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Institute of Problems of Chemical Physics of the Russian Academy of Sciences



This issue of the journal 'Russian Chemical Reviews' is fully composed of papers contributed by staff researchers of the Institute of Problems of Chemical Physics of the Russian Academy of Sciences (IPCP RAS), one of the leading research institutes of the Division of Chemistry and Materials Science of the RAS. In 1956, Academician N N Semenov, the former director of the Institute of Chemical Physics (ICP) of the USSR Academy of Sciences and a Nobel Prize Winner, and F I Dubovitsky, Corresponding Member of the USSR Academy of Sciences, set up an affiliated branch of ICP in the village of Chernogolovka (Noginsk Region near Moscow) with the primary goal to carry out large-scale research in combustion and explosion processes. In 1972, the affiliated branch was rearranged into a section of ICP and in 1991 the section was reorganised into the Chernogolovka Affiliation of ICP (presently, IPCP RAS).

The main lines of research pursued at IPCP RAS are as follows:

— general problems of chemical physics;

— structures and compositions of molecules and solids; kinetics and mechanisms of complex chemical reactions;

— physical chemistry of combustion and explosion;

— preparation and modification of polymers;

— biological processes and systems.

Noteworthy, all these studies have a common basis, *viz*., study of kinetics and mechanisms of diverse chemical and biological conversions.

The Institute has at its disposal a unique experimental base: proving grounds; specialised reinforced premises for large-scale studies of fast processes; chemical, technological and microbiological pilot plants; a vivarium; cryogenic equipment; a multi-access analytical centre for experimental support of investigations in the framework of projects of the Russian Foundation for Basic Research (RFBR) and state-sponsored research programmes of the Russian Ministry for Industry, Science and Technology.

The computer centre of IPCP is equipped with the most up-to-date computing system RM 600 E60\E20 (Siemens, FRG) which is integrated into the computer network of the Chernogolovka Research Centre and provides facilities for other research institutes of the RAS residing in Chernogolovka as well as for Moscow State University (MSU), Moscow Institute for Physics and Technology (MIPT), Moscow Engineering and Physical Institute and many other research and educational institutions in Moscow, Kazan, Rostov-on-Don, Ivanovo and other cities. The establishment of a high-capacity computer centre at IPCP has made it possible to state new fundamental tasks:

— design of software tools for numerical simulation of development of hydrodynamic instability;

— development of an 'individual particles' technique for description of high-energy pulsed processes;

— study of phase transitions in organic crystals;

— quantum-chemical studies of mechanisms of chemical conversions in organic compounds.

Researchers at IPCP have developed new generations of software complexes based on the use of massively parallel technologies which allows one to reduce the computation time 10 – 20-fold and to carry out direct simulation of fire- and explosive-hazardous events at chemical and nuclear units.

The staff of the Institute consists of more than 800 researchers including 109 D.Sci. and 322 Ph.D's. A department of the MIPT is functioning successfully on the mode of IPCP. An affiliated branch of the Department of Chemistry of MSU was established in IPCP in 1995 owing to the joint efforts of IPCP RAS and the Department of Chemistry of MSU. The Moscow Regional Affiliation of MSU, which includes departments of chemistry, physics and geology, has been functioning at IPCP since 1997. The Institute provides degree research facilities to students of senior courses of MSU, MIPT and other higher educational establishments; postgraduate students prepare their doctoral theses on the

basis of the Institute. IPCP has three expert councils for Ph.D. and doctoral theses; the post-graduate courses offer research facilities in 16 scientific disciplines.

In recent years, the interest of talented young scientists in scientific research has increased considerably owing to the organisation in the Chernogolovka Research Centre of a continuous educational system: school – college – postgraduate courses. At present, 30 students of IPCP are carrying out diploma works and over 30 people are postgraduate students.

The Institute carries out research in the framework of various projects supported by the RFBR (about 100 research projects annually), the European Union (INTAS), the International Science and Technology Centre (ISTC) as well as in the framework of Federal purpose-oriented programmes and RF President's Grants for leading scientific schools and collaborates with more than 50 universities and institutions in Russia and abroad.

Such a broad range of research, which encompasses virtually all main areas of chemical physics, is reflected in the present structure of IPCP. The Institute has ten sections: combustion and explosion; kinetics of chemical and biological processes; kinetics and catalysis; extremal states of substances; polymers and composite materials; structures of substances; photochemistry; functional inorganic materials; chemical technology; mathematics. In-depth fundamental studies carried out at IPCP have provided results of fundamental importance in all these areas.

Methods for exact calculation of complex surfaces of potential energy and dynamics of elementary processes have been developed. The quantum theory of molecular rearrangements has been devised. The rate constants for the main elementary reactions occurring in gas, liquid and solid phases have been established both theoretically and experimentally. The mechanisms of action of metalloenzymes have been investigated. These data served as a basis for the construction of purely chemical systems for photocatalytic liberation of hydrogen and oxygen from water, oxidation of methane and catalytic reduction of hydrogen under mild conditions.

The mechanism of combustion of condensed compounds has been investigated and its general theory is developed. Some methods of control over combustion have been proposed. The regularities of heterogeneous and filtrational combustion have been analysed.

In-depth studies into various aggregate states of substances and chemical and phase conversions at high pressures and temperatures under intense shock and detonation waves have been carried out. The thermal properties of dense plasma characterised by strong interparticle interactions as well as thermodynamic and conducting properties of gaseous and liquid hydrogen under conditions of multiple shock-wave loading have been investigated. The ability of hydrogen, helium and xenon to pass to a highly conducting (metallic) state has been established. The transition of metals (particularly, of lithium and sodium) into dielectric states at high dynamic pressures has been detailed. The electrical resistance of fullerite C_{60} under dynamic conditions has been measured for the first time. It has been established that the temperature dependence of resistance of shock-loaded fullerite is reversible and typical of semiconductors.

In-depth studies are carried out at IPCP within the framework of a general problem: molecular structure – solid structure – physical and chemical properties of materials. This resulted in the preparation and investigation of a vast variety of superconductors, metals, photochromic materials, superionics, materials with a broad range of useful mechanical, electrical and optical characteristics, nanomaterials and fullerenes.

Chemical modification of various classes of antitumour cytostatics by incorporation of fragments of iminoxyl radicals (bioantioxidants) has resulted in the development of novel classes of drugs manifesting a broad range of antitumour activities as well as membrane protectors and antioxidants.

Adequate nitrosyl models of active [Fe – S] centres of non-heme proteins, a novel class of promising medicinal drugs, have been obtained for the first time. Some new methods for the synthesis of these conjugates, which contain simultaneously two biochemical functional groups, *viz*., the –NO group (radio- or chemosensitiser) and the –SR group (antibacterial and antiinflammatory agents, enzyme inhibitors, antimetabolites), have been developed.

The Institute combines fundamental research with the solution of applied practical tasks and is actively engaged in the development and commercialisation of advanced technologies and processes. The German company 'Linde' has purchased the Institute's license for highly selective synthesis of higher linear α-alkenes based on controlled dimerisation and oligomerisation of ethylene and started the construction of several plants utilising this technology in Saudi Arabia. A process for pilot-plant production of poly-α-alkene bases for synthetic lubricants has been developed by IPCP in collaboration with the petrochemical company 'Petroleum Industry of Serbia'. This technology has served as the basis for the construction of the first plant in the Russian Federation for the production of synthetic motor oils in the town of Nizhnekamsk (Tatarstan).

The Russian – Chinese Joint Venture 'Sychuan Mianyang Lier' has been established for industrial realisation of a technology for preparation of pyridine-type pesticides developed by IPCP RAS in collaboration with the Chinese Academy of Physical Engineering. In 1997, the production of 3,6-dichloropicolinic acid and Lier (which represents an analogue of Lontrel) was set in operation at the Mianyang plant belonging to the Company.

In-depth studies of non-equilibrium filtration combustion processes have led to the development of environmentally safe technologies and equipment for processing industrial and domestic wastes and low-grade combustible fuels aimed at production of thermal and electric energy. Commercial plants for processing quenching oils (JSC 'Electrostaltyazhmash', Electrostal', Moscow Region) and household wastes (Lappeenrantha, Finland) have been set up. The assembly of an incineration plant is near completion in Moscow.

Active engagement of IPCP RAS in the activities connected with commercialisation of its own achievements has led to the establishment, in 2001, with the assistance of the Academy of National Economy at the Government of RF and the British Council, of a new section, *viz*., a Centre for commercialisation, which is aimed at performing technological audits, legal regulation and market research. The experts at the British Council render permanent support for the newly established Centre in organising training seminars on technological audits. This undertaking has received further support. At the end of 2002, it was decided to establish an Innovation-Technological Centre of the RAS on the basis of the Chernogolovka Research Centre in order to meet the need for qualified personnel for innovation spheres. The agreement on its establishment has been made between the Russian Academy of Sciences, MSU, the Government of the Moscow Region and the Academy of National Economy of the RF Government. One of the main provisions of this agreement is education of specialists and acquisition of professional skills and knowledge in the field of technological management, which includes commercialisation of new developments, estimation of commercial potentials of novel technologies, attraction of investments and advancement of novel technologies and scientific and technological products in the market.

The Institute takes an active part in international and domestic scientific-and-industrial exhibitions. In the past five years, IPCP researchers participated in 61 exhibitions, such as the International Industrial Fair in Hannover (FRG), Salon of Innovations, Novel Technologies and Inventions at Pittsburg (USA), and domestic exhibitions 'Khimekspo' and 'Ekspogorod'. Many of them won prizes at popular international exhibitions ('Innovations: Novel Materials and Chemical Products', 'Science and Scientific Instruments', 'Salon of Industrial Property 'Archimed') and the national exhibition 'Technologies from Russia'. The developments of the Institute were highly appraised

by the Jury of the 51st Salon 'Brussels: Eureka-2002' where they were awarded three gold, one silver and one bronze medals.

Every year, researchers of IPCP publish about 350 papers in domestic and foreign journals and make about 400 reports at national and international conferences. In the past five years, 34 monographs of IPCP researchers came out of such highly reputed publishing houses as Gordon and Breach, Elsevier, Springer, Kluwer Academic, Nauka, Khimiya, *etc*. The Institute publishes books of collected papers on diverse problems of chemical physics, physical chemistry, combustion and explosion, chemical kinetics, physics and chemistry of polymers. The Institute owns more than 60 patents for advanced developments and technologies; of those, 30 patents were granted in the last five years.

The Institute supports the organisation of numerous national and international scientific conferences and symposia devoted to combustion and explosion, chemistry and physicochemistry of oligomers, physical and chemical characteristics of elementary chemical processes, crystal chemistry and catalysis.

Several researchers of IPCP were awarded the honorary title 'Honoured Scientist of Russia'. Among other rewards granted to IPCP members in the new millennium are the Government Prize of RF for innovative activity, RF prizes for young scientists for outstanding achievements in science and technology and the European Academy prizes for young Russian scientists. In 2002, Academician V E Fortov was awarded a prestigious prize of the Max Planck Society for a series of experimental and theoretical investigations on the properties of various substances under extremal conditions.

The reviews published in this issue do not cover the whole range of investigations carried out at IPCP; many of the research subjects are intended for consideration by the physical community only.

As was mentioned previously, one of the most actively developed lines of research at IPCP is chemical physics of the formation and modification of polymers, namely, the kinetics of the formation and destruction of polymers, macromolecular design, interphase events occurring in polymers and composite materials; design and investigation of polymers and composite materials possessing unique optical, electrical and magnetic properties, structural theory of macromolecules and phase formation in polymeric materials; physical methods for studies of polymeric materials, *etc*. This line of research is detailed in the review by G V Korolev 'Current trends in investigations into the microheterogeneous mechanism of three-dimensional radical polymerisation' and the review by D P Kiryukhin and I M Barkalov 'Chain chemical reactions at low temperatures'.

Yet another important trend which combines different lines of research carried out at IPCP is related to the study of kinetics, mechanisms and elementary acts of chemical reactions. Of particular interest is the study of short-lived intermediate species involved in these reactions. The review by E Ya Misochko, A V Akimov and I U Goldshleger 'Modern applications of matrix isolation technique to investigation of radical species generated in atom–molecular chemical reactions' describes one of the most efficient in contemporary chemical physics techniques for the study of transient products and its application to concrete systems. Special attention is given to the analysis of conditions for the stabilisation of radical intermediates generated in cryochemical reactions and combined applications of various spectroscopic techniques.

The fundamental line of research aimed at activation of hydrocarbons by transition-metal complexes is led by Academician A E Shilov. Some aspects of this problem have been considered in the review by V D Makhaev 'Structure of methane complexes according to the data of experimental and theoretical investigations', which is devoted to the analysis of relationships between the nature of the central metal atom and the ligands and coordination of methane within complexes with neutral atoms, ions and molecular fragments and the comparative study of structural regularities of methane and tetrahydroborate complexes.

The kinetics and mechanisms of thermal decomposition of high-energy compounds, their chemical stability and application safety have long been studied by F I Dubovitsky, Corresponding Member of RAS. The results of long-term exploratory works aimed at the synthesis of novel representatives of high-energy compounds of the triazine series and their analogues are presented in the review by A V Shastin, T I Godovikova and B L Korsunskii 'Nitro derivatives of 1,3,5-triazine: synthesis and properties'. This is the first attempt to systematise the published data on novel 1,3,5-triazine derivatives as high-energy and biologically active substances and reagents for organic synthesis. The ability of trinitromethyl groups of 1,3,5-triazine derivatives to undergo nucleophilic substitution presents unquestionable interest for the understanding of mechanisms of nucleophilic aromatic substitution in heterocyclic compounds.

These are only a few trends of research being carried out at IPCP. In one of the next issues of Russian Chemical Reviews we shall continue to get you acquainted with the results of our investigations. For more detailed information see our web-site (http://www.icp.ac.ru).

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