Foreword

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Abstract

Milestones of historical evolution of the Chemistry Department of the Lomonosov Moscow State University, which was formally separated from the physical-mathematical faculty of the University in 1929, are briefly outlined. Directions of studies carried out at the Department in the field of structural chemistry are overviewed with an emphasis on the works included in this issue.

Keywords Methodical aspects · Teaching chemistry · Crystallographic structures · Organic frameworks · Clusters · Complexes · Conformers · Intra- and intermolecular interactions · Electronic states · Force fields · Spectra · Thermodynamic properties · Catalysts · Biologically active compounds

This issue is devoted to the 90th anniversary of the Department of Chemistry of the M.V. Lomonosov Moscow State University. This University is the oldest and the most reputable in Russia. It was established in 1755 according to the decree signed by Empress Elizabeth I, the daughter of Peter the Great. The project of the University was elaborated chiefly by the outstanding scientist Mikhail V. Lomonosov and a man of education, count Ivan I. Shuvalov.

Initially, there were three faculties of the University, namely, the ground-level philosophical faculty, whose graduates (after three years of study) could either continue their education at the same faculty or apply to either of the two higher-level faculties, namely the law and medicine. The latter one included the chair of chemistry. Nearly half a century later, in 1804, in the spirit of the times, the University was restructured and four departments replaced the three faculties. The chair of chemistry became part of one of them, the new physical-mathematical department. In another half a century, during which the departments were again renamed into faculties, the rank and importance of chemistry increased so much that the head of the chair of chemistry, professor Rudolf Heimann, gave public lectures for industrialists and manufacturers.

By the end of the third quarter of the 19th century, in 1872, the prominent scientist Vladimir V. Markovnikov was invited

to head the chair of chemistry. He laid the novel methodical foundations of teaching chemistry and considered it absolutely necessary for the chemistry majors to carry out research in a chemistry laboratory. Moreover, the chair of chemistry was among the first to admit women as students who could later on receive the Philosophy Doctor degree in Chemistry. The initiative for laboratory research was further developed by the next head of the chair, professor Nikolai D. Zelinskii, who made the systematic work in a laboratory an indispensable part of the curriculum. This became a tradition continuing to the present day. In 1921 the chair of chemistry was transformed into the department of chemistry within the physical-mathematical faculty, and eight years later, on October 1, 1929, a separate Faculty of Chemistry was established. This date has become the official birthday of the Faculty of Chemistry, though its history is longer as described above.

The number of chairs within the Faculty (or, Department, as it is called nowadays) has gradually increased in time, from the original five (general and inorganic, physical, organic, analytical chemistry, and biochemistry) to the present seventeen (general, inorganic, organic, analytical, colloid, physical chemistry, electrochemistry, petroleum chemistry and organic synthesis, chemical kinetics, radiochemistry, chemical engineering and novel materials, high-molecular compounds, laser chemistry, medicinal chemistry and fine organic synthesis, chemistry of natural compounds, chemical enzymology, and fundamental principles of chemistry). On the whole, the research and teaching staff of the Department of Chemistry involves about 1800 specialists in all the branches of chemistry and at the frontiers with physics and biology. Most of these associates are involved in teaching, as professors giving basic

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courses, as associate or assistant professors giving seminars or practical classes as well as general special courses, and as researchers of different levels who supervise specialized laboratory work, course work, diploma (Master-degree equivalent) projects, as well as post-graduate PhD studies.

Among the total of more than a thousand students of the department, there are always a considerable number of international students. On the whole, about fifteen hundred citizens of Europe, Asia, the Americas, and Africa have earned (Master-degree equivalent) diplomas in chemistry at our Department. We are proud that the Editor-in-Chief of *Structural Chemistry*, Professor Istvan Hargittai is among our graduates.

The scope of scientific studies carried out at the Department is extremely broad and represent both experimental and theoretical investigations that are supplemented with engineering projects. Previously distinct spheres of theory and experiment have interpenetrated during the last decades, so that almost all research groups combine synthetic work and computational simulations in order to obtain more detailed knowledge about systems or processes of interest. The works collected in this issue represent only one segment of these studies, which in itself is rather versatile and focuses on the structure of the building blocks of matter in various phases (gas, solid, and liquid) and the stationary features and dynamic properties of the substances under investigation. Special attention is being paid to the inherent peculiarities of the electron density distribution and the nuclear configurations of the building blocks involved.

In particular, the issue contains papers devoted to the results of studies carried out at the chairs of physical chemistry, inorganic chemistry, organic chemistry, medicinal chemistry and fine organic synthesis, and electrochemistry. They deal with diverse aspects of the molecular structure studies, which are as follows:

- (i) Synthesis and structure studies of novel compounds, which, depending on the phase state of the substance, are carried out with the use of NMR, infrared absorption or Raman spectroscopy, as well as single-crystal x-ray diffractometry, and either assisted or not by semiempirical or nonempirical modeling, which helps in determining the role of diverse intra- and interparticle interactions that govern the formation of particular conformers or supramolecular ensembles, frameworks, and crystals [1–5];
- (ii) Synthesis of drugs, drug precursors, and other kinds of biologically active compounds and their biological testing with the use of different experimental spectral techniques supplemented with molecular modeling that provides tentative ideas about the underlying mechanisms of biological effects [6, 7];
- (iii) Clarifying details of the mechanisms of important biochemical processes at the most reliable level accessible in modern simulations, namely with the use of

combined quantum/classical models where the reaction site is described at the high quantum chemical level, while the effect of substantially extended dynamic neighborhood is taken into account as a properly tuned force field [8];

- (iv) Determining structure peculiarities and the possible catalytic activity of different immobilized or deposited atomic layers or nano-sized particles depending on the characteristics of substrates, which is of primary importance in view of the production of more efficient and relatively cheap catalysts [9, 10];
- (v) Investigation of possible conformers of the compounds with complex either flexible or, by contrast, strained structures with an emphasis on the methods that provide reliable description of such compounds and the effects produced by particular substituents, functional groups, or ligands; as well as conformational analysis of molecules in different electronic states in relation to the differences in their absorption and fluorescence spectra determined by intramolecular transformations [11–13];
- (vi) Studying diverse molecular ensembles with the use of experimental and theoretical approaches, the latter involving either molecular dynamics or stationary nonempirical modeling, with an aim to clarify the nature and strength of intermolecular forces that stabilize particular kinds of solvation shells or local neighborhoods of foreign particles, as well as the structural kinds of dynamically changing clusters, agglomerates, and conglomerates of molecules that may be present in the bulk of liquids [14];
- (vii) Discovering peculiarities of the hydrogen-bonded complexes and building blocks, which are of primary importance in the case of gas-phase, liquid, and solid systems, with an emphasis on the changes, which accompany phase transitions, and spectral fingerprints observed both in the experimental infrared absorption spectra and simulated spectra retrieved from quantum chemical calculations [15–19];
- (viii) Modifying and improving the existing or constructing new schemes that provide more reliable description of the vibrational states of molecules with an emphasis on either efficient algorithms of determining force field parameters in the case of large molecular systems or the accurate representation of anharmonic interacting vibrations of relatively small molecules [20];
- (ix) Estimating accurate thermodynamic functions, particularly enthalpies of formation, of different compounds, especially those which are energy-rich ones, with the use of complex multilevel simulation schemes based on high-level quantum chemical methods [21].

Methodologically, the investigations are focused on (i) structural peculiarities of particles tightly related to their

electronic, rovibrational, and magnetic-resonance spectra, interpretation of which requires continuous development and improvement of already existing procedures; (ii) interrelated features of the electron density distribution and various, practically important local and bulk characteristics of particles and material building blocks that predetermine their adsorption/absorption power and reactivity including catalytic activity; (iii) spectral characteristics of molecules in different phases (gas, liquid, and solid) where different approaches and schemes are constructed to predict not only the probable transition frequencies and intensities of individual particles, but also the changes imposed by particular neighborhoods, which is especially important in the case of fluorescent markers or photovoltaic units.

This is by no means complete list of the directions of studies at the Chemistry Department, yet it is a relatively good representation of its research directions.

Dear readers of the Journal! We hope that you find interesting papers in the issue and will be glad if their presentation will encourage you to visit Moscow State University and to find partners for future joint work!

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References

- Bushmeleva AS, Tafeenko VA, Zakharov VN, Lobova AA, Aslanov LA (2019) Ammonium cyamelurates: synthesis and crystalline structures. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1187-0>
- Karpova EV, Zakharov MA, Medovik MG (2019) Structure and thermal behavior of two bimetallic carboxylates: Cs [M(CCl₃COO)₃(H₂O)₃], M=Co, Ni. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1258-2>
- Shestimerova TA, Kuznetsov AN, Shevelkov AV (2019) Silver-chalcogen frameworks: crystal and electronic structure of [Ag₃S](NO₃) and a comparison with [Ag₄Te](SO₄). *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1237-7>
- Zakharov MA, Ivanov AS, Arkhipova EA, Desyatov AV, Savilov SV, Lunin VV (2019) Structure and properties of new dicationic ionic liquid DBTMEDA (BF₄)₂. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1260-8>
- Marochkin II, Kuznetsov VV, Rykov AN, Makhova NN, Shishkov IF (2019) Molecular structure study of 1,2,3-trimethyldiaziridine by means of gas electron diffraction method. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1213-2>
- Zefirov NA, Evteeva YuA, Wobith B, Kuznetsov SA, Zefirova ON (2019) Adamantyl-substituted ligands of colchicine binding site in tubulin: different effects on microtubule network in cancer cells. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1219-9>
- Alexeev AA, Nurieva EV, Lyssenko KA, Grishin YuK, Zefirova ON (2019) Novel structural type of bridged urea derivatives bearing azatricyclo [4.3.1.0^{3,8}] decane moiety. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1252-8>
- Kapusta DP, Firsov DA, Khrenova MG, Grigorenko BL, Nemukhin AV (2019) Effect of solvation water shells on enzyme active sites in zinc-dependent hydrolases. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1206-1>
- Rybakov AA, Bryukhanov IA, Larin AV, Todorova S, Zhidomirov GM (2019) Different limits for convergent Pd-Pd lengths in Pd slabs grown over different oxides. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1230-1>
- Golosnaya MN, Pichugina DA, Kuz'menko NE (2019) Structure and reactivity of gold cluster protected by triphosphine ligands: DFT study. *Struct Chem* 30. <https://doi.org/10.1007/s11224-019-01292-2>
- Pisarev SA, Shulga DA, Palyulin VA, Zefirov NS (2019) Lone pairs vs. covalent bonds: conformational effects in bicyclo[3.3.1] nonane derivatives. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1240-z>
- Grineva OV (2019) How do halogen atoms influence the competition between all-trans and hairpin conformers of unbranched alkanes? *Struct Chem* 30. <https://doi.org/10.1007/s11224-019-1281-y>
- Godunov IA, Terentiev RV, Maslov DV, Yakovlev NN, Bataev VA, Abramnikov AV (2019) The structure of 2-methylpropanal molecule in the S₁ lowest excited singlet electronic state: theoretical and experimental studies. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1243-9>
- Abramovich A (2019) Features of molecular light scattering and structure of the chlorobenzene–o-dichlorobenzene solutions. *Struct Chem* 30. <https://doi.org/10.1007/s11224-019-01293-1>
- Slovokhotov YuL (2019) Organic crystallography: three decades after Kitaigorodskii. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1254-6>
- Sosulin IS, Tyurin DA, Feldman VI (2019) CHF₃ ... H₂O complex revisited: a matrix isolation and ab initio study. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1232-z>
- Korneichuk AYA, Senyavin VM, Kuramshina GM (2019) Molecular structure of 4-piperidinemethanol in gas, solutions and solid state: spectral and theoretical investigations. *Struct Chem* 30. <https://doi.org/10.1007/s11224-019-01296-y>
- Shilyaeva EA, Novakovskaya YuV (2019) Certain features of graphite oxide functional groups as drawn from simulations and experiment. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1248-4>
- Belega ED (2019) The dynamics of solid and liquid phases of water octamer, decamer, and dodecamer. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1249-3>
- Kochikov IV, Stepanova AV, Kuramshina GM (2019) Ab initio molecular force fields fitted in Cartesian coordinates to experimental frequencies of isotopic species using symmetry constraints: application to indole and pyrrole molecules. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1262-6>
- Dorofeeva OV, Ryzhova ON (2019) Enthalpies of formation of diamantanes in the gas and crystalline phase: comparison of theory and experiment. *Struct Chem* 30. <https://doi.org/10.1007/s11224-018-1220-3>