilizer aggregation in the appropriate medium (P. Kubát).

- e) Description of a new rotation-vibration band and of the potential energy function of NeH^+ in the ground electronic state (S. Civiš).
- f) First detection and high resolution spectroscopic study of FCO_2 radical (Z. Zelinger).
- g) Building up the Joint Laboratory of High Resolution Microwave Spectroscopy established in collaboration with the Institute of Chemical Technology Prague. The spectrometer has shown in test experiments sub-Doppler resolution up to 120 GHz and ranks among the top instruments of this kind in the world. Its continuous calibration on the international time standard takes place through satellites and enables an absolute precision of 10^{10} to be achieved (Š. Urban).

TOPIC 6. Phospholipids in Biological Systems (Fluorescence Spectroscopy)

Grant projects

1. Participation in the over-all project "Structure and Dynamics of Complex Molecular Systems and Biomolecules".
P. Hobza, MEYS, 2000-2004.
2. Interactions of cation compounds with DNA molecule.
M. Hof, EC/KONTAKT (MEYS) and CZ-PL, 2002-2003.

Main result in 2003

Refinement of the newly developed method for accurate determination of diffusion coefficients and twodimensional density of phospholipids in biomembranes using confocal fluorescence correlation spectroscopy. Its successful application to characterization of planar phospholipid bilayers and to determination of phospholipid mobility on a liquid/liquid interface (M. Hof).

DEPARTMENT OF COMPLEX MOLECULAR SYSTEMS

All three topics dealt with in the Department are subject of an over-all project "Structure and dynamics of complex molecular systems and biomolecules" in which three institutes of the Academy of Sciences and the Institute of Chemical

Technology, Prague are engaged. The project is headed by P. Hobza and is supported in the years 2000 through 2004 by a grant of MEYS.

TOPIC 1. Structure and Dynamics of Atomic and Molecular Systems

Grant projects

1. A molecular kit: Computer simulations of molecular propellers and rotors.
J. Vacek, GA ASCR, 2000-2003.
2. An integrated approach to understanding the air-water interface in atmospherically relevant systems.
P. Jungwirth (a), NSF, 2002-2006.
3. Solvation of nitrate ion at the air-water interface.
M. Roeselová, NATO, 2003-2004.

Main results in 2003

- a) Computer simulation of salt crystallization from aqueous solution and trapping of reactive gases on liquid aerosols. Proposal of a new non-inductive mechanism of storm clouds charging (P. Jungwirth).
- b) Molecular dynamics simulation of aqueous salt nanodroplet collisions including description of the van der Waals interactions causing the droplet coalescence
(P.Jungwirth).
- c) Molecular dynamics simulation of the pickup and photodissociation of hydrogen halides in and on argon and neon clusters (P. Jungwirth).
- d) Clarification of the interplay of hydrophylic and hydrophobic forces by molecular dynamics simulation of the microsolvation of a charged anion with two separate charge centers in dependence on the number of water molecules (P. Jungwirth).
- e) "Exact" and "adiabatical" calculation of the energies of the bound vibrational states and of energy density spectra of the continuum vibrational states of the bifluoride anion (V. Špirko).

TOPIC 2. Structure and Dynamics of Molecules and Molecular Clusters with Biological Relevance

Grant projects

1. Structure and dynamics of complex molecular systems and biomolecules.
P. Hobza, MEYS, 2000-2004.
2. Properties of DNA on different length scale.
J. Šponer, VW, 2002-2004.

Main results in 2003

- a) Accurate calculations of stabilization energy for guanine-cytosine and adenine-thymine pairs and corresponding methylated pairs (P. Hobza, J. Šponer).
- b) Correlated *ab initio* study of nucleic acid bases and their tautomers in the gas phase, in a microhydrated environment and in aqueous solution (P. Hobza).
- c) Application of the calculated intermolecular and intramolecular indirect NMR spin-spin coupling constants for discrimination between the inner-shell and outer-shell binding motif of hydrated divalent cations Mg^{2+} and Zn^{2+} with a guanine base (P. Hobza, J. Šponer).

TOPIC 3. Quantum Chemical Studies of Zeolites and Their Chemistry

Grant project

1. Structure and dynamics of complex molecular systems and biomolecules.
P. Hobza, MEYS, 2000-2004.

Main results in 2003

- a) Highly accurate calculation of site-specific CO stretching frequencies for copper carbonyls adsorbed on the Cu-exchanged MFI zeolite (P. Nachtigall, D. Nachtigallová).

- b) Theoretical calculation of coordination of Li⁺ and K⁺ ions in zeolite ZSM-5. Several different sites of extra-framework metal ions were found. The Li⁺ ion preferably occupies the sites on top of the six-membered ring on the channel while K⁺ ion preferably binds on the channel intersection (P. Nachtigall).

DEPARTMENT OF CATALYSIS

TOPIC 1. Synthesis and Reactivity of Catalytic Materials

Grant projects

1. Selective oxidation of hydrocarbons catalyzed by Me-O/zeolite systems.
B. Wichterlová, GA ASCR, 2000-2003.
2. Structure of metal ions in crystalline oxide matrices.
Synthesis/structure/activity/selectivity relation in the development of catalysts for highly selective reactions.
B. Wichterlová, EC/COST (MEYS), 2000-2003.
3. Redox zeolitic catalysts for nitrogen oxides abatement using process gases.
Z. Sobalík, ASCR, 2000-2004.
4. Synthesis of ordered mesoporous aluminas and their application in catalysis.
J. Čejka (a), EC/KONTAKT (MEYS), 2000-2003.
5. Basic molecular sieve catalysts for side chain alkylation.
J. Čejka, GA ASCR, 2000-2003.
6. Computer simulation of the structure – reactivity relation in zeolites.
J. Šponer-Molnár, GA CR, 2001-2003.
7. Advanced nanostructured metal/metaloxo/matrix catalysts for redox processes. Application for NO_x reduction to nitrogen.
B. Wichterlová, EC/GROWTH, 2001-2004.
8. Mesoporous molecular sieves for catalytic applications.
J. Čejka, GA CR, 2002-2004.
9. Effect of gaseous additives and gas phase reactions on the course of catalytic redox reactions.
D. Kaucký, GA CR, 2002-2005.
10. Czech Zeolite Group.
J. Čejka, MEYS/INGO, 2002-2005.

11. Synthesis of fine chemicals via heterogeneous catalysis.
J. Čejka, GA CR, 2003-2005.
12. Control of negative charge distribution in skeleton of high-silica zeolites.
J. Dědeček, GA ASCR, 2003-2006.
13. European Federation of Catalysis Societies.
Z. Sobalík, INGO/MEYS, 2003-2005.
14. Catalytic ammoxidation of propane.
B. Wichterlová, GA CR, 2003-2005.
15. Contribution of non-zeolitic pores to the separating function of composite membranes containing zeolites.
O. Prokopová, GA CR, 2003-2005.

Main results in 2003

- a) The first analysis of aluminum distribution in the channel structure of high silica zeolites based on the distribution of divalent cations determined from characteristic spectra of CO^{2+} ions. This information is not available by other experimental methods. Using this analysis it has been shown that Al distribution in the zeolite skeleton is not statistical and that it depends on the chemical composition of the skeleton and on dynamical conditions of the synthesis. In this way it is possible to control Al distribution in the zeolite skeleton which determines distribution and thereby catalytic properties of protonic and cationic centers. Synthesis of ZSM-5 zeolites with controlled Al distribution have been proposed using different sources of Si and Al (B. Wichterlová, J. Dědeček, J. Čejka, Z. Sobalík).
- b) Analysis of the structure and activity of Fe- and Ag-zeolites and Ag-alumina in selective reduction of NO_x in exhaust gases of oxygen-deficient combustion processes, and identification of the particular reaction steps using combined analysis of the gas phase, surface reaction intermediates and structure of active centers (B. Wichterlová, Z. Sobalík, L. Čapek).
- c) Synthesis of new types of composite aluminosilicates and silicates with defined structure of mesopores bearing on their walls a thin layer of nano-microporous zeolitic structure. These materials are expected to find application in catalytic reactions of large molecules where shape-selectivity takes place (J. Čejka).
- d) Elucidation of the role played in MCM-22 zeolite by *i)* Mo ions and Mo carbides in methane hydrogenation; *ii)* proton and Lewis centers in oligomerization and aromatization of olefinic fragments from methane to a mixture of benzene, toluene and xylenes (Z. Sobalík, B. Wichterlová).

TOPIC 2. Interactions and Mobility of Molecules in Microporous Systems

Grant projects

1. New dealumination routes to the production of transport-optimized catalysts for crude oil conversion.
M. Kočířík, EC/GROWTH, 2001-2004.
2. Accessibility of the channel system in medium-sized pore zeolites for aromates. Computer simulation.
M. Kočířík, GA ASCR, 2001-2003.
3. Potentials of utilizing nanofilter layers for membrane separations of low hydrocarbons.
A. Zikánová (a), GA CR, 2001-2003.
4. Interactions of bentonites with the environment: the effect of geological history and actual conditions; application in active waste deep repositories.
M. Kočířík (a), GA CR, 2002-2004.
5. Polymer-based membrane composites for separation of small molecules.
M. Kočířík (a), GA CR, 2003-2005.

Main results in 2003

- a) Synthesis of asymmetric ceramic porous elements used for gas filtration and as supports of membranes or catalysts. The basic porous bodies with average pore diameters around 10 micrometers which were developed in cooperation with Carborundum Electrite Ltd., consist of fused corundum and ceramic bond and have defects of maximum size from 0.8 to 1.2 micrometers (M. Kočířík, A. Zikánová).
 - b) Development of a mathematical model of dynamics of catalytic processes in fixed bed reactors which takes into account diffusion in macropores of the dealuminated zeolite catalyst for fluid catalytic cracking, and provides algorithms for process simulation (A. Zikánová, M. Kočířík).
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TOPIC 3. Sol – Gel Microstructured Materials

Grant project

1. Transparent thin films of mesoporous titania and mesoporous silica with embedded dye molecules as effective photocatalysts for pollutant mineralization and as optical gas sensors.
J. Rathouský, DFG, 2002-2004.
2. Study on new active silicas with highly effective and highly selective adsorption activity towards specific chemical species.
J. Rathouský, P&G, 2002-2003.

Main results in 2003

- a) Preparation of photocatalytically active organized mesoporous thin films of TiO₂ with highly stable surface hydrophobicity which has basic importance for photocatalytic degradation of hydrophobic organics dissolved in water. The photon efficiency surpasses that of the films of anatase nanoparticles currently used for photodegradation of organic compounds (A. Zukal, J. Rathouský).
- b) Development of new silica adsorbents using special doping. The prepared materials meet the sorption activity and selectivity required by the intended applications. Testing and optimization of the sorbents was performed jointly with two potential industrial producers (J. Rathouský, A. Zukal).

TOPIC 4. Organometallic Catalysis

Grant projects

1. Reactivity of pending double bonds in the coordination sphere of titanium.
K. Mach, GA ASCR, 2000-2003.
2. Zirconocene - acetylene chemistry: applications in organometallic synthesis and catalysis.
M. Horáček, GA CR, 2000-2003.
3. Silicon-based ansa-titanocene complexes: synthesis, properties and catalytic activities.
K. Mach, GA CR, 2002-2004.

- Catalysts for olefin metatheses and related polymerizations anchored on mesoporous molecular sieves.
H. Balcar, GA CR, 2002-2004.

Main results in 2003

- Preparation of metallocenes M^{II} from zirconocene chlorides and titanocene chlorides. Activation of C-H bonds in the prepared metallocenes leads to their rearrangement into more stable complexes under formation of M-H and M-C bonds. The rearrangement products were used for the synthesis of heterobinuclear Ti/Fe complexes and Ti (III) complexes. In this way new catalysts for terminal alkyne dimerization were obtained (K. Mach, M. Horáček).
- Preparation of a trinuclear titanocene complex with an *in situ* formed bis(alkoxy)organyl pincer ligand bearing two ferrocenylacetylene groups. Preparation of a series of new titanium and zirconium complexes with substituted cyclopentadienyl ligands applicable as single-site catalysts for ethylene polymerization (K. Mach).
- Preparation of a series of semi-sandwiched titanium complexes for styrene polymerization. Some derivatives are efficient catalysts for syndiotactic polymer even in the presence of small amounts of methylalumoxane as a co-catalyst (K. Mach, M. Horáček).
- Experimental evidence that hybrid catalysts which were prepared by immobilization of $[Rh(1,5\text{-cyclooctadiene})Cl]_2$ on mesoporous molecular sieves of various structure and pore size are in polymerization of phenyl acetylene and 4-ethynyl-N-{4[(trimethylsilyl)ethynyl]benzylidene}aniline to high molecular polymers more active and selective than homogeneous catalysts. The increasing accessibility of catalytic centers in mesopores entails increasing polymerization rate (MCM-41 < MCM-48 < SBA-15) and decreasing molecular weight of the polymer (H. Balcar).

DEPARTMENT OF ELECTROCHEMISTRY

TOPIC 1. Electrochemistry of Liquid Interfaces and Membranes

Grant projects

- New electrochemical methods for quantitative detection of 8-hydroxy-2-deoxy-guanosine in urine.
Z. Samec (a), GA CR, 2001-2003.

2. Quasielastic laser scattering on phospholipid monolayers.
Z. Samec, GA CR, 2001-2003.
3. Formation of surface films from monomers adsorbed at liquid/liquid interface.
V. Mareček, EC/KONTAKT (MEYS), 2002-2004.
4. Emulsification of liquid interfaces.
Z. Samec, EC/KONTAKT (MEYS), 2002-2004.
5. Polymerization of adsorbed layers at the liquid/liquid interface.
V. Mareček, GA CR, 2003-2005.

Main results in 2003

- a) Controlled preparation of a silicate film on the interface of two immiscible electrolytes by a modified sol-gel technique using the potential-dependent adsorption of a template ion and its transfer from the organic to the aqueous phase where it reacts with silicate ion as a precursor (V. Mareček).
- b) Realization of an amperometric electrode for polyions based on a polarizable PVC membrane and its application to determination of the heparine polyion in pharmaceuticals by cyclic voltammetry (Z. Samec).
- c) Determination of kinetic parameters and elucidation of the reactive mechanism of polymerization at liquid/liquid interfaces induced by hydroxyl ions formed by the potential-controlled Fenton reaction (V. Mareček).

TOPIC 2. Electrocatalysis

Grant projects

1. Structure and (photo)electrochemical properties of oxide semiconductors modified by photoredox active molecules.
L. Kavan (a), EC/COST (MEYS), 1999-2003.
2. Synthesis and characterization of new carbon materials with polyine structure.
L. Kavan, EC/KONTAKT (MEYS), 2002-2004.
3. Template mesoscopic TiO₂ for electrodes and photocatalysts.
L. Kavan, GA CR, 2003-2005.

4. Innovative multi-purpose thin-film UV reactor.
L. Kavan, EC, 2003-2005.
5. Charge transfer in organized supramolecular systems of fullerenes.
L. Kavan, GA ASCR, 2003-2006.
6. Nanostructure and photovoltaic properties of titanium oxide modified by sensibilizing dyes.
P. Janda, GA CR, 2001-2003.
7. The exploitation of alkali alkynides for the electrochemical and chemical preparation of long-chain oligoynes and carbon nanotubes.
J. Hlavatý, GA CR, 2003-2005.
8. Soft solution based synthesis of nano-microcrystalline Li insertion materials and their electrochemical characterization.
P. Krtil, EC/KONTAKT (MEYS), 2002-2004.
9. Low temperature synthesis of electrochemically active phases in the Li-Ti-O, Li-Mn-O and Li-Fe-Mn-O systems; their electrochemical characterization.
P. Krtil, GA CR, 2003-2005.
10. *In-situ* gravimetric investigation of ion transfer and adsorption at the interface of two immiscible liquids.
P. Krtil, GA CR, 2003-2005.
11. Application of advanced oxidation processes for water purification utilizing solar energy combined with non-ionogenic selective sorption.
J. Jirkovský (a), GA CR, 2002-2004.
12. Mineralization of organic injurants using new solar energy-based photocatalysts.
J. Jirkovský, GA CR, 2002-2004.
13. Investigation of photoelectrochemical properties of colloid solutions of ferrioxide and titanium dioxide – a route to clarify the mechanism of natural photoprocesses and their application in photocatalytic decontamination of water utilizing solar energy.
J. Jirkovský, BARRANDE/COST (MEYS), 2003-2004.
14. Complementarity of homogeneous (Fe) and heterogeneous (TiO₂) photocatalysts for pollutant removal from the aquatic compartment.
J. Jirkovský, EC-IHP, 2003-2004.
15. New catalysts for pesticide degradation using solar energy.
J. Jirkovský, MEYS, 2002-2003.
16. Photocatalytic surfaces with selfcleaning properties. Development of technology for preparation of new materials with surfaces exhibiting

selfcleaning and disinfection effects based on photocatalysis utilizing energy of light.

J. Jirkovský (a), MPO, 2003-2005.

17. *In-situ* study of active mass and contact layers in electrodes of the lead accumulator.

K. Micka (a), GA CR, 2002-2004.

Main results in 2003

- a) Experimental proof of electrochemical doping of double wall carbon nanotubes and of a different activity of the inner and outer tube. This fact entails an easy deconvolution of tangential Raman modes by changing the applied potential (L. Kavan).
- b) Determination of the organization and reactivity of Au nanoparticles at the polarizable interface of two immiscible electrolytes (P. Krtil, Z. Samec).
- c) Elucidation of the pseudo-capacity effects in an interaction of Li ions with very thin TiO₂ (anatase) nano-plates prepared by hydrothermal recrystallization. Identification of an ideal structure for bimodal lithium chemisorption (L. Kavan).
- d) Development of a new method for doping of anatase single crystal based on an electrochemical reaction (L. Kavan, P. Janda).
- e) Elucidation of the anodic strengthening of Raman spectrum of intratubular fullerene which is specific for the fullerene C₆₀@SWENT peapod (L. Kavan).
- f) Utilization of ion liquids for doping of nanomaterials under extreme conditions (L. Kavan, P. Janda).
- g) The first proof of selectivity in electrochemical doping demonstrated on polydispersed HIPCO (High Pressure Carbon Monoxide) nanotubes (L. Kavan).
- h) Preparation of protected 3-triisopropylsilylethynylpyrrole which electrochemically polymerizes to poly(3-ethynylpyrrole) (J. Hlavatý).
- i) Preparation of single crystal lithium-titanium spinel Li₄Ti₅O₁₂ and of single crystal TiO₂ for high performance Li ion batteries (L. Kavan).
- j) Clarification of the function of oxide admixtures in MnO₂ cathodes for alkaline primary cells. Proposal of new types of complex oxide and oxichloride additives. Procedure of cathode mixtures preparation (P. Krtil).

- k) Elucidation of the synergism occurring in combined homogeneous and heterogeneous photocatalytic systems containing dissolved Fe(III) salts and solid TiO₂ particles. Fe(III) aggregates that exhibit only negligible photochemical activity are continuously transformed into highly photoactive monomeric Fe(III) species on irradiated TiO₂ surface. This finding can be used in practice for highly effective photocatalytic degradation of organic pollutants which is friendly to the environment due to low concentrations of both photocatalysts (J. Jirkovský).

TOPIC 3. Organic and Organometallic Electrochemistry

Grant projects

1. Electrochemistry of nanostructures on heterogeneous interphases. Formation, properties and electron transfer reactions. L. Pospíšil, EC/COST (MEYS), 1999-2003.
2. Organometallic and metallo-organic building blocks for photonic materials. A. Vlček, EC/COST (MEYS), 1999-2003.
3. Effect of electron distribution on the reactivity of oximes towards esters. J. Ludvík (a), GA CR, 2001-2003.
4. Characterization of electrochemical and adsorption properties of supramolecular structures of selected pesticides. M. Hromadová, GA CR, 2002-2004.
5. Electronic properties, structure and reactivity of the azine group C=N-N=C and mechanism of biologically important azines degradation. J. Ludvík, GA ASCR, 2003-2005.
6. Electron transfer in supramolecular complexes, large molecules with more active centers and in organized structures. L. Pospíšil, GA CR, 2003-2005.

Main results in 2003

- a) Formulation of two mechanisms of the intramolecular electron-transfer acceleration for transition metal complexes in the normal and inverted regions of Marcus theory. One mechanism consists in a combination of large electronic coupling between the ligands and vibrational activation of the precursor state. The other mechanism operates through vibrational activation of the product in a combination with its high reorganization energy. Research on electron interaction between redox centers and

intramolecular electron transfer affords enabling knowledge for development and design of molecular devices (A. Vlček, jr., J. Fiedler).

- b) Electrochemical detection of the electronic transfer of information via ethynyl or ethane-diyl bridge in different positions of purine bases. Correlation with cytostatic activity (J. Ludvík).
- c) Characterization of low lying excited states in $[(N^N)IrCl(C_2H_5)]^+$ and $[(N^N)Ir(C_2Me_5)]$ complexes ((N^N) stands for 2,2'-bipyridin or 1,4-diazabutadiene), and application of TD DFT quantum chemical calculations to clarify different shifts in the spectra after replacement of 2,2'-bipyridine by 1,4-diazabutadiene (S. Zálíš).
- d) A novel way of protein labeling by means of a fragment of $(\eta^5\text{-cyclopentadienyl})\text{tricarbonyl manganese}$ and its use for determination of bovine serum albumin. The detection limit of the method is 2 orders of magnitude lower compared with spectroscopic determination (L. Pospíšil).
- e) Synthesis of a supramolecular complex of cyclodextrines and cyclopentadienyl dicarbonylmethyliron, and its application to redox activation of carbonylation reaction accompanied by suppression of undesired side reactions due to the protecting effect of the cyclodextrine cavity (L. Pospíšil).

TOPIC 4. Electroanalytical Chemistry

Grant projects

- 1. Interactions of peptides, proteins and DNA with electrodes, and new electrochemical methods for biochemistry and molecular genetics.
L. Novotný (a), University of Buenos Aires, 2002-2004.
- 2. Response of plants to abiotic stress by selected heavy metals.
I. Šestáková (a), GA CR, 2002-2004.
- 3. Characterization of cancer-related metalloproteins and their interaction with DNA.
I. Šestáková (a), MEYS, 2002-2005.

Main results in 2003

- a) Experimental establishment of unexpected catalytic evolution of hydrogen in aqueous solutions of sodium methoxide. Outline of possible connections with homogeneous reactions of methoxide in various systems (M. Heyrovský).

- b) Voltammetric determination of the structure of phytochelatin complexes with metals in plants (I. Šestáková, T. Navrátil).
- c) Application of elimination voltammetry with linear scan to monitoring of the damaged DNA interaction with osmium complexes (T. Navrátil, B. Yosypchuk).
- d) Development of mercurous sulphate electrode based on solid silver amalgam and proof of its long-term stability (B. Yosypchuk, L. Novotný).
- e) Development and testing of silver composite electrodes as a sensor suitable for replacing mercury electrode (T. Navrátil).

4. PUBLICATION AND POPULARIZATION ACTIVITIES

4.1. Synopsis of Papers Published in 2003

Members of the Institute are authors or co-authors of 216 research papers which appeared in 2003 in reviewed periodicals, proceedings of conferences, and monographs.

In addition, 5 popularization papers in professional publications appeared and 3 patent applications were filed.

Contributions in non-professional journals and newspapers are not included.

Table 4.1. Publications issued in 2003

Type of publication	Number
Research papers in periodicals	184
Research papers in conference proceedings	23
Contributions in monographs	9
Popularization papers	5
Patent applications	3

Members of the department of chemical physics, complex molecular systems, catalysis and electrochemistry were authors or co-authors of 91, 26, 38 and 82 of the issued publications, respectively.

Authors of 55 publications were exclusively members of the Institute. In 111, 58 and 26 publications authors from institutions abroad, universities in the Czech Republic, and other institutions in the Czech Republic, respectively, participated.

In the following list of published papers, members of the Institute are given with their full names.

4.2. Research Papers in Periodicals

1. Pittner Jiří
Continuous Transition between Brillouin-Wigner and Rayleigh-Schrödinger Perturbation Theory, Generalized Bloch Equation, and Hilbert Space Multireference Coupled Cluster.
J. Chem. Phys. 118(24), 10876-10889 (2003).
2. Čurík Roman, Čársky Petr
Vibrationally Inelastic Electron Scattering on Polyatomic Molecules by the Discrete Momentum Representation (DMR) Method.
J. Phys. B - Atomic, Molecular and Optical Physics 36, 2165-2177 (2003).
3. Puiggros O. R., Pittner Jiří, Čársky Petr, Stampfuss P., Wenzel W.
Multireference Brillouin-Wigner Coupled Cluster Singles and Doubles (MRBWCCSD) and Multireference Doubles Configuration Interaction (MRD-CI) Calculations for the Bergman Cyclization Reaction.
Collect. Czech. Chem. Commun. 68(12), 2309-2321 (2003).
4. Fišer J., Boublík T., Polák Rudolf
Combining Rule for Interaction Energies of the (CO)₂, (N₂)₂ and CO-N₂ Complexes.
Mol. Phys. 101(23/24), 3409-3418 (2003).
5. Polák Rudolf, Fišer J.
A CASSCF/icMRCI Study of the Nuclear Electric Field Gradient in Low-Lying Electronic States of N₂⁺/N₂.
Chem. Phys. 290(2), 177-188 (2003).
6. Polák Rudolf, Fišer J.
On the Behavior of the Low-Lying 2.SIGMA.+ Electronic States of NO.
Chem. Phys. Lett. 377(5/6), 564-570 (2003).
7. Polák Rudolf, Fišer J.
The Rovibrational Dependence of the ¹⁴N Nuclear Quadrupole Coupling Constants in the X₂.SIGMA.+ and B₂.SIGMA.+ States of CN from the Multireference CI Approach.
Collect. Czech. Chem. Commun. 68, 509-528 (2003).
8. Durand P., Paidarová Ivana
Ionization of the Hydrogen Atom from Weak to Strong Static Electric Fields.
Eur. Phys. J. D - Atomic, Molecular and Optical Physics 26, 253-259 (2003).

9. Kalus R., Paidarová Ivana, Hrivňák D., Paška P., Gadea F.X.
Modelling of Kr_n^+ Clusters ($n = 2-20$) I. Structures and Energetics.
Chem. Phys. 294(2), 141-153 (2003).
10. Paidarová Ivana, Durand P.
Quantum Resonance Line Profiles and Dynamics.
Collect. Czech. Chem. Commun. 68(3), 529-553 (2003).
11. Pick Štěpán
A Tight-Binding Study of Surface Magnetic Anisotropy of the Co
(0001) and Its Perturbation by Cu and CO.
Solid State Commun. 127, 531-534 (2003).
12. Pick Štěpán, Dreyssé H.
On the Gas Adsorption Effect upon Electronic Structure of
Ferromagnetic Co(0001).
Surf. Sci. 540, 389-394 (2003).
13. Pick Štěpán, Stepanyuk V. S., Baranov A. N., Hergert W., Bruno P.
Effect of Atomic Relaxations on Magnetic Properties of Adatoms and
Small Clusters.
Phys. Rev. B 68, 104410.1-104410.5 (2003).
14. Zahradník Rudolf, Šroubková Libuše
Polyacetylenes and Cumulenes, Potential Elements for Molecular
Machines and Precursors of Carbon Clusters: A Theoretical Study.
Helv. Chim. Acta 86, 979-1000 (2003).
15. Herman Zdeněk
Collisions of Slow Polyatomic Ions with Surfaces: The Scattering
Method and Results.
J. Amer. Soc. Mass Spectrom. 14, 1360-1372 (2003).
16. Franceschi P., Thissen R., Žabka Ján, Roithová Jana, Herman
Zdeněk, Dutuit O.
Internal energy effects in the reactivity of CO_2^{2+} doubly charged
molecular ions with CO_2 and CO .
Int. J. Mass Spectrom. 228, 507-516 (2003).
17. Gluch K., Fedor J., Matt-Leubner S., Parajuli R., Mair C., Stamatovic
A., Echt O., Lifshitz C., Harvey J., Hagelberg F., Herman Zdeněk,
Probst M., Scheier P., Märk T. D.
Energetics and Dynamics of Decaying Cluster Ions.
Eur. Phys. J. D - Atomic, Molecular and Optical Physics 24(1/3), 131-
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21. Navrátil Tomáš, Šenholdová-Dlasková Z., Heyrovský Michael, Přistoupilová K., Přistoupil T. I.
Thiodiglycolic Acid in Urine. Atherosklerosa. Hyperhomocysteinemie 2003,
p. 67-69, Praha 2003.
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Relationships between Metabolism of Homocysteine and Physiological Formation of Thiodiglycolic Acid.
Atherosklerosa. Hyperhomocysteinemie 2003, p. 81-84, Praha 2003.
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Voltammetric Determination of Thiodiglycolic Acid in Urine of Persons Exposed and Non-Exposed to Vinylchloride Monomer (in Czech).
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4.4. Contributions in Monographs

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Basics of Optical Spectroscopy.
In: *Handbook of Spectroscopy* (Günter, G. - Tuan, V. D., Ed.), Chap. 3,
pp. 39-47. Wiley-VCH, Weinheim 2003
2. Sablinkas V., Steiner G., Hof Martin
Applications of Optical Spectroscopy.
In: *Handbook of Spectroscopy* (Günter, G. - Tuan, V. D., Ed.), Chap. 6,
pp. 89-168. Wiley-VCH, Weinheim 2003.
3. Wilson S., Hubáč I., Mach P., Pittner Jiří, Čársky Petr
Brillouin-Wigner Expansions in Quantum Chemistry
Bloch-Like and Lippmann-Schwinger-Like Equations.
In: *Advances Topics in Theoretical Chemical Physics* (Maruani, J. -
Lefebvre, R. - Brändas, E. J., Ed.), pp. 71-117. Kluwer Academic,
Dordrecht 2003.
4. Paidarová Ivana, Durand P.
Modelling Quantum Resonances I. Dynamics of Interacting Resonances.
In: *Advanced Topics in Theoretical Chemical Physics* (Maruani, J. -
Lefebvre, R. - Brändas, E. J., Ed.), pp. 271-294. Kluwer Academic,
Dordrecht 2003.
5. Durand P., Paidarová Ivana
Modeling Quantum Resonances II. Overview of Collision Theory.
In: *Advanced Topics in Theoretical Chemical Physics* (Maruani, J. -
Lefebvre, R. - Brändas, E. J., Ed.), pp. 295-310. Kluwer Academic,
Dordrecht 2003.
6. Jungwirth Pavel
Physical Properties and Atmospheric Reactivity of Aqueous Sea Salt
Micro-Aerosols.
In: *Water in Confining Geometries* (Buch, V. - Devlin, J. P., Ed.),
pp. 277-293. Springer, Berlin 2003.
7. Vohlídal J., Pacovská M., Sedláček J., Svoboda J., Zedník J., Balcar
Hynek
Polymerizations Catalyzed with Rhodium Complexes.
In: *Novel Metathesis Chemistry: Well-Defined Initiator Systems for
Specialty Chemical Synthesis, Tailored Polymers and Advanced Material
Applications* (Imamoglu, Y. - Bencze, L., Ed.), pp. 131-154. Kluwer
Academic, Dordrecht 2003.

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Mesoporous Molecular Sieves Immobilized Catalysts for Polymerization of Phenylacetylene and its Derivatives.
In: *Novel Metathesis Chemistry Well-Defined Initiator Systems for Specialty Chemical Synthesis, Tailored Polymers and Advanced Material Applications* (Imamoglu, Y. - Bencze, L., Ed.), pp. 155-165. Kluwer Academic, Dordrecht 2003.
9. Kavan Ladislav, Dunsch L., Kataura H.
Charge Transfer at Carbon Nanotubes with Encapsulated C60 and C70 (Peapods).
In: *Fullerenes, vol. 13: Fullerenes and Nanotubes: The Building Blocks of NExt Generation Nanodevices* (Guldi, D. M. - Kamat, P. V. - D'Souza, F., Ed.), pp. 323-332. The Electrochem. Soc., Pennington 2003.

4.5. Patents

1. Steiner G., Salzer R., Hof Martin, Beneš Martin
Method and Construct for Intesifying the Fluorescence Emission in Fluorescence Correlation Spectroscopy (in German).
DE Pat. No. DE 100 58 577 C2. Patented 7 August 2003.
2. Gonsiorová O., Bortnovskij O., Wichterová Blanka, Čejka Jiří
Synthesis of Zeolite Beta (in Czech).
Office for Industrial Ownership, Prague, 2003.
3. Corzani I., Rossi S., Rathouský Jiří, Zukal Arnošt
Doped Absorbent Materials with Enhanced Activity.
US Pat. No. WO 03/013719 A1. Patented 20 February 2003.

4.6. Popularization Papers

1. Zahradník Rudolf
A contribution in "Stories of Czech Science" (in Czech).
(L. Koubská, K. Pacner, S. Speváková).
Academia, Prague 2003.
2. Jungwirth Pavel
Aerosols and atmospheric chemistry (in Czech).
Vesmír 82(4), 196 (2003).
3. Hanuš Vladimír, Herman Zdeněk, Lamr K.
Mass spectrometry and large molecules (in Czech).
Vesmír 82(6), 312 (2003).
4. Weber Jan, Pelouchová Hana, Janda Pavel
Tunnel microscopy and spectroscopy in electrochemistry (in Czech).
Čs. čas. fyz. 53(2), 128-131 (2003).
5. Heyrovská Rajalakshmi, Kodymová J., Krupková O., Musilová J.
Women in physics. A few words on an international „physical conference without physics“ (in Czech).
Čs. čas. fyz. 53(1), 36-38 (2003).

4.7. Further Major Activities in the Popularization of Science

- a) Five broadcast interviews of Z. Herman on occasion of awarding him the National Prize "Česká hlava 2003", November and December 2003.
- b) A broadcast relation of Z. Herman on the chemistry in crossed molecular beams in the program Meteor, 28 November 2003.
- c) An appearance of Z. Herman on the chemistry in crossed molecular beams in the program Popularit, November 2003.
- d) Participation of P. Jungwirth in debate on the perspectives of Czech science in the program "Tea for the third one", Czech TV, August 2003.
- e) Tour of the Institute for 77 visitors within the framework of the "Days of the open door 2003", 7 and 8 November 2003.
- f) Seminar "Contemporary polarography" given by M. Heyrovský for Prague secondary school teachers, 15 October 2003.
- g) Lecture „Physical chemistry of surfaces on a nanostructure scale“ given by Z. Knor in the Ch.Doppler gymnasium in Prague 5, 27 November 2003.

4.8. Organization of Local Conferences

Participation in the organization of the seminar “Modern Electrochemical Methods XXIII”. Jetřichovice, 20 through 22 May 2003, co-organizers T.Navrátil and L. Novotný, 45 participants.

5. LECTURES AND SEMINARS

Lectures and seminars organized in the Institute included

- annual Brdička Lecture,
- annual Student Seminar,
- institute seminars,
- departmental seminars.

In addition, research teams organized their internal colloquiums to discuss specific partial problems, methodical questions, progress in work, etc.

5.1. Brdička Lecture

The Institute has organized since 1991 annually a festive lecture to commemorate Professor Rudolf Brdička (1906-1970), the founder and director of one of the constituent parts of the present Institute. Invited speakers have been outstanding internationally recognized scientists active in some field related to the research currently pursued in the Institute.*

* BRDIČKA LECTURES

1. (1991): Edgar HEILBRONNER (Eidgenössische Technische Hochschule, Zürich)
"The old Hückel formalism".
 2. (1992): Kamil KLIER (Lehigh University, Bethlehem, Pennsylvania)
"Physical chemistry in two dimensions".
 3. (1993): Joshua JORTNER (Tel Aviv University, Tel Aviv)
"Clusters - a bridge between molecular and condensed matter chemical physics".
 4. (1994): David J. SCHIFFRIN (The University of Liverpool)
"Electrochemistry in two-dimensional systems".
 5. (1995): Josef MICHL (University of Colorado, Boulder, Colorado)
"A molecular kit for new materials".
 6. (1996): Gerhard ERTL (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin)
"Self-organization in surface reactions".
 7. (1997): Roger PARSONS (The University of Southampton)
"Electrochemistry in the last 50 years: from Tafel plotting to scanning tunneling".
 8. (1998): G. Barney ELLISON (University of Colorado, Boulder, Colorado)
"The chemical physics of organic reactive intermediates in combustion and atmospheric processes".
 9. (1999): Henry F. SCHAEFFER III (University of Georgia, Athens, Georgia)
"The third age of quantum chemistry".
 10. (2000): Alexis T. BELL (University of California and Lawrence Berkeley Laboratory, Berkeley, California)
"Progress towards the molecular design of catalysts - lessons learned from experiments and theory".
 11. (2001): Mario J. MOLINA (Massachusetts Institute of Technology, Cambridge, MA)
"The Antarctic Ozone Hole".
 12. (2002): Jean-Marie LEHN (Université Louis Pasteur, Strasbourg and Collège de France, Paris)
"Selforganization of Supramolecular Nanodevices"
-

The 13th Brdička Lecture entitled

**„Elementary Processes in Catalysis:
Looking at and Learning from “Naked” Transition Ion”**

was delivered on 2 June 2003 by Prof. Dr. Drs.h.c. **Helmut SCHWARZ** of Technical University Berlin.

5.2. Annual Student Seminar

The annual seminar of Ph.D. students and advanced undergraduates working on their diploma theses took place in Třešť from 3 to 5 June 2003. Contributions were presented by 29 Ph.D. students and 5 undergraduates. Each student was awarded a financial premium according to the shown performance.

5.3. Institute Seminars

Of nine Institute seminars presented in 2003, six were held by members of the Institute and three by speakers from abroad.

09.01.	Z. Samec <i>Heyrovský Institute</i>	Quasi-elastic light scattering at the polarised liquid interface
06.02.	S. Civiš <i>Heyrovský Institute</i>	Utilization of high power laser systems for simulation of lightnings and impact of an extraterrestrial body into the early atmosphere of Earth. Can such an impact synthesize life precursors?
06.03.	G. Meijer <i>FOM-Institute for Plasmaphysics “Rijnhuizen”, University of Nijmegen, Fritz-Haber- Institut der Max-Planck- Gesellschaft, Berlin</i>	Deceleration and trapping on neutral polar molecules
03.04.	J. Čejka <i>Heyrovský Institute</i>	From zeolites to mesoporous alumina and back
15.05.	L. Kavan <i>Heyrovský Institute</i>	Electrochemistry of carbon nanostructures
04.09.	M. Kawai <i>RIKEN-The Institute of Physical and Chemical Research, Wako-Shi</i>	Chemistry of molecules at surfaces

	H. S. Kato <i>RIKEN-The Institute of Physical and Chemical Research, Wako-Shi</i>	Reaction promotion of water in hydrogen bond network on surfaces
10.10.	J. Michl <i>University of Colorado, Boulder</i>	Artificial surface-mounted molecular rotors
06.11.	Z. Sobalík <i>Heyrovský Institute</i>	Approach to analysis of active sites and their functioning in heterogeneous catalysis
04.12.	P. Janda <i>Heyrovský Institute</i>	Visualization, analysis and nanostructurization of surfaces by <i>in situ</i> SPM methods

5.4. Departmental Seminars

66 seminars were held in departments by members of the Institute and by hosted speakers both from domestic and foreign institutions.

TABLE 5.1. SYNOPSIS OF DEPARTMENTAL SEMINARS

Department	Seminars given by			Total
	internal speakers	hosted speakers from CR	from abroad	
Chemical Physics	6	2	14	22
Complex Molecular Systems	1	4	5	10
Catalysis	16	0	8	24
Electrochemistry	8	0	2	10

DEPARTMENT OF CHEMICAL PHYSICS

INTERNAL SPEAKERS

17.02.	Š. Pick	Calculations of magnetic anisotropy of small Co clusters on Cu(001) surface
03.03.	J. Žabka	Study of CO ₂ ²⁻ ion reactivity towards neutral molecules (Ar, ¹³ N ₂ , CO ₂ , NO, CO) using synchrotron radiation
31.03.	J. Vacek	Molecular kit: computer simulations of molecular rotors
09.06.	Z. Zelinger	Simulation of atmosphere pollution in aerodynamic tunnel and its comparison with measurements in real atmosphere

- 10.10. I. Paidarová Shape of spectral lines and the dynamics
- 03.11. P. Pracna Small molecules from the view of high precision vibration-rotation and rotation spectroscopy

HOSTED SPEAKERS

- 10.01. D. K. Böhme
York University, Toronto Novel chemistry initiated by atomic metal ions
- 17.03. K. Vèkey
*Chemical Research Center,
Hungarian Acad. Sci., Budapest* MASSKINETICS: Simulation of ion activation and dissociation
- 14.04. D. Smith
Keele University, UK Selected ion flow tube mass spectrometry in medicine
- 25.04. W. H. Miller
University of California, Berkeley Using semiclassical theory to add quantum effects to classical molecular dynamics simulation
- 12.05. J. Horáček
*Fac. Math. Phys., Charles
University* Origin of molecular hydrogen and its role in the Universe
- 26.05. P. Jensen
Bergische Universität, Wuppertal Molecular structure determination: Coulomb explosion imaging vs. quantum chemistry and spectroscopy for CH₂⁺
- 27.06. M. McEwan
*Canterbury University,
New Zealand* Things that ions can do
- 10.07. W. C. Lineberger
University of Colorado, Boulder Femtosecond detachment probes of molecular rearrangement dynamics
- 21.07. R. Flannery
*Georgia Institute of Technology,
Atlanta* Atomic and molecular processes in ultra cold Rydberg plasmas
- 23.07. H. Yasumatsu
*Toyota Technological Institute,
Ichikawa* Scattering and deposition of size-selected clusters by impact onto solid surface
- 04.08. A. Hess
Vanderbilt University, Nashville The cyclization of squalene to lanosterol and hopanoids
- 30.09. J. Michl
University of Colorado, Boulder Sigma electron delocalization

- | | | |
|--------|---|--|
| 14.10. | M. Allan
<i>University Fribourg</i> | Recent experiments in electron -
molecule scattering |
| 01.12. | R. Schiller
<i>Hungarian Acad. Sci., Budapest</i> | Dispersive diffusion and chemical
reactions - a semiconductor electrode
impedance |
| 9.12. | K. Vèkey
<i>Chemical Research Center,
Hungarian Acad. Sci., Budapest</i> | Activation of ions in the gas phase and
the theory of mass spectra |
| 15.12. | J. Kolmaš
<i>Oriental Institute, AS CR</i> | Prince of pilgrims or the largest travel
book of the world (Süng-cang travel to
the Holy Land of Buddhism 629-645) |

DEPARTMENT OF COMPLEX MOLECULAR SYSTEMS

INTERNAL SPEAKERS

- | | | |
|--------|------------|--|
| 29.09. | P. Žďánská | Quantum chemistry methods for
resonance phenomena |
|--------|------------|--|

HOSTED SPEAKERS

- | | | |
|--------|--|---|
| 10.03. | N. B. Leontis
<i>Bowling Green State University</i> | RNA structural bioinformatics |
| 24.03. | V. Kareš
<i>Masaryk University, Brno</i> | String theory – a theory of everything? |
| 28.08. | F. Tureček
<i>University of Washington, Seattle</i> | Peptide and proteins radicals:
agreements and disagreements between
theory and experiment |
| 15.09. | D. Knopf
<i>ETH Zürich</i> | Thermodynamic properties and
nucleation processes of aerosol particles
of the upper troposphere and lower
stratosphere |
| 13.10. | S. Bradforth
<i>University of Southern California</i> | Probing ultrafast reaction dynamics in
water – photodetachment and
photodissociation |
| 31.10. | M. Holthausen
<i>Universität Marburg</i> | Biomimetic models for dinuclear copper
proteins: Structure and oxidation
chemistry from a quantum chemical point
of view |
| 10.11. | J. Zamastil
<i>Fac. Math. Phys., Charles
University, Prague</i> | TBA |

- | | | |
|--------|---|--|
| 24.11. | P. Kužel
<i>Inst. Physics, AS CR</i> | Time resolved terahertz spectroscopy of molecular systems |
| 08.12. | R. Bulánek
<i>University Pardubice</i> | FTIR study of small molecules interaction with metal cations in zeolites |

DEPARTMENT OF CATALYSIS

Internal speakers

- | | | |
|--------|----------------------------|--|
| 18.03. | A. Zukal | Morphological parts of mesoporous molecular sieves |
| 15.04. | O. Prokopová | Evaluation of cylindrical membranes |
| 29.04. | M. Boldiš | Simulation of non-isothermal dynamical sorption |
| 13.05. | R. Hamtil | Olefin metathesis on heterogeneous catalysts |
| | J. Klisáková | Catalysts for acylation reactions |
| 20.05. | J. Pinkas | Synthesis of new catalysts for olefin polymerizations |
| 27.05. | J. Schwarze | Structure and reactivity of Fe centers in zeolites |
| | V. Kreibich | Structure of Fe centers for benzene oxidation by N ₂ O |
| 24.06. | P. Sazama
O. Bortnovsky | Cracking of C ₅ and C ₄ olefins on molecular sieves |
| 15.10. | L. Brabec | Silicalite-1 and hydrofluoric acid: etching of crystals and polycrystalline layers |
| 29.10. | P. Sazama
O. Bortnovsky | Cracking of C ₄ up to C ₆ olefins on zeolite catalysts |
| 11.11. | J. Dědeček | MAS NMR of zeolites. Current possibilities and the first results |
| 18.11. | M. Zukalová | Organized porous TiO ₂ (anatase): synthesis and characterization |
| 25.11. | G. Košová | Synthesis of new types of zeolites |
| 02.12. | P. Prokešová | Micro/mesoporous composite materials |

09.12. A. Zikánová
Development of non-stationary permeation and diffusion methods for testing of nanofiltration membranes and their application

Hosted speakers

21.03. D. J. Suh
Korean Institute of Chemical Technology
Synthesis and characterization of catalytic aerogel materials

01.04. J. R. Agger
University Manchester
Zeolite crystal growth

05.05. J.-C. Guillemin
Ecole Nationale Supérieure de Chimie, Rennes
Vinylamine and other unsaturated heterocompounds. Synthesis and spectroscopic studies

12.06. W. Schmidt
Max-Planck-Institut für Kohlenforschung, Mülheim
Exotemplating, nanocasting and matrix-assisted growth of high surface area materials

17.06. J. P. Pariente
Institute of Catalysis and Petrochemistry, Madrid
Synthesis of zeolites: From first principle to new materials

15.09. J. F. Harrod
McGill University, Montreal
Poetry in motion: A modest proposal as to how titanocene derivatives catalyze diverse chemical reactions

27.10. U. Rosenthal
Universität Rostock
Titanocene and zirconocene complexes of bis(trimethylsilyl)acetylene – the way from silicon to titanium and via zirconium back to silicon

7.11. H. van Bekkum
University of Delft
Zeolites in the synthesis of fine chemicals

DEPARTMENT OF ELECTROCHEMISTRY

INTERNAL SPEAKERS

- 24.01. T. Navrátil Electrochemistry of biological systems with more redox centers
- 07.02. B. Schneider Solvation of DNA
- 21.02. P. Janda Charge transfer reactions on carbon nanostructures
- 31.03. J. Hlavatý Preparation of stable protected 3-ethynylpyrroles for electrochemical polymerization
- 04.04. M. Rejňák Electrochemical properties of benzothiophene derivates
- 24.10. A. Vlček Ultrafast electron transfer ligand-ligand and ligand-metal
- 07.11. P. Krtíl Phase transitions during Li insertion into transition metal oxides
- 21.11. J. Ludvík Correlation of electrochemical behavior and structure of organic molecules (bond length, electron delocalization)

HOSTED SPEAKERS

- 07.03 J. Růžička
University of Washington, Seattle Electrochemical application of the FIA (flow-injection analysis) methods
- 18.04. S. Szunerits
Center of Atomic Energy (CEA), Grenoble The use of optical fiber bundles combined with electrochemistry for chemical imaging

6. INTERNATIONAL CONTACTS

6.1. Synopsis

The Institute was collaborating with several dozens of foreign universities and research institutions within the framework of multilateral research networks and bilateral agreements (Chap. 3). The Institute continued to serve as the main coordinator of the project "Advanced nanostructured metal/metaloxo/matrix catalysts for redox processes. Application for NO_x reduction to nitrogen" of the 5th EC framework programme GROWTH.

Members of the Institute published 111 papers jointly with authors from institutions abroad (Chap. 4).

The Institute functioned as Marie Curie Training Site of EC in quantum chemical methods and quantum molecular dynamics; and as a member of two Research Training Networks of EC concerning generation, stability and reaction dynamics of multiply charged ions, and electron and positron induced chemistry (EPIC) (Sect. 6.2).

Visitors from abroad gave 35 lectures and seminars in the Institute (Chap. 5). The Institute organized 9 international conferences (Sect. 6.3). Members of the Institute acted in editorial or advisory boards of scientific periodicals and in international scientific organizations and bodies (Chap. 8)

6.2. Working Stays

Of several tens of visitors from abroad, 22 spent 30 days or more at the Institute working on joint projects (Table 6.1.).

Table 6.1. Working stays of researchers from abroad in 2003 (30 days or longer)

Name	Country	Length (days)	Host	Department
M. Kaciorowska	Poland	365	J. Hrušák	<u>Chemical Physics</u>
J. Jašík	Slovakia	273	Z. Herman	
I. Ypoliy	Slovakia	273	Z. Herman	
P. Papp	Slovakia	212	P. Čársky	
P. Hrušč	Slovakia	120	P. Čársky	
S. Kardahakis	Greece	90	P. Čársky	
Y. Lykhach	Ukraine	89	Z. Bastl	
K. Nikiforov	Russia	76	Z. Knor	
W. Majewski	Poland	33	Z. Bastl	
N. Alov	Russia	31	Z. Bastl	
J. Michl	USA	30	P. Čársky	
H. Valdez Gonzales	Spain	30	P. Čársky	

				<u>Complex Molecular Systems</u>
W. Zierkiewicz	Poland	196	P. Hobza	
T. Kral	Poland	134	M. Hof	
B. Minofar	Iran	30	P. Jungwirth	
				<u>Catalysis</u>
J. Pawlesa	Poland	91	J. Čejka	
P. Šabo	Slovakia	90	Z. Sobalík	
C.D. Radu	Romania	49	Z. Sobalík	
O. Bartels	Germany	30	J. Rathouský	
Y. Rohlifing	Germany	30	J. Rathouský	
				<u>Electrochemistry</u>
D. Fattakhova	Russia	90	P. Krtil	
G. Ekmekci	Turkey	60	J. Ludvík	

6.3. International Scientific Meetings Arranged by the Institute

1st Pittsburgh - Prague Symposium on Complex Molecular Systems.
Prague, 6 - 7 February 2003, organizers P. Hobza and P. Jungwirth. 45 participants including 7 from the U.S.A.

MCInet (Multiply Charged Ions), 2nd Summer School 2003.
Třešť, 27 - 30 April 2003, organizers Z. Herman and J. Hrušák. 27 participants including 16 from abroad.

36th Heyrovský Discussion "Electrochemistry of Biological Systems and Their Models".
Třešť, 15 - 19 June 2003, organizer J. Ludvík. 56 participants including 30 from abroad.

13th International Symposium on Electron - Molecule Collisions and Swarms (a satellite of the XIIIth ICPEAC).
Průhonice near Prague, 30 July - 2 August 2003, co-organizer P. Čársky. 109 participants including 98 from abroad.

8th Conference on Methods and Applications of Fluorescence: Spectroscopy, Imaging and Probes.
Prague, 24 - 27 August 2003, organizer M. Hof. 305 participants including 275 from abroad.

5th Czech-German Summer Academy.
Prague, 14 - 27 September, 2003, co-organizer S. Černý. 101 Ph.D. students and undergraduates (14 from Czech Republic, 3 from Slovakia, 84 from Germany) and 12 lecturers (6 from Czech Republic, 5 from Germany, 1 from Netherlands).

2nd Central European Symposium on Theoretical Chemistry.
Nové Hrady, 25 - 28 September 2003, organizers P. Čársky and J. Hrušák. 78 participants including 68 from abroad.

8th Seminar of Ph.D. Students on Organometallic Chemistry.
Hrubá Skála near Turnov, 29 September - 3 October 2003, organizer K. Mach.
96 participants including 71 from abroad.

35th Symposium on Catalysis.
Prague, 3 - 5 November 2003, organizer J. Čejka. 105 participants including 22 from
abroad.

7. COOPERATION WITH UNIVERSITIES IN THE CZECH REPUBLIC

Acronyms used:

CU – MAT	Charles University, Prague, Faculty of Mathematics and Physics
CU – MED	Charles University, Prague, 3 rd Faculty of Medicine
CU – SCI	Charles University, Prague, Faculty of Science
CUA – AGR	Czech University of Agriculture, Prague, Faculty of Agronomy
CTU – NUC	Czech Technical University, Prague, Faculty of Nuclear Physics and Engineering
ICHT – ENG	Institute of Chemical Technology, Prague, Faculty of Chemical Engineering
ICHT – ENV	Institute of Chemical Technology, Prague, Faculty of Environmental Technology
ICHT – TEC	Institute of Chemical Technology, Prague, Faculty of Chemical Technology
MU – SCI	Masaryk University, Brno, Faculty of Science
TUB – CHEM	Technical University of Brno, Faculty of Chemistry
UPAR – TEC	University of Pardubice, Faculty of Chemical Technology

7.1. Lecture Courses for Undergraduates and Ph.D. Students

Synopsis

Semester	Number of courses	Hours per semester
Summer 2003	12	290
Winter 2003	25	544
Total	37	834

Number of lecturers from the Institute: 27

Number of faculties involved: 10

DEPARTMENT OF CHEMICAL PHYSICS

Lecturer	Lecture course	Faculty	Semester	Hours
P. ČÁRSKY (WITH J. FIŠER, CU – SCI)	Structure of molecules	CU – SCI	W	26
M. HOF	Molecular physics	CTU – NUC	S	30
M. HOF	Fluorescence spectroscopy: Principles and biological applications	CTU – NUC	W	30
Z. KNOR	Chemistry and physics of surfaces and interfaces	CU – SCI	W	30
Z. KNOR (WITH B. WICHTERLOVÁ)	Adsorption and catalysis	ICHT – TEC	S	20
J. PITTNER	Methods of analytical gradients	CU – SCI	W	30
J. PITTNER	Structure of molecules	CU – SCI	W	26
Š. URBAN	Selected chapters of chemical physics	ICHT – ENG	W	36
Š. URBAN	Molecular spectroscopy	ICHT – ENG	S	36
S. CIVIŠ	Spectroscopic methods II: Laser analytical spectroscopy	CU-SCI	W	12

DEPARTMENT OF COMPLEX MOLECULAR SYSTEMS

Lecturer	Lecture course	Faculty	Semester	Hours
P. HOBZA	Theoretical and computational chemistry	CU – SCI	S	40
P. JUNGWIRTH	Classical and quantum molecular dynamics	CU – MAT	W	28
P. NACHTIGALL	Introduction to quantum chemistry	UPAR – TEC	W	28
P. NACHTIGALL	Quantum chemistry – spectroscopy	UPAR – TEC	W	28
P. NACHTIGALL	Methods of quantum chemistry	UPAR – TEC	S	28
P. SCHNEIDER	Determination and description of molecular structure	CU – SCI	W	30

V. ŠPIRKO	Atomic and molecular spectroscopy	CTU – NUC	W	25
J. VACEK	Computer simulations of biomacromolecules	CU – MAT	W	13

DEPARTMENT OF CATALYSIS

Lecturer	Lecture course	Faculty	Semester	Hours
J. ČEJKA	Principles and methods of heterogeneous catalysis	ICHT – TEC	W	28
J. ČEJKA	Zeolites and microporous inorganic materials: synthesis, structure, characterization and application	ICHT – TEC	W	30
J. ČEJKA (WITH J. VOHLÍDAL, CU – SCI)	Principles and methods of heterogeneous catalysis	CU – SCI	W	21
J. ČEJKA	Chemical principles of industrial manufacturing	CU – SCI	W	45
J. NOVÁKOVÁ	Stable isotopes in the study of catalytic reaction intermediates (within the course "Nuclear chemistry experiments")	CTU – NUC	W	4
Z. SOBALÍK	Spectroscopical characterization of heterogeneous catalysts	UPAR – TEC	W	28
Z. SOBALÍK (WITH J. KRÝSA, ICHT – TEC)	Experimental methods in electrochemistry and catalysis	ICHT – TEC	W	8
B. WICHTERLOVÁ (WITH Z. KNOR)	Adsorption and catalysis	ICHT – TEC	S	10

DEPARTMENT OF ELECTROCHEMISTRY

Lecturer	Lecture course	Faculty	Semester	Hours
L. KAVAN	Selected spectral methods	CU – SCI	W	28
L. POSPÍŠIL	Electrochemistry	ICHT – ENV	S	30
I. ŠESTÁKOVÁ	Electrochemistry (within the course "Special analytical chemistry")	CUA – AGR	S	2+4
J. LUDVÍK	Electrochemistry	ICHT-ENG	W	32

Z. SAMEC	Physical chemistry	CU-SCI	S	42
L. NOVOTNÝ	Electroanalysis	UPAR-TEC	S	26
L. NOVOTNÝ	General and applied electrochemistry	UPAR-TEC	W	26
T. NAVRÁTIL	Medical chemistry and biochemistry	CU-MED	W	8
P. KRTIL	Electrochemical power sources	ICHT-ENG	S	15
V. MAREČEK	Experimental methods in electrochemistry	CTU	S	7
A. VLČEK	Photochemistry, electrochemistry and electron transfer	CU-SCI	W	28

7. 2. Training Courses for Undergraduates

Synopsis

Semester	Number of courses	Hours per semester
Summer 2003	11	163
Winter 2003	9	89
Total	20	252

Number of course leaders from the Institute: 16

Number of faculties involved: 7

DEPARTMENT OF CHEMICAL PHYSICS

Course leader	Training course	Faculty	Semester	Hours
Z. BASTL	<i>Electron microscopy</i>	CU – SCI	S	10
P. KUBÁT	<i>Laser kinetic spectroscopy</i>	CU – MAT ICHT – TEC	W	12
M. HOF	<i>Fluorescence correlation spectroscopy</i>	CU-SCI	W	4
J. PITTNER	<i>Analytical gradient methods</i>	CU – SCI	W	14

Š. URBAN	<i>Selected chapters of molecular physics</i>	ICHT – ENG	S	17
Š. URBAN	<i>Molecular spectroscopy</i>	ICHT – ENG	S	18
Z. ZELINGER	<i>Laser analysis and its application to investigation of atmospheric pollution</i>	CU – SCI	S	20

DEPARTMENT OF COMPLEX MOLECULAR SYSTEMS

Course leader	Training course	Faculty	Semester	Hours
J. VACEK	<i>Computer simulations of biomacromolecules</i>	CU – MAT	W	13

DEPARTMENT OF CATALYSIS

Course leader	Training course	Faculty	Semester	Hours
L. BRABEC	<i>Scanning electron microscopy</i>	CTU – NUC	S	2
L. BRABEC	<i>Scanning electron microscopy</i>	CU – SCI	W	4
K. MACH	<i>Electron spin resonance</i>	CTU – NUC	S	12
J. NOVÁKOVÁ	<i>Mass spectrometry</i>	CTU – NUC	S	18
J. NOVÁKOVÁ	<i>Mass spectrometry</i>	CU – SCI	W	12
A. ZIKÁNOVÁ	<i>Flow methods in sorption measurements on solids</i>	CTU – NUC	W	12
B. WICHTERLOVÁ	<i>Reaction kinetics in catalysis</i>	CTU-NUC	S	6
B. WICHTERLOVÁ	<i>Reaction kinetics in catalysis</i>	CU-SCI	W	6

DEPARTMENT OF ELECTROCHEMISTRY

Course leader	Training course	Faculty	Semester	Hours
V. MAREČEK, A. LHOTSKÝ	<i>Fundamentals of electrochemical methods</i>	CTU – NUC	S	10
T. NAVRÁTIL	<i>Electrochemical methods</i>	CU – SCI	S	18
T. NAVRÁTIL	<i>Medical chemistry and biochemistry</i>	CU – MED	W	12
I. ŠESTÁKOVÁ	<i>Electrochemical methods</i>	CUA – AGR	S	32

7.3. Supervision of Theses

94 Ph.D. Theses and 8 Diploma Theses were supervised by members of the Institute's staff, in most cases jointly with teachers at universities. On 64 Ph.D. theses worked students imbursed at least partially by the Institute. On 30 Ph.D. theses worked students imbursed by other institutes or graduates who did not have the status of Ph.D. students.

10 undergraduates participated for different periods of time in the work of the Institute as auxiliary research assistants.

Supervised Ph.D. Theses

DEPARTMENT OF CHEMICAL PHYSICS

Student	Faculty	Thesis title	Supervisor in the Institute	Start	Remark
M. Šimečková	CU-MAT	Hyperfine effects in high resolution spectra of molecules	Š. Urban	1999	
M. Střížík	CU - SCI	Application of laser opto-acoustic and differential absorption LIDAR spectroscopy to the study of atmospheric pollution	Z. Zelinger	1999	Defended in 2003
M. Beneš	CU-MAT	Fluorescence correlation spectroscopy: Characterization of planar phospholipid bilayer systems for protein-membrane interactions	M. Hof	2000	
J. Roithová	ICHT-ENG	Dynamics of reactions of molecular dications	Z. Herman	2000	Defended in 2003
J. Kubišta	UPAR-TEC	Mass spectrometric studies of ion rearrangements		2001	
P. Kania	ICHT-ENG	Microwave spectroscopy	Š. Urban	2001	
D. Babánková	CU-SCI	Application of high-power lasers	S. Civiš	2001	
M. Polášek	CU-SCI	Mass spectrometry of organic molecules		1996	Defended in 2003
V. Horká	CU-SCI	High resolution spectroscopy of ions	S. Civiš	2001	
D. Poláčková	UPAR-TEC	Effect of radiation-induced modification of surfaces on their chemical properties	Z. Bastl	2001	Terminated in 2002
J. Sýkora	CU-SCI	Solvent relaxation in biomolecules	M. Hof	2002	
A. Benda	CU-SCI	Single molecule spectroscopy on biomembranes and their model systems	M. Hof	2002	
J. Humpolíčková	CU-SCI	Determination of fluorescence lifetimes in single macromolecular assemblies	M. Hof	2002	
O. Demel	CU-SCI	Development and application of the MRBWCC method with inclusion of connected triplets	J. Pittner	2002	
K. Bezpalcová	CU-MAT	Physical modelling of streaming and diffusion in urban agglomeration	Z. Zelinger	2002	
K. Dryahina	CU-MAT	Studies of ion - molecules processes	P. Španěl	2003	

P. Hrubý	ICT-ENG	Energetic and electronic factor in surface effects on metals	Z. Knor	2003	
J. Šmydke	CU-MAT	Analytical gradient for the multireference Brillouin-Wigner Coupled Cluster Method	J. Pittner P. Čársky	2003	
L. Stříteská	ICT-ENG	Microwave spectroscopy	Š. Urban	2003	
P. Nikolič	CU-MAT	Optoacoustic laser spectrometry of ozone and atmospheric pollutants	Z. Zelinger	2000	Defended in 2003

DEPARTMENT OF COMPLEX MOLECULAR SYSTEMS

Student	Faculty	Thesis title	Supervisor in the Institute	Start	Remark
M. Roeselová	CU-MAT	Quantum dynamics and spectroscopy in cryogenic clusters	P. Jungwirth	1995	Defended in 2003
N. Špačková	MU-SCI	Molecular interactions in DNA and DNA-intercalator complexes	J. Šponer	1997	
F. Ryjáček	CU-SCI	Structure, dynamics and energetics of DNA: Computer simulations and quantum chemical studies	P. Hobza	1998	
M. Davidová	CU-MAT	Theoretical study of the structure and reactivity of transition metal – zeolite systems	P. Nachtigall	1999	
E. Hudečková	CU-MAT	Spectroscopy and control of photochemical processes in cryogenic clusters	P. Jungwirth	1999	
P. Slavíček	CU-MAT	Ultrafast quantum dynamics in clusters	P. Jungwirth	1999	
M. Šindelka	CU-MAT	Dynamics and chemical reactivity of highly excited rotation-vibration states of polyatomic molecules	V. Špirko	1999	
M. Hanus	CU-SCI	Theoretical study of complex molecular systems	P. Hobza	1999	
J. Chocholoušová	CU-MAT	Theoretical study of the structure, properties and dynamics of aminoacids, peptides and their complexes with DNA	P. Hobza	2000	Defended in 2003
P. Jurečka	CU-SCI	Theoretical study of the structure, properties and dynamics of aminoacids, peptides and their complexes with DNA	P. Hobza	2000	
A. Prokop	CU-MAT	Computer simulations of molecular propellers	J. Vacek	2000	

D. Řeha	CU–SCI	Theoretical study of ligand interactions with DNA	P. Hobza	2000
M. Kalhous	CU–MAT	Solution of multidimensional Schrödinger equation	V. Špirko	2000
J. Kučera	UPAR–TEC	Theoretical and experimental study of structure and properties of basic centres in zeolites	P. Nachtigall	2001
M. Šilhan	UPAR–TEC	Theoretical studies of structure and properties of transition metals bound in molecular matrices	P. Nachtigall	2001
J. Černý	ICT–ENG	Theoretical study of excited states of nucleic acid bases	P. Hobza	2002
J. Rejnek	CU–SCI	Thermodynamical calculations of nucleic acid bases complexes	P. Hobza	2002
J. Honzíček	UPAR–TEC	A study of vanadocene fragments interaction with bioligands	P. Nachtigall	2002
M. Mucha	CU–MAT	Molecular simulations of clusters and surfaces	P. Jungwirth	2002
Shai Ronen	Tel Aviv University	Experimental and theoretical description of dipole bound electrons	P. Jungwirth	2002
P. Dobeš	CU-SCI	Calculation of thermodynamic characteristics of DNA with ligands	P. Hobza	2003
L. Zendlová	CU-SCI	Theoretical and experimental study of bases and base pairs of nucleic acid	P. Hobza	2003
L. Vrbka	CU-SCI	Structure and dynamics of ions on the solid and fluid phase interface	P. Jungwirth	2003
J. Řezáč	CU-SCI	QM/MM calculations on DNA fragments	P. Hobza	2003
J. Fanfrlík	CU-SCI	Evaluation of hydration free energy	P. Hobza	2003
R. Vácha	CU-SCI	Molecular simulations of atmospheric aerosols	P. Hobza	2003
E. Mrázková	CU-SCI	The nature of improper hydrogen bond	P. Hobza	2003
T. Šedivcová	CU-MAT	Theoretical study of molecular ions and their detection in the instellar space	V. Špirko	2003
T. Kubař	CU-SCI	Parameterization of the force field for nucleic acid modelling	P. Hobza	2003

DEPARTMENT OF CATALYSIS

Student	Faculty	Thesis title	Supervisor in the Institute	Start	Remark
O. Bortnovsky		Synthesis of zeolite Beta. Structure and activity of its Lewis center	B.Wichterlová	1998	Defended in 2003
L. Čapek	UPAR–TEC	Selective catalytic reduction of NO _x by hydrocarbons	B.Wichterlová	1998	
M. Boldiš	ICHT–BIO	Application of molecular sieves to isolation of fermentation products	M. Kočířik	2000	
P. Hrabánek	ICHT–TEC	Study of permeation and separation properties in coherence with application in membrane reactors	A. Zikánová	2000	
M. Slabová – Staňková	ICHT–ENG	Highly ordered nanostructures of titanium dioxide	A. Zukal	2000	
V. Kreibich	ICHT–TEC	Structural chemistry of zeolite catalysts and redox catalysis	B.Wichterlová	2000	
L. Lukešová	CU–SCI	Titanocene catalysts for olefin polymeration	K. Mach	2000	
P. Mokrejš	CU–SCI	Interaction of bentonites with surroundings in dependence on the bentonite history and actual physico-chemical conditions	A. Zikánová	2000	
J. Pinkas	CU–SCI	Low-valent titanocene – amid complexes	K. Mach	2000	
H. Jirglová	ICHT–ENG	Adsorption equilibria, sorption kinetics and dynamics of polydisperse structure materials	M. Kočířik	2001	
V. Gábová	ICHT–TEC	Al distribution in aluminosilica-based high-silica molecular sieves	J. Dědeček	2001	
K. Juristová	ICHT–TEC	Preparation and characterization of SiO ₂ -based microporous membrane materials for application in separation technologies and catalysis	A. Zikánová	2001	
G. Košová	ICHT–TEC	Synthesis of zeolite catalysts for selective reactions of heterocycles	J. Čejka	2001	
K. Novoveská	UPAR–TEC	Selective oxidation of alkanes	B.Wichterlová	2001	
P. Prokešová	ICHT–TEC	Synthesis of zeolite-based composite materials for catalytic applications	J. Čejka	2001	
O. Gonsiorová	ICHT–TEC	Synthesis and post-synthesis modifications of zeolites	B.Wichterlová	2001	
M. Schwarze	CU–SCI	Redox catalysis on molecular sieves	Z. Sobalík	2001	
P. Sazama	UPAR–TEC	Acidobasic transformations of hydrocarbons on zeolites	B.Wichterlová	2001	

M. Fryčová-Šnáblová	ICHT–TEC	Polymer-loaded solvents	M. Kočířik	2002
J. Klisáková	ICHT–TEC	Synthesis of zeolite catalysts for acylation reactions	J. Čejka	2002
M. Zukalová	CU-SCI	Titanium oxide-based organized nanostructure materials	J. Rathouský	2002
R. Hamtil	ICHT - TEC	Heterogeneous catalysators of olefin metatheses on base of mesoporous molecule sieves	H. Balcar	2002
P. Štěpánek	CU-SCI	Redox catalysis on zeolites in dynamical regimes	Z. Sobalík	2003
P. Topka	ICHT - TEC	Molecular sieves for olefin metatheses	J. Čejka	2003

DEPARTMENT OF ELECTROCHEMISTRY

Student	Faculty	Thesis title	Supervisor in the Institute	Start	Remark
M. Dřevínek	ICHT–TEC	Multichannel electrochemical detection for high-efficiency separation	L. Novotný	1995	
P. Bašová	CU–SCI	Electroanalysis and electrochemistry of selected biologically active substances	L. Novotný	1996	
Z. Dlasková	UPAR–TEC	Voltammetry of selected injurants and their metabolites in body liquids	L. Novotný	1997	Defended in 2003
R. Jirásek	ICHT–ENG	Preparation of nanostructured anatase for electrochemical applications	L. Kavan	1998	Interrupted in 2001
B. Josypčuk	UPAR–TEC	Voltammetric and electrosorption analysis of selected ecologically and biologically active substances	L. Novotný	1998	Defended in 2003
H. Pelouchová	CU–SCI	Immobilized mediator on a TiO ₂ (anatase) single crystal. Study of electrochemical microscopy with scanning probe technique	P. Janda	1998	Defended in 2003
V. Dorčák	CUA–AGR	Application of electrochemical methods to the study of plant metallothioneins and their complexes with heavy metals	I. Šestáková	1999	
J. Houser	TUB–CHEM	Potentialities of new voltammetric methods for solution of selected problems of the environment protection connected with the analysis of wastes with monomeric and polymeric matrice	L. Novotný	1999	

V. Chudoba	CU–SCI	Spectro-electrochemical study of selected ecologically important metal complexes	L. Novotný	1999	Defended in 2003
J. Pícha	ICHT–TEC	Synthesis of aryl-methyl-ketoximes and study of their properties	J. Ludvík	1999	
H. Hoffmannová	ICHT–ENG	Study of electrochemically initiated intermediates	P. Krtil	2000	
H. Měšťánková	ICHT–TEC	Comparative investigation of phenylurea derivatives degradation in aqueous TiO ₂ suspensions and Fe(III) solutions	J. Jirkovský	2002	
D. Rozbroj	ICHT–ENG	Electrochemical study of azo-methine bonds	J. Ludvík	2001	
R. Fadrná	UPAR–TEC	Electrochemical study of selected bioactive systems using electroanalytical sensors	L. Novotný	2001	
S. Šebková	UPAR–TEC	Electroanalysis of selected ecologically significant compounds and complexes using suitable experimental arrangement of electrodes	L. Novotný	2001	
P. Čížková	CUA–AGR	Application of electrochemical techniques to the study of uptake and metabolism of heavy metals in plants	J. Šestáková	2001	
T. Kotrba	ICHT–ENG	Quantum chemical calculations of spectroscopic parameters of molecules	S. Záliš	2002	
J. Jirkovský	ICHT–TEC	In-situ spectroscopic methods used in studies of lithium insertion into oxides of transition metals	P. Krtil	2003	
T. Kostlánová	CU-SCI	Solvothermal synthesis on nanocrystalline insertion hosts in Li-Ti-O systems and their electrochemical characterization	P. Krtil	2003	
M. Kolář	ICHT–ENG	The study of degradation of pollutants through heterogeneous catalysis	J. Jirkovský	2003	
J. Šebera	CU – SCI	Quantum chemical interpretation of spectra of molecular and complex systems	S. Záliš	2003	
M. Rejňák	ICHT- TEC	Electrochemical study of benzothiophene derivatives	J. Ludvík	2003	
P. Mořkovská	UPAR-TEC	Redox reactions inside molecular cavities	L. Pospíšil	2003	

7.4. Joint Projects and Publications

Members of the Institute's staff worked on 36 joint grant projects with universities in the Czech Republic (see Sect. 3). In 16 and 20 joint projects they acted as project leaders and associated contractors, respectively.

37 joint papers were published (see Sect. 4).

7.5. Membership in University Bodies

DEPARTMENT OF CHEMICAL PHYSICS

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| P. Čársky | ▪ Scientific Council of Technical University Liberec |
| Z. Herman | ▪ Branch Council for Physical Chemistry in the Ph.D. study program "Physical Chemistry" (Fac. Chem. Engng, Institute of Chem. Technol. Prague) |
| Z. Knor | ▪ Branch Council for Physics of Surfaces and Interfaces in the Ph.D. study program "Physics" (Fac. Mathem. and Phys., Charles Univ.)
▪ Branch Council for Physical Chemistry in the Ph.D. study program "Chemistry" (Fac. Chem. Engng, Institute of Chem. Technol. Prague)
▪ Examining Board for awarding Ph.D. degrees in physical chemistry (Fac. Science, Charles Univ.) |
| Š. Urban | ▪ Scientific Council of Fac. Chem. Technol., Institute of Chem. Technol. Prague
▪ Scientific Council of Fac. Chem. Engng., Institute of Chem. Technol. Prague
▪ Examining Board for state finals (Fac. Chem. Engng, Institute of Chem. Technol. Prague)
▪ Examining Board for awarding Ph.D. degrees in physical chemistry (Fac. Chem. Engng, Institute of Chem. Technol. Prague) |

DEPARTMENT OF COMPLEX MOLECULAR SYSTEMS

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| P. Hobza | ▪ Scientific Council of the Institute of Chem. Technol. Prague
▪ External membership in the Chair of Phys. and Macromol. Chem., Fac. Science, Charles Univ.
▪ Branch Council for Physical Chemistry in the Ph.D. study program "Physical and Macromolecular Chemistry" (Fac. Science, Charles Univ.)
▪ Branch Council for Physical Chemistry in the Ph.D. study program "Physical Chemistry" (Fac. Chem. Engng, Institute of Chem. Technol. Prague)

▪ Branch Council for Physical Chemistry in the Ph.D. study program "Application of Science" (Fac. Nuclear and Phys. Engng, Czech Technical Univ.) |
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- P. Jungwirth
- Branch Council for Biophysics, Chemical and Macromolecular Physics in the Ph.D. study program "Physics" (Fac. Mathem. and Phys., Charles Univ.)
 - Examining Board for awarding Ph.D. degrees in mathematical and computational modelling (Fac. Mathem. and Phys., Charles Univ.)

DEPARTMENT OF CATALYSIS

- J. Čejka
- Branch Council for Organic Technology in the Ph.D. study program "Chemistry and Chemical Technology" (Institute of Chem. Technol. Prague)
- M. Kočířík
- Scientific Council of Fac. Science, Univ. Ostrava
- K. Mach
- Branch Council for Inorganic Chemistry in the Ph.D. study program "Inorganic Chemistry" (Fac. Science, Charles Univ.)
 - Branch Council for Inorganic Chemistry in the Ph.D. study program "Inorganic Chemistry" (Fac. Chem. Technol., Univ. Pardubice)

DEPARTMENT OF ELECTROCHEMISTRY

- L. Kavan
- Branch Council for Inorganic Chemistry in the Ph.D. study program "Inorganic Chemistry" (Fac. Science, Charles Univ.)
- J. Ludvík
- Examining Board for state finals (Fac. Chem. Engng, Institute of Chem. Technol. Prague)
- V. Mareček
- Scientific Council of Fac. Science, Charles Univ.
 - Branch Council for Ph.D. studies in inorganic technology (Fac. Chem. Technol., Institute of Chem. Technol. Prague)
 - Branch Council for Ph.D. studies in analytical chemistry (Fac. Chem. Engng, Institute of Chem. Technol. Prague)
 - Examining Board for state finals in physical and analytical chemistry (Fac. Science, Charles Univ.)
 - Appointment Advisory Committee (Fac. Science, Charles Univ.)
- L. Novotný
- Examining Board for state finals in analytical chemistry (Fac. Chem. Technol., Univ. Pardubice)
- L. Pospíšil
- Scientific Council of Fac. Environ. Protection, Institute of Chem. Technol. Prague
 - Appointment Advisory Committee (Fac. Science, Charles Univ.)
- Z. Samec
- Scientific Council of Fac. Chem. Technol., Institute of Chemical Technol. Prague
 - Branch Council for Ph.D. studies in analytical chemistry (Fac. Science, Charles Univ.)
 - Examining Board for state finals in physical chemistry (Fac. Science, Charles Univ.)

8. OTHER ACTIVITIES

8.1. Membership in Editorial or Advisory Boards of Scientific Periodicals

P. Čásky	Theor. Chim. Acta Int. J. Mol. Sci. Collect. Czech. Chem. Commun.
J. Čejka	Collect. Czech. Chem. Commun.
V. Hanuš	Europ. Mass Spectrom.
Z. Herman	Chem. Soc. Rev. Vesmír
P. Hobza	Chem. Rev. Chem. Europ. J. Phys. Chem. Chem. Phys.
M. Hof	J. Fluoresc.
P. Janda	Collect. Czech. Chem. Commun.
L. Kavan	Carbon
K. Mach	Organometallics
K. Míka	J. Power Sources
J. Pittner	Collect. Czech. Chem. Commun.
L. Pospíšil	Collect. Czech. Chem. Commun.
Z. Samec	Electrochim. Acta
V. Špirko	J. Mol. Spectrosc. Chemtracts – Inorganic Chemistry
J. Šponer	J. Biomol. Struct. Dynamics
A. Vlček	Inorg. Chim. Acta Chemtracts – Inorg. Chem. Coord. Chem. Rev.
J. Volke	Chem. Listy

- B. Wichterlová Catal. Rev.
Microporous Mesoporous Mater.
Res. Chem. Intermed.
- R. Zahradník Adv. Quantum Chem.
Int. J. Quantum Chem.
Chem. Listy
Collect. Czech. Chem. Commun.

8.2. Officials and Elected Members of Scientific Organizations and Bodies (except universities - cf. Sect. 7.5.)

DEPARTMENT OF CHEMICAL PHYSICS

- Z. Bastl
- *J.M. Marci Spectroscopical Society* – member of the Committee and chairman of the Photoelectron Spectroscopy Section
 - *The Surface Analysis Society of Japan* – member
- P. Čárský
- *International Academy of Quantum Molecular Sciences* – member
 - *WATOC (World Association of Theoretical Organic Chemists)* – member of the Scientific Council
 - *Learned Society of CR* – member
 - *Czech Chemical Society* – member of the General Committee
 - *Ministry of Education of Slovak Republic, Commission for awarding DrSc. degrees in physical chemistry* – member
 - *American Chemical Society* - member
 - *American Institute of Physics* - member
- V. Hanuš
- *Learned Society of CR* – member
 - *European Academy of Sciences and Arts (Salzburg)* – member
- Z. Herman
- *Academy of Sciences of CR* – member of the Scientific Council
 - *MOLEC (International Conference on Molecular Collisions)* – member of the Steering Committee
 - *Czech National Committee for Chemistry* – member
 - *Czech Chemical Society* – member of the General Committee, chairman of the Group for Chemical Physics
 - *Ministry of Education, Youth and Sports of CR, Advisory Board for funding research and development in natural sciences* – member

- M. Hof
- *Society of Fluorescence* – national representative and member of the Permanent Steering Committee of the Conference “Series on Methods and Applications of Fluorescence: Spectroscopy, Imaging & Probes“
 - *International Scientific Advisory Board of the Academic Center for Biotechnology of Lipid Aggregates in Wroclaw* – member
- J. Hrušák
- *Academic Council of ASCR* – member
- Z. Knor
- *Ministry of Education, Youth and Sports of CR, Commission for awarding DrSc. degrees in physical chemistry and chemical physics* – member
 - *American Chemical Society* – member
- P. Kubát
- *Czech Society for Photobiology and Photodynamical Therapy* – member of the Committee
- P. Pracna
- *J.M. Marci Spectroscopical Society* – auditor
- Š. Urban
- *J.M. Marci Spectroscopical Society* – member of the Committee and chairman of the Molecular Spectroscopy Section
 - *Czech Committee for Collaboration with IIASA (Intern. Committee for Applied System Analysis) at the AS CR* – chairman
 - *IIASA* – member of the Council (chairman of the Membership Committee, member of the Executive Committee and the Program Committee)
- R. Zahradník
- *Academy of Sciences of CR* – honorary president
 - *Learned Society of CR* – member
 - *International Academy of Quantum Molecular Sciences* – member
 - *European Academy of Arts, Science and Literature (Paris)* – member
 - *European Academy of Sciences and Arts (Salzburg)* – member
 - *Academia Europaea (London)* – member
 - *European Academy for Environmental Affairs* – member
 - *WATOC (World Association of Theoretical Organic Chemists)* – fellow
 - *Swiss Chemical Society* – honorary member
 - *Society of German Chemists* – honorary member
 - *Croatian Academy of Sciences* – corresponding member
 - *Carolinum (Societas alumnorum et amicorum Universitatis Carolinae)* – honorary member

DEPARTMENT OF COMPLEX MOLECULAR SYSTEMS

- P. Hobza
- *Learned Society of CR* – member of the Committee
 - *European Academy of Arts, Sciences and Humanities (Paris)* – member
 - *Institute of Organic Chemistry and Biochemistry AS CR* – member of the Scientific Council
 - *Commission for Life Sciences at the Government Board for Research and Development* – vice-chairman
 - *Working group of the Accreditation Commission of CR* – member

DEPARTMENT OF CATALYSIS

- J. Čejka
- *Federation of European Zeolite Associations (FEZA)* – member of the Committee
 - *Czech Chemical Society, Group for Catalysis* – member of the Committee
 - *Czech Chemical Society, Czech Zeolite Group* – chairman
- M. Kočířik
- *IUPAC Commission on Colloid and Surface Chemistry including Catalysis* – national representative
- K. Mach
- *Royal Society of Chemistry (London)* – fellow
- Z. Sobalík
- *Czech Chemical Society, Group for Catalysis* – vice-chairman
 - *European Federation of Catalysis Societies (EFCATS)* – member of the Board for CR
- B. Wichterlová
- *European Federation of Catalytic Societies (EFCATS)* – member of the Committee
 - *International Association of Catalysis Societies* – member of the Committee
 - *Grant Agency of CR, Branch Council for Natural Sciences* – member; *Sub-council for chemistry and biochemistry* – head
 - *Czech Chemical Society, Czech Zeolite Group* – member of the Committee

DEPARTMENT OF ELECTROCHEMISTRY

- L. Kavan
- *Grant Agency of CR, Scientific Committee 203* - member
 - *Institute of Rock Structure and Mechanics AS CR* – member of the Scientific Council
 - *Czech Chemical Society, Group for Electrochemistry* – member of the Committee
 - *Czech Society for Carbon Materials* - member of the Committee
 - *COST- D14* – member of the management Committee
 - *International Society of Electrochemistry* – member
 - *The Electrochemical Society (USA)* – member
- J. Ludvík
- *Czech Chemical Society, Group for Electrochemistry* – member of the Committee
 - *The Electrochemical Society (USA)* – member
- J. Langmaier
- *The Electrochemical Society (USA)* – member
- V. Mareček
- *Grant Agency of the Academy of Sciences* – vice-chairman
 - *Ministry of Education of Slovak Republic, Commission for awarding DrSc. degrees in inorganic technology and materials* – member
 - *The Electrochemical Society (USA)* – member
 - *International Society of Electrochemistry* – member
- L. Novotný
- *Czech National Committee of IWSA (International Water Services Association)* – member
- L. Pospíšil
- *COST - D15* – member of the Management Committee
 - *ESF Unit for Physical & Engineering Sciences* – expert referee for ESF Eurocores Programme in Self-Organized Nanostructures
- Z. Samec
- *Grant Agency of CR, Branch Council for Chemical Sciences* – member
 - *Czech Committee for Chemistry* – member
 - *IUPAC Fellow*
 - *International Society of Electrochemistry* – member
 - *The Electrochemical Society (USA)* – member
- A. Vlček
- *European Photochemistry Association* - member of the Executive Committee, member of the Standing Committee
 - *Royal Society of Chemistry* – fellow
 - *COST Action D14 “Functional Molecular Materials”* – vice-chairman of the Management Committee
 - *COST Project D14 “Organometallic and Metallo-organic Building Blocks for Photonic Materials”* – coordinator

8.3. Appointments, Conferments

Š. Urban

Appointment to Professor of Analytical Chemistry at the Institute of Chemical Technology, Prague

J. Čejka

Conferment of DrSc. degree by the Slovak Academy of Sciences

8.4. Awarded Prizes and Honors

RNDr. Oto Bludský, CSc.

Otto Wichterle Prize

Prof. RNDr. Zdeněk Herman, DrSc.

National Prize "Česká hlava 2003"

Ing. Gabriela Košová

Honourable mention of the Group for Catalysis of the Czech Chemical Society

Dr.rer.nat. Jiří Pittner

Otto Wichterle Prize

Ing. Pavla Prokešová

Prize of the Group for Catalysis of the Czech Chemical Society

Mgr. Jana Roithová, PhD.

Prize for the 2nd place in the 2003 competition of doctoral dissertations in chemistry in ČR, awarded by the French Embassy and the Company Rhodia

Prof. Ing. Rudolf Zahradník, DrSc.

Title „Chevalier dans l'Ordre des Palmes Académiques“ awarded by Prime Minister of France for services to the French culture

APPENDIX I

MAJOR INSTRUMENTATION AVAILABLE

Computer Facilities and Network

- 4-processor Alpha/Compaq ES40/667MHz/8GB RAM server (64-bit processor)
- cluster of Intel/Itanium 1 64-bit processors (6x) running under Linux OS
- cluster of 90 Pentium II/440 MHz and Pentium III/800 MHz processors running under Linux OS
- cluster of Hewlett-Packard workstations HP-785 (1x), HP-J280 (2x), HP-J200 (2x)
- cluster of Silicon Graphics workstations SGI/R8000 Power Indigo2, SGI/R4600 (2x) and SGI/R4400
- cluster of 44 Athlon 1800 MHz processors running under Linux OS
- Dell workstation 330, 1024 MB (2x)
- access to the Computational Center of the Academy of Sciences (SGI Power Challenge RACK 6xR8000) and other computational facilities equipped with SGI Power Challenge computers, NEC SX-4, DEC Alpha and others
- Ethernet 100 Mbit/s LAN, Novell NetWare 4.10 server
- direct connection to the campus network and to the Internet (ATM Metropolitan Network, TEN-34)

Instrumental Equipments

Spectroscopic laboratories

- infrared laser diode spectrometer (Aero Lasers, partly in-house construction)
- matrix isolation spectroscopy in IR and UV, Vis (Leybold)
- Lambda Physik LPX 205, COMPEX 102 and FL 3002 Dye Lasers
- laser kinetic spectrometer (Applied Photophysics)
- fluorescence correlation spectrometer ConfoCor (Carl Zeiss)
- emission/excitation spectrophotometer Fluorolog 3 (Jobin Yvon, France)
- fluorescence life-time system (IBNM Consultants, UK)
- system for synthesis of phospholipid membranes (Novodirect, Germany)
- UV-Vis absorption photospectrometer Helios (Unicam, France)

Reaction dynamics and organic mass spectrometry laboratories

- two special crossed-beam scattering machines of in-house construction: EVA for studies of ion-molecule processes and ion-surface interaction, GOLEM for studies of collisions of multiply-charged ions
- a selected-ion-flow-tube (SIFT) apparatus for studies of kinetics of ion-molecule reactions at thermal energies
- hybrid tandem mass spectrometer ZAB2-SEQ (Micromass, UK)
- high resolution double-focusing mass spectrometer VG 7070E

Surface science laboratories

- ESCA 310 high resolution electron spectrometer (Gammadata Scienta, Sweden)
- ESCA 3 Mk II and UVG electron spectrometers (VG Scientific, UK)
- SIMS spectrometer VT 250 (Tesla Vacuum Techniques, Czechoslovakia)
- UHV field ion and field emission microscopes with CCD camera for on-line image analysis
- UHV apparatus for thermal desorption with quadrupole mass spectrometer

Catalysis laboratories

- gas chromatographs with GC-FID, TCD, MSD (HP 5890, HP 6890, HP 5971A, HP 6850, Finnigan 9001)
- FTIR spectrometers Nicolet MX1, Nicolet Protégé 460, Nicolet Magna 550 with high temperature cells and MS gas analysis, Nicolet Avatar 320 with diffuse reflectance accessory
- FT-IR spectrometer Nexus 670 with in-situ high temperature cell
- UV-Vis-NIR spectrometer Perkin Elmer Lambda 19 with reflectance attachment and Harrick high temperature cell
- quadrupole mass spectrometers (QMA 125, QMG 421C, QMG 420)
- ESR spectrometer (ERS-220 DAW)
- XRD (Siemens D 5005)
- AMI-200 catalyst characterization system (Raczek Analysentechnik, Germany)
- NO/NO_x chemoluminescence analyzers (VAMET, CR)
- Advance Optima analytical system for N₂O (Hartmann & Brown, Germany)
- high-low pressure IR reactor (In-Situ Research Instruments, USA)
- scanning electron microscope Jeol JSM-03
- Accusorb Micromeritics sorptometer
- adsorption apparatus ASAP 2010 (Micromeritics, USA)
- high speed water sorption apparatus Hydrosorb 1000 (Quantochrom, USA)
- surface area and porosity analyzer (SY-LAB, Austria)
- super critical point dryer (Tousimis, USA)
- SCD 050 sputterset (BAL-TEC, Liechtenstein)
- dry box

Electrochemistry laboratories

- impedance systems: 2x FRA Solartron 1255 + EI 1287, 2x FRA Solartron 1250 + EI 1286
- potentiostat/galvanostats: 1x EG&G PAR 273A, 4x EG&G PAR 263A, 2x Eco Chemie AUTOLAB 30, 1x POS 2 Bank Elektronik
- signal and spectrum analyzers: 1x HP 35665A, 2x SRI SR 780, 1x Tektronix 495 P, 1x RF analyzer 1.3 GHz Agilent Technologies
- fluorescence detector HP-1000
- electrochemical quartz crystal microbalance PAS 5510, Poland
- HPLC chromatograph Merck-Hitachi (L4250 + L6200A + D2500)
- FTIR spectrometers: 1x Nicolet Impact 410, 1x Philips PU9800
- UV-Vis spectrometers: 1x HP 8452A, 1x HP 8453, 1x Ocean Optics
- scanning tunneling microscopes: Topometrix TMX 2010, NanoScope III Multimode, Digital Instruments
- PC-controlled Eco-Tribo Polarograph, Polaro Sensors, CR
- carbon analyzer TOC-V WS (Shimadzu)
- coulometric titrator (Metrohm)
- dry box Labstar 50

APPENDIX II

A BRIEF HISTORY OF THE INSTITUTE

The present Institute was established in 1972 through the merger of the Institute of Physical Chemistry and the Institute of Polarography, both of them parts of the Czechoslovak Academy of Sciences.

The **Institute of Polarography** was founded in 1950 under the directorship of **Professor Jaroslav Heyrovský**, and two years later became part of the newly constituted Czechoslovak Academy of Sciences. Research activities focused both on the theory of polarography and physico-chemical processes occurring at dropping and streaming mercury electrodes, and on the methodology, instrumentation and analytical applications of polarography.

The award of the 1959 Nobel Prize for Chemistry to Professor Heyrovský for the invention and development of polarography represented an important stimulus for the Institute and encouragement for the whole scientific community in the country.

The early sixties marked the start of a gradual extension of pursued research topics from polarography to other disciplines of general and applied electrochemistry, including different methods of electroanalysis, electrochemical power sources, and electrochemical processes at interfaces between immiscible electrolyte solutions with relevance to biological membranes.

When Professor Heyrovský retired, his former student Dr. Antonín A. Vlček who was engaged in electrochemical studies of inorganic coordination compounds, took over the position of director of the Institute in 1965.

The **Institute of Physical Chemistry**, with **Professor Rudolf Brdička** as director was established in 1955 by expanding the Laboratory of Physical Chemistry founded in 1953 within the framework of the forming Czechoslovak Academy of Sciences. As most of the first members of the Laboratory and of the Institute were awarded their degrees for research work in polarography, polarographic topics took precedence for some time in their work. In particular were pursued exact solution of mass transport to the dropping mercury electrode combined with chemical volume reactions accompanying the electron transfer process. However, the research program of the Institute gradually shifted to other disciplines such as mass spectrometry, dynamics of elementary collisions of ions and excited atoms with molecules, theory of the chemical bond, quantum chemistry, adsorption and heterogeneous catalysis, polymer science and organometallic chemistry, aerosol science, thermodynamics and kinetics of chemical reactions, molecular spectroscopy, and electron spectroscopy.

A difficult situation occurred after the invasion of the country by Warsaw Pact armies in 1968, when many members of the Institute, including several leading personalities emigrated to the West. After a transition period following the untimely death of Professor Brdička in 1970, the Institute was in 1972 amalgamated with the Institute of Polarography under the name **J. Heyrovský Institute of Physical Chemistry and Electrochemistry**, with Professor A. Vlček as director.

In 1988 the Institute moved to a new building constructed on the Academy Campus in Prague 8. This event represented a radical improvement of working conditions and was crucial for the further development of the Institute.

The profound political changes in the country in the years 1989/1990 started a new era of the Academy. The Institute gained a large measure of autonomy and its structure and management were extensively reformed. In 1990 the Scientific Council of the Institute elected Dr. Rudolf Zahradník, a theoretical and quantum chemist, as director. In order to overcome the consequences of central planning in scientific work and to increase the efficiency of the Institute, its staff was reduced almost by half, and research in some fields was even terminated. Grant system of funding research projects was introduced. Abolition of restrictions imposed on contacts with the scientific community abroad opened the way to a wide international cooperation and integration of the Institute into a number of research networks. Also a rapid and extensive modernization and improvement of the experimental equipment and computer facilities started.

Because of his election as President of the Academy of Sciences of the Czech Republic in 1993, Professor Zahradník resigned from the position of director of the Institute and Dr. Vladimír Mareček, an electrochemist specializing in processes at interfaces of immiscible solutions, was elected his successor for a 4-year term. The name of the Institute was shortened to **J. Heyrovský Institute of Physical Chemistry**. In 1997, Dr. Mareček was re-elected director of the Institute for the next term. When he stepped down from this position effective December 31, 2000 due to personal reasons, Dr. Petr Čársky, a quantum and theoretical chemist, was elected to director for the next four years.



Professor J. Heyrovský (right) and professor R. Brdička, directors of the two parent institutes (1952)