

SIXTY YEARS OF THE J. HEYROVSKÝ INSTITUTE OF PHYSICAL CHEMISTRY, ACADEMY OF SCIENCES OF THE CZECH REPUBLIC, PRAGUE (1953–2013)

ZDENEK HERMAN a SLAVOJ ČERNÝ

J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Dolejškova 3, 182 23 Prague 8

Introduction

The present J. Heyrovský Institute of Physical Chemistry was founded with the formation of the Czechoslovak Academy of Sciences in 1952 as the Laboratory of Physical Chemistry. It started to operate on 1st January, 1953. Its first Director was Professor Rudolf Brdička (1906–1970), a member of the Academy and professor at Charles University. The Laboratory grew rapidly; in 1955 it became the Institute of Physical Chemistry. The original locations of the Institute were rooms at the Chemical Institute of Charles University, at its Albertov center. In 1957 the Institute moved to a former state office building on Máchova Street in Vinohrady. After the death of Professor Brdička, the Institute merged with the Institute of Polarography of the Academy of Science in 1972. The J. Heyrovský Institute of Physical Chemistry and Electrochemistry was formed, with Professor Antonin A. Vlček (1927–1999) as Director. At that time the Institute consisted of laboratories of different sizes scattered all over Prague. The main center of the former Institute of Physical Chemistry was in Máchova Street with about 100 researchers. Smaller groups, such as molecular spectroscopy, aerosols and quantum chemistry, were located elsewhere. The main center of the former Institute of Polarography, and the Director's Office, were on Vlašská Street, with smaller units on Opletalova Street and in Hostivař. In 1988, the Institute was consolidated in a new building at the Academy Center in Kobylisy (Prague 8, Dolejškova 3); at that time the Institute had about 240 employees. On 1st January 1993, with the dissolution of Czechoslovakia and the Czechoslovak Academy of Sciences, the Institute became part of the Academy of Sciences of the Czech Republic; its name thereafter shortened to J. Heyrovský Institute of Physical Chemistry. Its directors were subsequently Rudolf Zahradník, Vladimír Mareček, Petr Čárský and the present Director Zdeněk Samec. Today the Institute has about 165 employees, 115 of whom are scientists.

Beginnings

The doctoral students of Professor Jaroslav Heyrovský and Professor Rudolf Brdička, mainly physical



Fig. 1. Professor Rudolf Brdička, the first Director of the Institute

chemists from the polarographic school of Professor Heyrovsky, were responsible for the main research at the original Laboratory.

However, the Laboratory's main task was to develop new areas of physical chemistry: Vladimír Čermák, Vladimír Hanuš, Čestmír Jech, and Josef Cabicar started construction of a mass spectrometer; Ivo Kössler and Bohumír Matyska applied infrared spectroscopy to studies of polymers, including their synthesis; Otto Grubner and Miloš Rálek studied separation processes and the development of gas chromatography; Jaroslav Koutecký laid the foundations of the theoretical department with his work on the quantum theory of surface states. Vladislav Daneš came from the Institute of Chemical Technology to start a research group in heterogeneous catalysis. Research in polarography continued, too. The award of a 1954 State Prize to Professor Brdička and Jaroslav Koutecký (for theoretical studies in polarography) added to the good reputation of the young Institute. A second 1954 State Prize was awarded to the same team for construction of the first mass spectrometer in the country.

Máchova Street (1957–72)

At the end of 1957 the Institute moved from its location at Albertov to more spacious accommodation on Máchova Street, where it shared one floor with several departments of the Academy's Institute of Physics, and hosted its library. The Institute was then about 80 strong, with a small administration group, glassblowers, and a very effective mechanical workshop.

Conditions for research and contact with foreign scientific institutions were rather modest in the fifties. Instrument purchase from abroad was all but impossible: all necessary mechanical, vacuum, and electronic equipment had to be made in-house. The supply of journals to the library was limited. Foreign travel and conference participation was restricted. Meetings with foreign scientists were largely limited to international conferences held in Czechoslovakia.

The Institute was organized into departments by line of research. In 1958 the prominent chemical thermodynamics group of Eduard Hála, Emerich Erdős and collaborators from the Institute of Chemical Technology, joined the Institute; later on in 1964 they moved to the Academy's Institute of Chemical Process Fundamentals. The period 1958–59 led to a considerable strengthening of research in heterogeneous catalysis, when several research teams of younger scientists were formed (involving Pavel Jirů, Kamil Klier, Vladimír Ponec and Zlatko Knor). Work on mechanisms and kinetics of catalytic reactions laid the foundations for the



Fig. 2. The building in 7, Máchova Street

experimental investigation of catalyst structure, surface centers, and interacting surface complexes. Rudolf Zahradník established a theoretical research group in quantum chemistry and its applications mainly to organic chemistry. Květoslav Spurný joined with his group working on the physics and chemistry of aerosols and their practical applications. In 1963 the department of infrared spectroscopy led by Josef Pliva joined from the Institute of Organic Chemistry and Biochemistry: this constituted a considerable broadening of the Institute's research program, especially the construction of a large classical high-resolution infrared spectrometer (led by Rostislav Sovička).

Research in the sixties led to a series of significant results: the work of Jaroslav Koutecký and Mojmir Tomášek in the quantum theory of surface phenomena on metals and semiconductors¹, and the spectroscopy of polycyclic hydrocarbons by Josef Paldus, Rudolf Zahradník and Petr Hochman². Jiří Čížek developed the method of coupled clusters³, currently one of the basic methods in calculation of molecular properties in quantum chemistry. Vladimír Hanuš gained international recognition in organic mass spectrometry for his work on rearrangement of organic cations⁴. Investigation of collision processes of ions and electronically excited neutrals by the mass spectrometric method (by Vladimír Čermák and Zdeněk Herman) led to fundamental information on the kinetics of chemical reactions of ions and ionization reactions of neutrals⁵. Theoretical studies of the highest quality by Pliva's department addressed the fine structure of infrared spectra for small polyatomic molecules⁶. In heterogeneous catalysis, work on chemisorption on clean metal surfaces (by Vladimír Ponec and Zlatko Knor⁷), the mechanism of selective catalytic oxidation reactions, and oxygen bond strength in metal oxides (by Kamil Klier^{8,9}, Pavel Jirů and Jana Nováková^{8,10}) achieved international recognition. Otto Grubner, Miloš Rálek, Kamil Klier and Pavel Jirů started their novel investigation into the structure and sorption properties of zeolites¹¹. New science benefitted significantly from the support of the Institute's technical groups. The electronics group of Miroslav Pacák and Ladislav Hládek played an important role in apparatus construction, by developing tailor-made devices, as did the high-quality glassblower service of Alexander Černý and Josef Šaněk, and the excellent work by Josef Protiva and colleagues at the mechanical workshop.

The sixties heralded a somewhat improved political climate. Visits to western universities and research institutions were more prevalent, as was participation in conferences abroad – although arranging these usually involved difficult and lengthy administrative procedures; many applications were rejected by state authorities.

The unique atmosphere of the Institute in the sixties is noteworthy. The environment of enthusiasm, tolerance, cooperation and critical respect of others' work was due in large part to the exceptional personality of Professor Brdička. His authority isolated the Institute from external

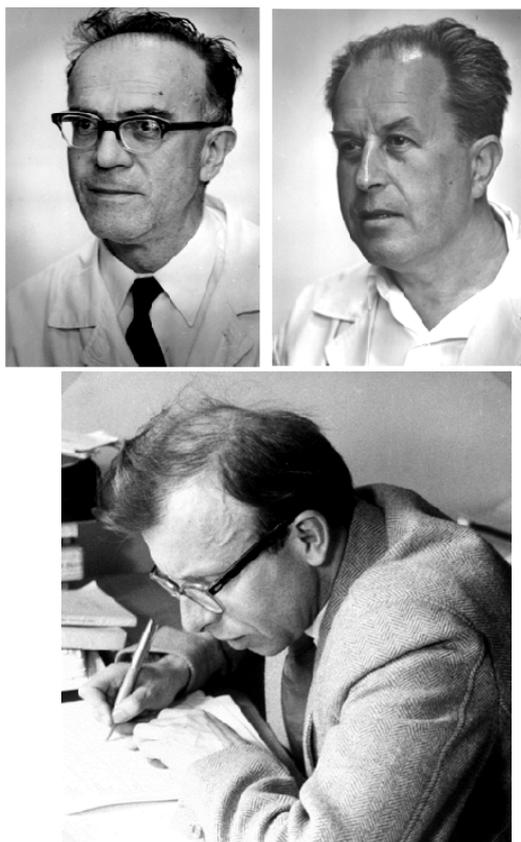


Fig. 3. Vladimír Hanuš (1923–2007), Scientific Secretary 1953–1963, then Deputy Director of the Institute; Vladimír Čermák (1920–1980); Jaroslav Koutecký (1922–2005)

political influence to a certain extent. The founding members of the Institute, educated by Professors Heyrovský and Brdička, contributed by stressing a tradition of concentrated, dedicated and honest research. This atmosphere was generally appreciated by staff, and presumably contributed to low rate of staff departure from the Institute up until 1968. The Institute's scientists met weekly on Saturdays to discuss progress and future research. Professor Brdička was in constant contact with the researchers, visiting laboratories and discussing progress. During the sixties the Institute organized the annual Symposium on Heterogeneous Catalysis (together with the Institute of Chemical Process Fundamentals) at Liblice castle. Until the eighties the annual Joint Czech-Polish Symposium on Catalysis was held alternately in each country. Since 1969 the Institute organized an annual meeting at Bechyně castle, where researchers reported recent progress and future plans; after merging with the Institute of Polarography in 1972, these meetings continued at Liblice. The Institute's relatively young staff enjoyed a rather lively social life: a long tradition of joint events with the sister Institute of Polarography, which

included a football match, continued.

The political events of 1968 influenced the Institute deeply. Many key staff emigrated, or stayed abroad. The theoretical department effectively fell apart: the Institute lost Jaroslav Koutecký, Josef Paldus, Jiří Čížek, Petr Hochman, Josef Pliva, Zdeněk Cihla, František Jenč, Josef Michl and Cyril Párkányi. The catalysis department lost Otto Grubner, Miloš Rálek, Vladimír Ponec, Kamil Klier and Milan Štolka. The aerosols group lost Květoslav Spurný and Gustav Kubie. The Institute was further weakened when Professor Brdička died of a heart attack in June 1970. Deputy Director Vladimír Hanuš directed the Institute until 1972, when it merged with the Institute of Polarography and continued as the J. Heyrovský Institute of Physical Chemistry and Electrochemistry. Antonín A. Vlček, Director of the Institute of Polarography since 1965, became Director.

After 1969 the Institute was under heavier pressure from the Communist Party organization. The newly appointed Presidium of the Academy decided that all employees abroad were required to repatriate before the end of 1969, or be regarded as emigrants. For some time no scientific titles were awarded, and many politically motivated changes in personal assignments and Academy structure were imposed.

The J. Heyrovský Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences (1972–1989)

Political vetting in 1972 led to removal of key scientists including Vladimír Čermák and Rudolf Zahradník from leading positions and to substantial organizational changes in the joint Institute under Antonín A. Vlček's directorship. His deputies, Robert Kalvoda and Dušan Papoušek, were party members. The scientific secretary was Bohumír Matyska. The Institute's scientific staff were organized in three divisions: chemical physics (Head Mojmir Tomášek, deputy Jan Vojtík), electrochemistry (Head Jiří Říha, deputy Zdeněk Zábanský) and heterogeneous processes (Head Ondřej Kadlec, deputy Arnošt Zukal). Each division consisted of departments.

The new enlarged Institute was even more scattered across Prague. An internal newsletter (Kurýr) was established to keep staff informed regarding seminars, lectures, Director's decisions and other administrative announcements. Scientists met annually, as mentioned before, at a two-day conference.

The Institute did rather well scientifically, despite reductions in foreign contacts from previous years due to travel restrictions. Many colleagues from abroad, using existing contracts between the Academy and foreign institutions, visited Prague for extended stays to work on the Institute's specialized equipment. This facilitated continued collaborations with Western Europe and the



Fig. 4. Antonín A. Vlček (1927–1999), Director of the Institute 1972–1990

United States. The Institute's electrochemical division maintained successful Heyrovský Discussions with strong international participation. The conference on quantum chemistry, first organized by Rudolf Zahradník in 1972 and revived in 1979 under Jan Vojtik grew from former Microsymposia on Quantum Chemistry to become the International Symposium on Elementary Processes and Chemical Reactivity. The International Conference on High-Resolution Infrared Spectroscopy regularly attracted scientists from abroad.

Apparatus also improved gradually. A commercial electron spectrometer ESCA (electron spectroscopy for chemical analysis) was purchased from VG for heterogeneous catalysis research. A new double-focusing mass spectrometer with a computer (JMS-D100 of JEOL, Japan) was acquired for Vladimír Hanuš in organic mass spectrometry.

More importantly, in-house construction of specialized equipment enabled unique experiments to be devised and conducted in Prague, attracting the attention and promoting visits from scientists based outside Czechoslovakia. From previous studies of ionization reactions of excited neutrals, Vladimír Čermák developed Penning ionization electron spectroscopy (PIES) which, by accurate measurement of the energy of the electron released in the ionization process, enabled the internal states of particles and their interactions¹² to be investigated. Čermák continued these studies until his untimely death in 1980. Zlatko Knor constructed an autoemission electron and ion projector and used it successfully – at single atom level – in studies of chemisorption and catalytic phenomena on metal surfaces¹³. Slavoj Černý introduced adsorption microcalorimetry on vacuum-evaporated metal films¹⁴. The development of an instrument incorporating crossed beams of ions and molecules made it possible to study the dynamics of ion-molecule collisions by the scattering method (Zdeněk Herman¹⁵); new experimental

information on the mechanisms of elementary chemical reactions, necessary also for parallel theoretic studies, was obtained.

Theoretical research suffered due to the paucity of local computing resources. Any computational progress depended largely on the unselfish help of foreign colleagues who made it possible to carry out calculations at their home institutions. Important theoretical work included semi-empirical calculations of radicals (by Rudolf Zahradník and Petr Čásky¹⁶), followed by investigation of weak interactions (Rudolf Zahradník and Pavel Hobza¹⁷). The latter opened a broad field of theoretical studies into clusters and later biomolecules. Other studies concerned development of methods for calculation of potential

hypersurfaces related to the investigation of elementary reactions (Rudolf Polák¹⁸) and calculations on Penning ionization in connection with Vladimír Čermák's work¹⁹. Surface state calculations were performed by Mojmir Tomášek and Štěpán Pick. Fine structure calculations for small polyatomic molecules continued in the work of Dušan Papoušek, Vladimír Špirko, Štěpán Urban and Petr Pracna²⁰.

In electrochemistry, Antonín A. Vlček's work in the Department of redox processes investigated relations between the structure of inorganic complexes and coordination compounds and their electrochemical behavior²¹. Electrocatalytic studies addressed

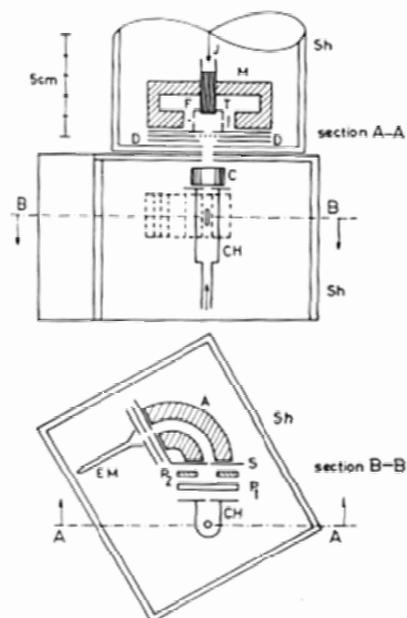


Fig. 5. V. Čermák's electron spectrometer for PIES studies¹⁰. Upper: excited particles source with molecular beam and deflection analyzer of released electrons with crossed molecular beam of investigated molecules (perpendicularly to the figure plane). Lower: 127° deflection electron analyzer viewed perpendicularly

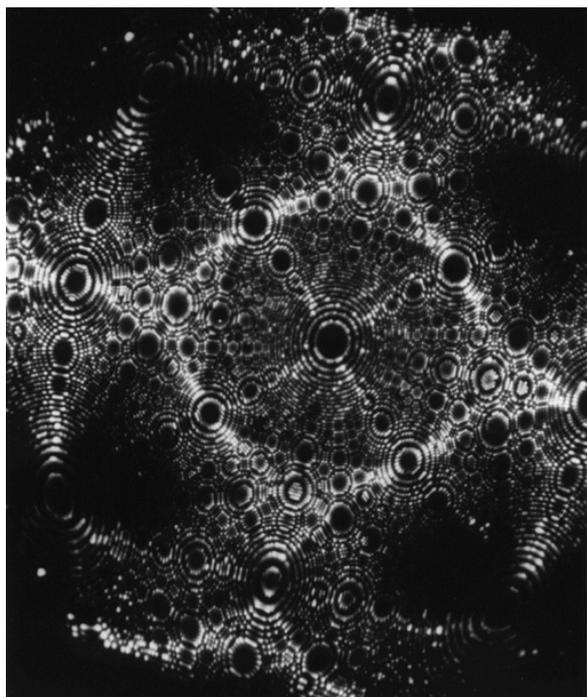


Fig. 6. Ion autoemission projector of Z. Knor (FIM)¹³: the Pt tip at 20 K

carbonylation of methane, conversion of nitrogen to ammonia and its dependence on ambient temperature and pressure. The kinetics of redox processes, adsorption and corrosion inhibition were studied by Jaroslav Kůta and collaborators²², theory of adsorption processes and ion-selective electrodes by Jiří Koryta²³

The organic electrochemistry group continued research in electro-synthesis, electro-luminescence²⁴ and radical formation in electrochemical reactions. A new discipline, electrochemistry on the interface of two immiscible liquids, was developed by Jiří Koryta, Zdeněk Samec and Vladimír Mareček²⁵. First studies in bio-electrochemistry appeared²⁶. Michael Heyrovský investigated the influence of light on electrode processes²⁷. Important subjects of electrochemical research were electrochemical current sources and their relation to fuel cells and suitable catalysts (by Jiří Mrha and Jiří Jansta²⁸); the preparation of new plastic electrodes for storage batteries²⁹; and investigations of lithium cells³⁰. Applied studies were directed towards the development of automatic monitoring of sulphur dioxide for city stations (by Jiří A.V. Novák and Jiří Tenygl) and oxygen electrodes for bio-applications (Lubomír Šerák³¹). Automatic measurement of electrode impedance (Lubomír Pospíšil³²) created further possibilities for kinetic and adsorption studies.

Experimental instrumentation was also gradually developed in the division of heterogeneous processes. Alongside equipment for kinetics studies, a series of

spectroscopic methods was introduced (including infra-red, near infra-red, UV-visible, mass spectrometric, electron spin resonance and X-ray) to investigate catalysts and reaction intermediates^{33–35}, and transport characteristics of porous materials (Milan Kočířík³⁶). Studies by Pavel Jirů and collaborators (Blanka Wichtelová, Ludmila Kubelková and Jana Nováková) on acido-basic and redox catalytic properties of zeolites with proton centers³³ and doped with metal atoms or oxidic particles^{34,35} received international acknowledgement. Studies of homogeneous catalysts, in particular titanium complexes, and their use in polymerization reactions was

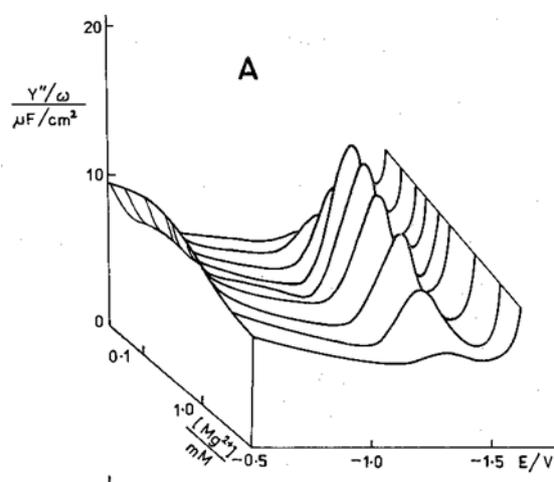


Fig. 7. An example of face-resolved polarography with alternating current. Optimization of composition of a catalyst based on Mo-Mg-methoxo-cluster (electrocatalytic conversion of nitrogen to ammonia at room temperature and pressure)

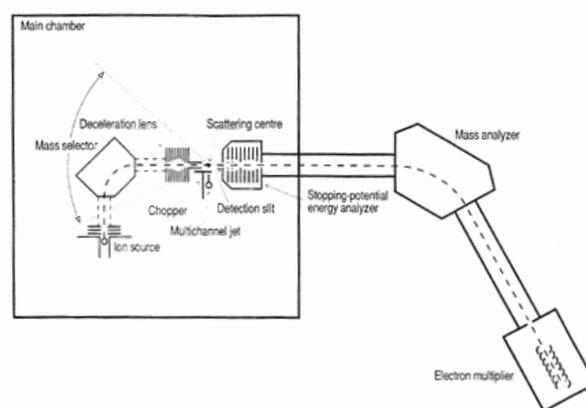


Fig. 8. Schematics of the apparatus for studies of the single-collision dynamics of ion processes based on the scattering in crossed beams (Z. Herman¹⁵)



Fig. 9. Prominent electrochemists of the Institute in the seventies and eighties: Jiří Koryta (1922–1994), Jaroslav Kůta (1924–1980), Jiří Volke (1926–2011), Jiří A.V. Novák (1913–2002)

conducted by Bohumír Matyska and Karel Mach³⁷. The group of Emerich Erdős studied equilibria in gas-solid phase systems and their practical applications. In April 1988 the Institute moved to a new building in Kobylišy, co-locating with the Institutes of Physics, of Plasma Physics, of Thermomechanics, of Information Theory and Automation, and of Informatics and Computing Techniques). Finally, the Institute was united under one roof. The Institute had at that time about 260 employees.

5. Post 1989

The political and social changes following 1989 again influenced both the Academy of Sciences and the Institute profoundly. After 18 years of directorship, Antonín A. Vlček resigned in 1990 and – after his return from abroad – Rudolf Zahradník was elected Director by the Science Council of the Institute. The science division of the Institute initially comprised 23 research teams each reporting directly to the Director. Later the earlier structure of three divisions was re-adopted (Chemical Physics, Electrochemistry, Heterogeneous Processes). The number of employees gradually reduced to about 150, but despite this research output was maintained. Many younger

colleagues took advantage of new opportunities to travel and stay longer abroad, some staying abroad permanently. Others accepted positions at Czech universities. Nevertheless the Institute continued to consolidate. Pavel Hobza returned to form a theoretical group investigating complex molecular systems and biomolecules. Computer simulations of different systems were developed, including: the structure and dynamics of DNA and other biologically relevant compounds³⁸; many-body water-salt systems (Pavel Jungwirth³⁹) and zeolites (Petr Nachgall⁴⁰). Vladimír Špirko⁴¹ studied the theory of elementary processes. In 2003 the group left for the Academy's Institute of Organic Chemistry and Biochemistry.

In 1992, with the division of Czechoslovakia, the Institute became part of the Academy of Sciences of the Czech Republic. In March 1993 Rudolf Zahradník relinquished the directorship to become President of the Academy of Sciences. Vladimír Mareček (1993–2001) was elected Director under new regulations restricting directorships to a maximum of two four-year terms. He was succeeded by Petr Čárský (2001–2009) and the present Director, Zdeněk Samec.

Securing Czech or foreign research grants became important in financing projects. In 1997 the Institute established its International Advisory Board consisting of respected foreign scientists to evaluate the quality and impact of the Institute's research, equipment and organization on a periodic basis. The Coordinating Scientist of this Board, Professor J.P. Toennies (Director of the Max-Planck Institute for Fluid Dynamics in Göttingen), concluded after careful comparison with institutes of the Max-Planck Society, that the Institute's productivity was comparable to that of a middle-ranking Max-Planck Institute.



Fig. 10. The new building of the Institute (Dolejškova 3, Prague 8) in the Academy Center Kobylišy (since 1988)



Fig. 11. Directors of the Institute after 1990: Rudolf Zahradník (1928), Vladimír Mareček (1944), Petr Čárský (1942), Zdeněk Samec (1947)

The Institute has organized important international conferences and been involved in European research programs for decades. Since 1991 the annual festive Brdička Lecture has been presented by an outstanding foreign scientist, including several Nobel Prize winners. The Institute has strived to apply research results in practice, for example through: licensing rights; the preparation and analysis of aerosols (Bedřich Binek) for the German firm Sartorius in the end of the sixties; and production of hydrogen generators (František Dousek). In the seventies and eighties the Institute had numerous contracts with different industrial organizations and institutions, in particular in heterogeneous and homogeneous catalysis. In 1991 it established Ecochem with a hydrogeologic and analytical firm. Cooperation with Polaro-Sensors in production of modern polarographic instrumentation was another example of these efforts.

The Institute continued its large scale educational role. About 30–40 graduate students, registered at their home universities, carry out their doctoral work in the Institute annually.

Another reorganization of the Institute took place in 2006, when developments of new research themes, in particular material and biochemical research, led to broadening the Institute's scope and the formation of new departments. The present Institute consists of the following

ten departments (with department heads in parentheses):

- Theoretical Chemistry (Jiří Pittner)
- Spectroscopy (Svatopluk Civiš)
- Ion and Cluster Chemistry (Patrik Španěl)
- Biophysical Chemistry (Martin Hof)
- Structure and Dynamics in Catalysis (Jiří Dědeček)
- Synthesis and Catalysis (Jiří Čejka)
- Electrochemical Materials (Ladislav Kavan)
- Biomimetic Electrochemistry (Zdeněk Samec)
- Molecular Electrochemistry (Magdaléna Hromadová)
- Low-dimensional Systems (Martin Kalbáč)

The Institute's activities are focused primarily on theoretical and experimental investigations of chemical and physico-chemical phenomena on the level of single atoms and molecules. This includes the structure and dynamics of substances and reaction mechanisms in the gaseous, liquid and solid phases and their interfaces. Topics of particular relevance include chemical catalysis and sorption, electrochemical and biological processes, including the preparation and characterization of new catalytic, sorption, electrode and other special materials.

The research interests of specific departments is as follows. In *the Department of Theoretical Chemistry*, research addresses: development of the multi-reference method of coupled clusters⁴²; development and application of methods to describe excited states with non-adiabatic transitions⁴³; computation of interaction between electrons and polyatomic molecules to describe electron scattering and vibrational excitation⁴⁴; quantum resonance modelling; and quantum chemical modelling of the properties and catalytic activity of zeolites⁴⁵. *The Department of Spectroscopy* deals with laser spectroscopy and high-resolution spectroscopy of radicals and ions⁴⁶ and their application in atmospheric and material research⁴⁷, and with the chemistry of high-power laser sparks^{48,49}. Investigations within *the Department of Ion and Cluster Chemistry* concern: kinetics of ion-molecule reactions by the SIFT (selected-ion-flow-tube) and its use in quantitative analysis of volatile compounds, in particular breath analysis for medical applications (Patrik Španěl⁵⁰); structure and dynamics of molecular clusters with respect to their characterization and reactivity, mainly in connection with the investigation of processes in the atmosphere (Michal Fárník^{51,52}); studies of radicals by CRD (cavity-ring-down) spectroscopy; and dynamics of ion-molecule reactions by a combination of special methods and mass spectrometry⁵³. *The Department of Biophysical Chemistry* has four research themes involving fluorescence spectroscopy, namely: atomic level membrane biophysics using fluorescence spectroscopy and theoretical simulation⁵⁴; development and application of fluorescence spectroscopy to cell biology⁵⁵; elucidation of the relationship between the dynamics and hydration of enzymes and their activity by means of fluorescence spectroscopy⁵⁶; and localization and clustering of membrane proteins using high-resolution fluorescence spectroscopy⁵⁷.

The Department of Structure and Dynamics in Catalysis deals with preparation, identification, characterization and dynamic behavior of nano-structured materials and their relation to catalytic activity. A suite of spectroscopic and kinetic methods, complemented by theoretical modelling, provides atomic- or molecular- level information regarding the structure of activity centers and their environment. This in turn aids characterization of activity and selectivity in redox and acido-basic reactions^{58–60}, especially in connection with the development of zeolite catalysts for selective oxidation of nitrogen^{61,62}. *The Department of Synthesis and Catalysis* works mainly on the synthesis of new zeolite, their two-dimensional analogues and hierarchic materials using a new synthetic mechanism^{63,64}. Materials so prepared are evaluated for adsorption of carbon dioxide, hydrogen, and organic substances, as well as in catalytic reactions relevant for petrochemical and other chemical processes. The chemistry of elements of the organometallic subgroups of the periodic table is also studied, as is preparation and characterization of metallocene complexes with cyclopentadienyl ligands, non-metallocene complexes of the chelate type, and chemistry of low-valence complexes. Catalytic reactions leading to transformation of unsaturated hydrocarbons by means of transition metal complexes, polymerization reactions, oligomerization of alkynes and relationships between the structure, physical and chemical properties of transition metals and their catalytic activity are also studied⁶⁵.

The Department of Electrochemical Materials deals with synthesis and characterization of nanocrystalline, supramolecular and composite materials suitable for electrochemistry, photo-electrochemistry, and photocatalysis, in particular with carbon materials such as nanotubes, fullerenes, nano-diamond and polyenes⁶⁶. More and more attention is given to studies of graphene⁶⁷. Electrode materials based on TiO₂ (ref.⁶⁸), ternary oxides and phosphates have also been studied. The aim is to develop systems for solar energy conversion, for production of solar fuels and for accumulation of electric energy in lithium- and sodium-ion batteries. The investigation in photo-catalysis is oriented to mechanisms of pollutant degradation, reaction on CO₂, and to practical questions of water and air purification. Research in *the Department of Biomimetic Electrochemistry* includes: polarization phenomena on the interface of two immiscible liquids⁶⁹; preparation and characterization of transition metal complexes and their salts in neutral- and charged-particle transfer between two liquid phases⁷⁰; development and studies of new electrode types and electrochemical biosensors⁷¹; experimental and theoretical studies of excited states of transition metal compounds in photocatalysis and in solar energy conversion; and theoretical characterization of poly-nuclear complexes with bridging ligands including interpretation of their spectral and electrochemical properties. *The Department of Molecular Electrochemistry* deals with electrochemical examination of organic, organometallic and coordination compounds on

the level of single molecules, in order to understand reaction mechanisms of their redox processes in different media. Efforts to correlate experimental and theoretical results elucidate the relationship between structure and reactivity⁷². Electrochemically-generated radical intermediate products and their subsequent reactions are studied by means of a series of spectrometric methods^{73,74}, including sono-electrochemistry, electrochemically-generated luminescence, AFM/STM microscopy and impedance measurement. *The Department of Low-Dimensional Systems* considers chemistry on surfaces, interfaces, thin films, and surface interactions on metals and semiconductors. Preparation of solid substances, surface films, and nano-materials (carbon nano-tubes, graphen, MoS₂) are of particular interest, as are spectroscopic and microscopic studies of their chemical properties and electronic composition^{75–77}.

At present the Institute has 165 employees, including 45 graduate students. Scientists at the Institute publish around 250 articles in peer-reviewed journals annually.

The authors wish to thank the following colleagues (in alphabetical order) for valuable comments: Petr Čárský, Jiří Ludvík, Rudolf Polák, Lubomír Poslíšil, Vladimír Špirko, Blanka Wichlerlová. The authors gratefully acknowledge the Institute's current department heads for their contributions to Section 5 on current research activities.

REFERENCES

1. Koutecký J.: *Phys. Status Solidi I*, 554 (1961).
2. Koutecký J., Paldus J., Zahradník, R.: *J. Chem. Phys.* 36 3129 (1962).
3. Čížek J.: *J. Chem. Phys.* 45, 4256 (1966).
4. Hanuš V., Čermák V.: *Collection Czech. Chem. Commun.* 2, 1602 (1959); Dolejšek, Z., Hanuš V., Prinzbach H.: *Angew. Chemie* 74, 902 (1962).
5. Čermák V., Herman Z.: *J. Chim. phys.* 87, 717 (1960); Herman, Z., Čermák, V.: *Nature* 199, 588 (1963).
6. Cihla Z., Plíva J.: *Collection Czech. Chem. Commun.* 28, 1232 (1963).
7. Ponec V., Knor Z., Černý S.: *Disc. Faraday Soc. No. 41*, 149 (1966).
8. Klier K., Nováková J., Jirů P.: *J. Catal.* 2, 479 (1963).
9. Klier K.: *J. Catal.* 8, 14 (1967).
10. Jirů P., Wichterlová B., Křivánek M., Nováková J.: *J. Catal.* 11, 182 (1968).
11. Klier K., Rálek M.: *J. Phys. Chem. Solids* 29, 951 (1968).
12. Čermák V., Yench A.J.: *J. Electron Spectrosc. Rel. Phenomena* 1, 167 (1977).
13. Knor Z.: *Surf. Sci.* 70, 286 (1978).
14. Černý S., Smutek M., Buzek F.: *J. Catal.* 38, 245 (1975).
15. Hierl P.M., Pacák V., Herman Z.: *J. Chem. Phys.* 67, 2678 (1977).

16. Zahradník R., Čárský P.: *J. Chem. Phys.* 74, 1235; 1240; 1249 (1970).
17. Hobza P., Zahradník R.: *Weak Intermolecular Interaction*. Elsevier, Amsterdam 1980.
18. Polák R.: *Chem. Phys.* 16, 353 (1976).
19. Vojtík J., Paidarová I., Schneider F.: *Chem. Phys.* 114, 369 (1987).
20. Papoušek D., Špirko V.: *Top. Curr. Chem.* 68, 59 (1976).
21. Vlček A. A.: *Coord. Chem. Rev.* 43, 39 (1982).
22. Pospíšil L., Kůta J.: *J. Electroanal. Chem.* 101, 39 (1979).
23. Koryta J.: *Anal. Chim. Acta* 23, 1 (1990).
24. Ludvík J., Pragst F., Volke J.: *J. Electroanal. Chem.* 180, 141 (1984).
25. Samec Z., Mareček V., Homolka D.: *Faraday Disc.* 77, 197 (1984).
26. Bresnahan W. T., Moiroux J., Samec Z., Elving P. J.: *Bioelectrochem. Bioenerget.* 7, 125 (1980).
27. Heyrovský M.: *J. Chem. Soc., Faraday Trans. I* 82, 585 (1986).
28. Trojáněk A.: *Surface Technol.* 15, 93 (1982).
29. Mrha J., Krejčí I., Braunstein B., Koudelka V., Malík J., v knize: *Power Sources*, (Thompson, J., ed.), str. 153. Academic Press, London 1979.
30. Papež V., Novák P., Pflüge, J., Kmínek J., Nešpůrek S.: *Electrochim. Acta* 32, 1087 (1987).
31. Šerák L.: *Sci. Total Environ.* 37, 107 (1984).
32. Pospíšil L.: *Chem. Listy* 74, 694 (1980).
33. Kubelková L., Nováková J., Nedomová K.: *J. Catal.* 124, 441 (1990).
34. Kubelková L., Seidl V., Nováková J., Bednářová S., Jirů P.: *J. Chem. Soc. Faraday Trans. I* 80, 1367 (1984).
35. Tvarůžková Z., Wichterlová B.: *J. Chem. Soc., Faraday Trans. I* 79, 1591 (1983).
36. Kočířík M., Zikánová A.: *Ind. Eng. Chem. Fundamentals* 13, 347 (1974).
37. Mach K., Varga V., Antropiusová H., Poláček J.: *J. Organometal. Chem.* 333, 205 (1987).
38. Dąbkowska I., Jurečka P., Hobza P.: *J. Chem. Phys.* 122, 204322 (2005).
39. Brown E. C., Mucha M., Jungwirth P., Tobias D. J.: *J. Phys. Chem.* 109, 7934 (2005).
40. Nachtigall P., v knize: *Zeolites and Ordered Mesoporous Materials: Progress and Prospects*, (Čejka J., van Bekkum H., ed.), str. 243. Elsevier, Amsterdam 2005.
41. Mrugała F., Špirko V., Kraemer W. P.: *J. Chem. Phys.* 118, 0547 (2003).
42. Paldus J., Pittner J., Čárský P., v knize: *Recent Progress in Coupled Cluster Methods* (Čárský P., Paldus J., Pittner J., ed.), str. 455. Springer, Berlin 2010.
43. Barbatti M., Ruckebauer M., Plasser F., Pittner J., Granucci G., Persico M., Lischka H.: *WIREs Comput. Mol. Sci.* 4, 26 (2014).
44. Čárský P., Čuřík R., v knize: *Low-Energy Electron Scattering from Molecules, Biomolecules and Surfaces* (Čárský P., Čuřík R., ed.), str. 263. CRC Press, Taylor&Francis Group, Boca Raton 2012.
45. Sklenák S., Dědeček J., Li Ch., Sierka M., Sauer J.: *Angew. Chem. Int. Ed.* 46, 7286 (2007).
46. Civiš S., Kubát P., Nishida S., Kawaguchi K.: *Chem. Phys. Lett.* 418, 448 (2006).
47. Kafunková E., Taviot-Gueho C., Bezdička P., Klementová M., Kovář P., Kubát P., Pospíšil J., Lang K.: *Chem. Mater.* 22, 2481 (2010).
48. Ferus M., Kubelík P., Civiš S.: *J. Phys. Chem. A* 115, 12132 (2011).
49. Ferus M., Nesvorný D., Šponer J., Kubelík P., Michalčíková R., Shestivska V., Šponer J., Civiš S.: *Proc. Natl. Acad. Sci.* 112, 657 (2014).
50. Španěl P., Smith D.: *Mass Spectrom. Rev.* 30, 236 (2011).
51. Lengyel J., Pysanenko A., Kočíšek J., Poterya V., Pradzynski C. C., Zeuch T., Slaviček P., Fárník M.: *J. Phys. Chem. Lett.* 3, 3096 (2012).
52. Lengyel J., Kočíšek J., Poterya V., Pysanenko A., Svrčová P., Fárník M., Zaouris D. K., Fedor J.: *J. Chem. Phys.* 137, 034304 (2012).
53. Herman Z.: *Mol. Phys.* 111, 1697 (2013); Herman Z. *Int. J. Mass Spectrom.* 378, 113 (2015).
54. Sýkora, J., Brezovský J., Koudeláková T., Lahoda M., Fořtová A., Chernovets T., Chaloupková R., Štěpánková V., Prokop Z., Kutá-Smatanová I., Hof M., Damborský J.: *Nature Chem. Biol.* 10, 428 (2014).
55. Cebecauer M., Humpolíčková J., Rossy J., v knize: *Methods in Enzymology*, Vol. 505, str. 273. Elsevier, Amsterdam 2012.
56. Dědeček J., Čapek L., Kaucký D., Sobalík Z., Wichterlová B.: *J. Catal.* 211, 198 (2002).
57. Sklenák S., Dědeček J., Li Ch., Wichterlová B., Gábová V., Sierka K., Sauer J.: *Angew. Chem. - Int. Ed.* 46, 7286 (2007).
58. Jurkiewicz P., Cwiklik L., Jungwirth P., Hof M.: *Biochimie* 94, 26 (2012).
59. Štefl M., Šachl R., Olžýnska A., Amaro M., Savchenko D., Deyneka A., Hermetter A., Cwiklik L., Humpolíčková J., Hof M.: *Biochim. Biophys. Acta - Biomembranes* 1838, 1769 (2014).
60. Dědeček J., Sobalík Z., Wichterlová B.: *Catal. Reviews Sci. & Eng.* 54, 135 (2012).
61. Dědeček J., Čapek L., Sazama P., Sobalík Z., Wichterlová B.: *Appl. Catal. A - General* 391, 244 (2011).
62. Sazama P., Čapek L., Drobná H., Sobalík Z., Dědeček J., Arve K., Wichterlová B.: *J. Catal.* 232, 302 (2005).
63. Roth W. J., Nachtigall P., Morris R. E., Wheatley P. S., Seymour V. R., Ashbrook S. E., Chlubná P., Grajciar L., Položij M., Zukal A., Shvets O., Čejka J.: *Nat. Chem.* 5, 623 (2013).
64. Roth W. J., Nachtigall P., Morris R. E., Čejka J.: *Chem. Rev.* 114, 4807 (2014).
65. Gyepes R., Varga V., Horáček M., Kubišta J., Pinkas

- J., Mach K.: *Organometallics* 29, 3780 (2010).
66. Kavan L., Dunsch L.: *Chemphyschem* 8, 974 (2007).
 67. Kavan L.: *Top. Curr. Chem.* 348, 53 (2014).
 68. Kavan L.: *Chem. Rec.* 12, 131 (2012).
 69. Samec Z.: *Pure Appl. Chem.* 76, 2147 (2004).
 70. Samec Z., Langmaier J., Trojáněk A., Zálíš S., v knize: *Handbook of Porphyrin Science* (Kadish K. M., Smith K. M., Guilard R., ed.), Vol. 34, str. 97. World Scientific Publishing, Singapore 2013.
 71. Josypčuk B., Barek J., Josypčuk O.: *Anal. Chim. Acta* 778, 24 (2013).
 72. Josefík F., Mikýšek T., Svobodová M., Šimůnek P., Kvapilová H., Ludvík J.: *Organometallics* 33, 4931 (2014).
 73. Liška A., Rosenkranz M., Klíma J., Dunsch L., Lhoták P., Ludvík J.: *Electrochim. Acta* 140, 572 (2014).
 74. Sokolová R., Hromadová M., Ludvík J., Pospíšil L., Ginnarelli S.: *Electrochim. Acta* 55, 8336 (2010).
 75. Frank O., Dresselhaus M. S., Kalbáč M.: *Acc. Chem. Res.* 48, 111 (2015).
 76. Costa S. D., Weis J. E., Frank O., Bastl Z., Kalbáč M.: *Carbon* 84, 347 (2015).
 77. Weis J. E., Costa S. D., Frank O., Bastl Z., Kalbáč M.: *Chem. Eur. J.* 21, 1081 (2015).

Note from the Editor

It was my pleasure to read this interesting article about the history of one of the oldest and internationally most respected Institutes of the Czech Academy of Science. I am working in the field of electroanalytical chemistry, so that my destiny is closely connected with this Institute in which I have found many outstanding teachers and I am proud to acknowledge their decisive influence on my professional carrier. Moreover, I have found in this Institute many fascinating collaborators and friends that profoundly enriched my professional and personal life. That is why I have found much interesting information in this valuable article. Nevertheless, one piece of very important information is missing there, namely on the

outstanding contribution of Prof. RNDr. Zdeněk Herman, DrSc., a co-author of the article. During my frequent travels abroad I had encountered his name earlier than I have had the pleasure to meet him personally. And I have realized that his name has always been pronounced by foreign experts with great respect and admiration and was inseparably connected with his pioneering work on crossed molecular beams and his studies on molecular dynamics and kinetics. Prof. Herman and all people in his Institute (as well as the whole Czech scientific community) can be proud of the results of this research and its international recognition. Of course I admire Prof. Herman's modesty which led him to refuse putting his name on the list of the outstanding personalities of this Institute. Nevertheless, I consider it to be my professional and human duty to state that the results of his fascinating work are of much higher importance than it would seem from the marginality of his mentions on it in the article; this is due solely to his extreme modesty. I am aware of the utmost importance of the big investment into modern chemical infrastructure and its instrumentation. Nevertheless, deep in my heart I am convinced that it is real personalities which present the most important asset for the development of any scientific discipline. The personalities like prof. Herman, to which the coming scientific generation could look up at with esteem and admiration, as at an example worth of following. Last but not least I would like to thank to all staff-members, postdocs and PhD students of this Institute, both past and present, for everything they have done for the good name of our country and our chemistry. We should be grateful for anything a Czech chemist can be proud of during his stay abroad. Undoubtedly, the Heyrovský Institute of Physical Chemistry of the Czech Academy of Sciences is among these assets, thanks to its past achievements, its presence, and the enthusiasm of both past and present staff members. And I would like to wish them much success in attaining their research goals and respectable representation of our science on international forum.

*On behalf of the editorial board of Chemické Listy
Jiří Barek*