Scientist, Teacher, Enthusiast

Boris Filipovych Minaev

On the 75th anniversary

Cherkasy
2018

UDK 54(092)Minaev
S40

Scientist, Teacher, Enthusiast. **Boris Filipovych Minaev: On the 75th anniversary.** / V. A. Litvin, V. A. Minaeva, N. N. Karaush-Karmazin, G. V. Baryshnikov. – Cherkasy: Chabanenko Yu. A., 2018. – 80 p.
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The book covers the main periods of life, scientific and pedagogical activity of Boris F. Minaev: Doctor of Chemical Sciences, Professor, Academician of the Academy of Sciences of the Higher School of Ukraine, Honored Worker of Science and Technology of Ukraine and contains an overview of his most important scientific works. The book reflects Minaev's great contribution to scientific research and informs the reader about his achievements in the field of physical organic chemistry and molecular electronics.

The book is dedicated to the 75th anniversary of the B. Minaev's birthday and to the 55th anniversary of his scientific activity.

UDK 54(092)Minaev

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The Head of the Department of Chemistry and Nanomaterials Science at the Bohdan Khmelnytsky National University, Professor Boris Minaev celebrates the 75th anniversary this year. At the same time, we mark another remarkable date – 55 years of his scientific activity.

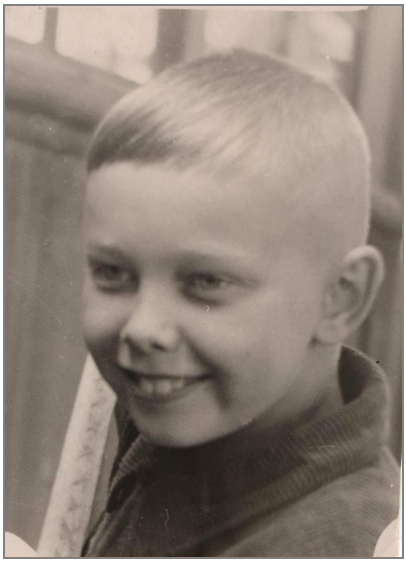
B. F. Minaev was born on 21 September, 1943 in the city of Sverdlovsk (now Yekaterinburg) in a family of nonmanual workers. His father, Filip Prokopovich, at that time worked as Deputy Chairman of the Sverdlovsk Regional Executive Committee, supervised Uralmash and other large Ural plants, where the Second-World-War Soviet Victory weapon was created.

After the war, the father supervised the Novgorod and Semipalatinsk Regional Executive Committee, the Ministry of Building Materials Industry in Kazakhstan Republick, therefore the family often moved from one part of the Soviet Union to another. Mother, Tetyana Mykolayivna, was a teacher, she taught history at school and raised three children of her own.

Filip Prokopovych Minaev, father, 1951

Tetyana Mykolayivna Minaeva, mother, 1951

In 1962 B. Minaev graduated from secondary school No. 3 in Karaganda and entered the Physics Department of the V. V. Kuibyshev Tomsk State University (TSU). His first scientific research was devoted to the calculations of nitrocompounds by the Hückel method. He started this study in his third-year at the University.



Boris Minaev's childhood, 1949

Minaev B. with his elder brother, 1950

Pupil of the 6th form of the secondary school No. 15 Almaty, 1956

Boris Minaev's youth, 1959

As a 5th-year student he passed a pre-diploma practice at the Institute of High-Molecular Compounds of the USSR Academy of Sciences in Saint Petersburg, based on the results of which Minaev wrote his first scientific paper “On the relative stability of various hydrogen-bonded configurations of purine and pyrimidine derivatives” in co-authorship with Yu. G. Baklanova, I. E. Milevskaya and Yu. E. Eisner (Molecular biology. USSR, 1968, No 2. P. 303–309).

B. F. Minaev– 5th-year student
during the pre-diploma practice
(Institute of High-Molecular Compounds of the USSR
Academy of Sciences, St. Petersburg, 1966)

In 1967 Boris Minaev graduated from the University and entered the post-graduate course at the Optics and Spectroscopy Department of the Tomsk State University. Even then, the young PhD student was fascinated by the quantum chemistry methods, which he used to calculate the electronic and spectral properties of molecules [1–4]. In those years the first lasers were created under the supervision of Professor N. A. Prilezhaeva at the Optics and Spectroscopy Department of the Tomsk State University and the first computers were used to calculate molecules and their spectra. Natalia A. Prilezhaeva was a successor and former of Academician A. N. Terenin and spoke about his discovery of the triplet nature of phosphorescence. In addition to the gas discharge spectra, Prof. Prilezhaeva was interested in the theory of excited states of molecules. She fostered this interest in her graduate student.

Since 1970, B. Minaev worked as a junior researcher at the Academician V. D. Kuznetsov Siberian Physics-Technical Institute, and a year later he moved to the Department of Organic Chemistry of the Tomsk State University. In early 1973 he defended his PhD dissertation for the degree of candidate of physical and mathematical sciences on the topic: "Spin-orbital coupling effects in the optical and EPR spectra of molecules and radicals". Even in the earliest papers of the young scientist, we can trace the desire for deeper understanding of the regularities in the molecular spectra of various classes of compounds (from two-atomic molecules [4] to large charge-transfer systems [1] and biopolymers) on the basis of fundamental theories. Boris Minaev also developed methods for calculating the effects of spin-orbital coupling (SOC) based on the Hartree-Fock Self-Consistent-Field method and configuration interaction method for excited states. Accounting SOC and calculation of the phosphorescence lifetime for the aromatic molecules allowed B. Minaev to

explain for the first time the role of strongly coupled σ-electrons in the spectra of this wide class of organic compounds [2, 3]. Earlier, these σ→π* transitions were practically not considered. The coloring of organic molecules and dyes was justified due to π→π* transitions. To explain the phosphorescence lifetime [1–4], the σ→π* transitions serve as a source of «intensity borrowing» for forbidden triplet-singlet radiation, therefore the young graduate student paid much attention to the study of σ-electron excitations. B. Minaev has shown that the first σ→π* transitions in aromatic compounds occur in the near-UV region, but due to their low intensity they are overlapped by the more intense π→π* transitions [2, 3].

Working at the Organic Chemistry Department of the Tomsk State University (1971–1974), B. Minaev has developed the theory of spectra for the charge transfer complexes with the example of nitroaromatic compounds and has explained the properties of the Mesenheimer complexes [5]. The research experience of the SOC effects allowed Minaev to carry out the first systematic calculations of the g-factor anisotropy of the electron paramagnetic resonance (EPR) spectra based on the self-consistent field theory for a large number of radicals [6]. A quarter century later, he performed the first non-empirical calculation of the g-factors together with colleagues from Sweden [151]. Now this priority is universally recognized. Recently, the theoretical aspects of the phosphorescence of molecules over the last 50 years have been summarized and published in a highly rated journal Chemical Reviews of the American Chemical Society [7] (Impact factor 52.613). This review has also considered the problem of optical detection of magnetic resonance (ODMR), zero field splitting and g-splitting in the EPR spectra for triplet states as well as the problems of molecular electronics dependent on spin statistics of charge carriers in amorphous semiconductors.

CHEMICAL REVIEWS

Review

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Theory and Calculation of the Phosphorescence Phenomenon

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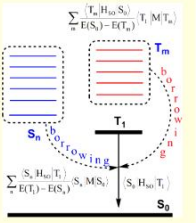
ABSTRACT: Phosphorescence is a phenomenon of delayed luminescence that corresponds to the radiative decay of the molecular triplet state. As a general property of molecules, phosphorescence represents a cornerstone problem of chemical physics due to the spin prohibition of the underlying triplet-singlet emission and because its analysis embraces a deep knowledge of electronic molecular structure. Phosphorescence is the simplest physical process which provides an example of spin-forbidden transformation with a characteristic spin selectivity and magnetic field dependence, being the model also for more complicated chemical reactions and for spin catalysis applications. The bridging of the spin prohibition in phosphorescence is commonly analyzed by perturbation theory, which considers the intensity borrowing from spin-allowed electronic transitions. In this review, we highlight the basic theoretical principles and computational aspects for the estimation of various phosphorescence parameters, like intensity, radiative rate constant, lifetime, polarization, zero-field splitting, and spin sublevel population. Qualitative aspects of the phosphorescence phenomenon are discussed in terms of concepts like structure−activity relationships,



From 1974 to 1988 Boris Minaev first worked as Asssitant Professor of the Theoretical Physics Department and then as a head of the Physical Chemistry Department at the Karaganda State University. At that time Minaev developed his famous theory of the singlet-triplet transitions intensity in the visible and near-IR specrtal regions of molecular oxygen. In the upper layers of the atmosphere these weak transitions have a purely magnetic nature and occur due to a very specific spin-orbital coupling in the O_2 molecule [8].

In 1978 Minaev showed that the well-known red Fraunhofer line of the sunlight absorbed by the atmosphere does borrow its intensity from the EPR magnetic transition between spin sublevels of the ground triplet state in the O_2 molecule. This unusual nature of optical absorption was discovered in molecular spectroscopy for the first time [9]. Two years later, following the same principles, Minaev explained the specific luminescence enhancement of the singlet ($a^1\Delta_g$) oxygen in solutions [10].

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, VOL. XVII, 367–374 (1980)

Intensities of Spin-Forbidden Transitions in Molecular Oxygen and Selective Heavy-Atom Effects*

B. F. MINAEV

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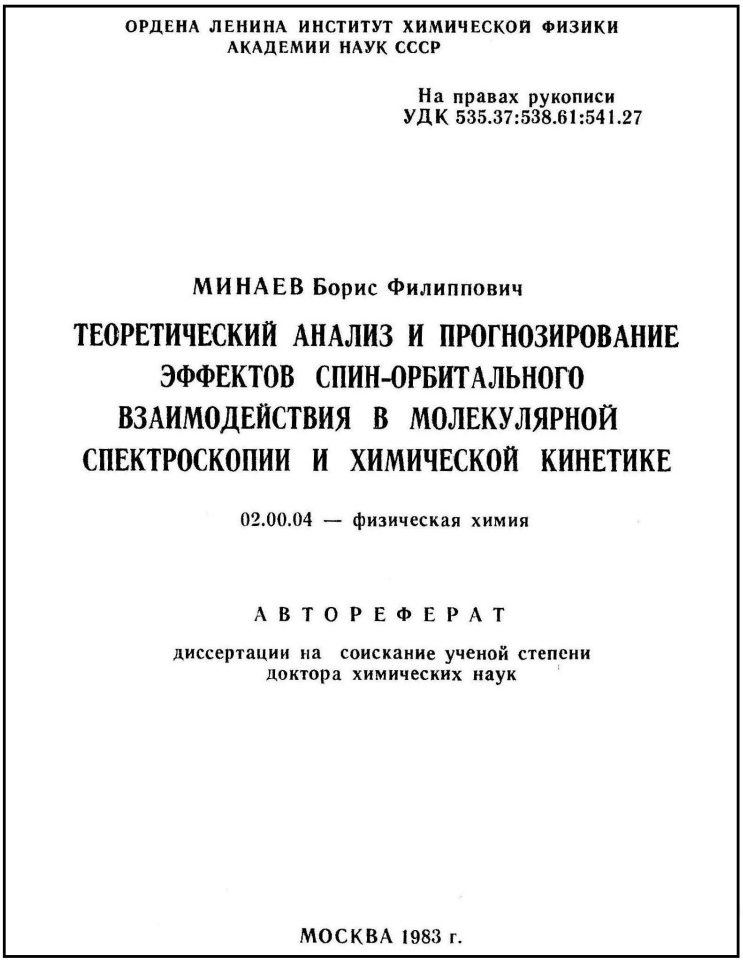
Abstract

Intensities of $a\,^1\Delta g \leftarrow X\,^3\Sigma_g^-$ and $b\,^1\Sigma_g^+ \leftarrow X\,^3\Sigma_g^-$ transitions in molecular oxygen have been calculated on the basis of the INDO method taking into account spin-orbit coupling by perturbation theory. The transitions are magnetic dipole in nature. The first of them ($a - X$) steals its intensity from $^3\Pi_g$-$^3\Sigma_g^-$ and $^1\Pi_g$-$^1\Delta_g$ transitions, which are determined by the orbital angular-momentum operator. This source is not the principal one for the intensity of the second (b-X) transition. Its intensity is stolen principally from microwave transitions between spin sublevels of the ground $^3\Sigma_g^-$ state. The last source explains the large difference in intensities of the a-X and b-X transitions. Calculated oscillator strengths are in a good agreement with experiment. The same integrals that determine the intensity also determine the parameters of the spin Hamiltonian for the ground $^3\Sigma_g^-$ state. These parameters are in a good agreement with experiment also, showing the validity of the whole calculation. In a condensed phase the investigated transitions are enhanced by intermolecular exchange interaction. It is known that an external heavy atom (EHA) enhances the b-X transition of oxygen in solution, but does not influence the a-X transition. In the collision complex O_2-EHA, which has a geometry without inversion symmetry, the microwave transitions between spin sublevels of the "$^3\Sigma_g^-$" state obtain electric-dipole moments, which are stolen from the charge-transfer transition. This mechanism explains the selective effect of EHA.

In 1984 B. Minaev has defended his doctoral dissertation for specialty 02.00.04. – physical chemistry. The doctoral dissertation topic was the following: «Theoretical analysis and prognostication of spin-orbit coupling effects in molecular spectroscopy and chemical kinetics». In a letter signed by the head Academician V. A. Legasov, the Expert Council of the Higher Attestation Commission of the USSR allowed B. Minaev to acquire a doctorate in chemical sciences on the basis of defence of the author's abstract without writing the whole dissertation. The defense took place in the N. N. Semenov Institute of Chemical Physics of the USSR Academy of Sciences in Moscow and triggered a great interest in the scientific community. The Dissertation Council of the Institute consisted of leading scientists of the Academy of Sciences of the USSR (among them two Nobel laureates).

In 1984 Boris Minaev headed a newly created Quantum Chemistry Department at the Karaganda State University which was the second (after Moscow State University) in the Soviet Union. During this time he trained six PhDs and two doctors of science.



ОРДЕНА ЛЕНИНА ИНСТИТУТ ХИМИЧЕСКОЙ ФИЗИКИ
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МИНАЕВ Борис Филиппович

ТЕОРЕТИЧЕСКИЙ АНАЛИЗ И ПРОГНОЗИРОВАНИЕ ЭФФЕКТОВ СПИН-ОРБИТАЛЬНОГО ВЗАИМОДЕЙСТВИЯ В МОЛЕКУЛЯРНОЙ СПЕКТРОСКОПИИ И ХИМИЧЕСКОЙ КИНЕТИКЕ

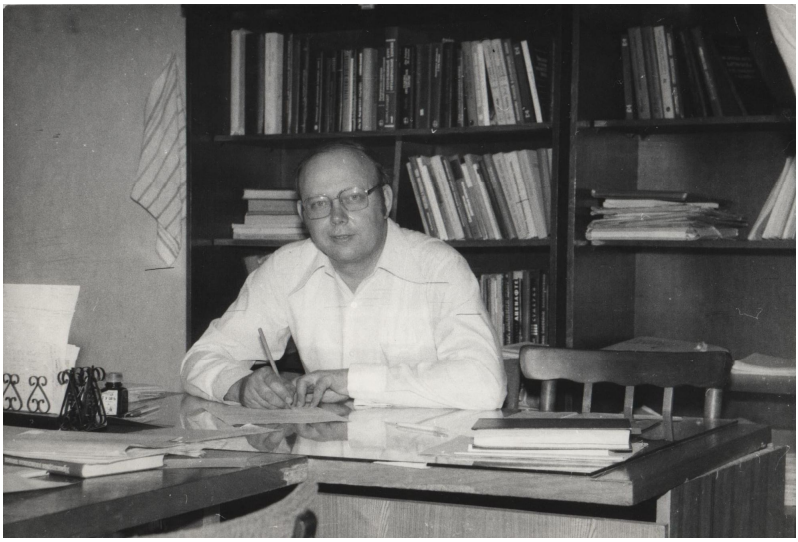
02.00.04 — физическая химия

АВТОРЕФЕРАТ

диссертации на соискание ученой степени
доктора химических наук

МОСКВА 1983 г.

Boris Minaev with colleagues from the Organic Chemistry Department, Karaganda State University, 1975



In the Quantum Chemistry Laboratory (Karaganda, 1985)

Boris Minaev with colleagues and PhD students of the Quantum Chemistry Department, Karaganda State University, 1985

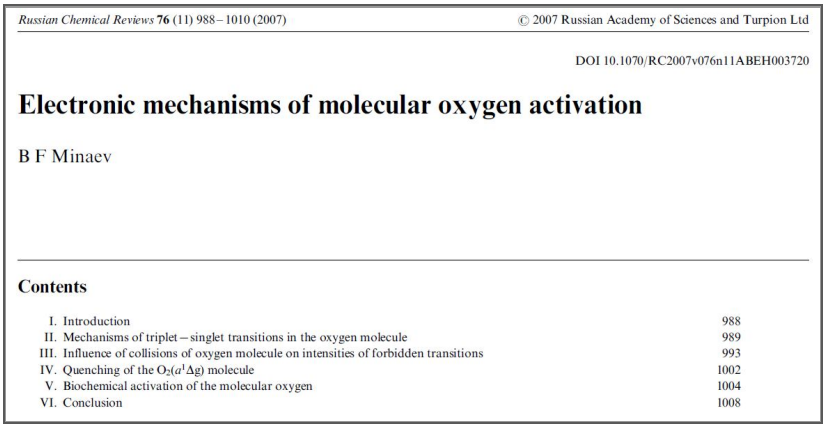
At that time B. Minaev's scientific school took a strong position in the quantum chemistry of the former USSR and gained wide popularity abroad. Working at the Karaganda State University, Prof. Minaev developed the optical detection of magnetic resonance (ODMR) theory in the low-temperature phosphorescence spectra of molecular crystals and the emission intensity of singlet oxygen in the gas phase and solutions, which was topical at that time. This theory was first reported by B. Minaev in 1982 at the All-Union School of Quantum Chemistry (Karkaralinsk, near Karaganda), but the theory was widely recognized only after 1997, when German physicists have performed its direct verification based on impulse experiments [7].

The growth of chaos due to the restructuring and disintegration of the USSR forced B. Minaev to leave Kazakhstan. He was invited to take the post of head of the Chemistry Department at the branch of the Kiev Polytechnic Institute in Cherkasy. Since February 1988 he worked at this branch which was later reformed into the Cherkasy State Technological University (CSTU). During his work in CSTU B. Minaev taught three PhD in chemical sciences.

At the same time, Professor Minaev delivered lecture cources in Quantum Chemistry at the Bohdan Khmelnytsky National University of Cherkasy (ChNU). In 2007 he was appointed as a head of the Organic Chemistry Department of ChNU and later (2016) – the head of the Department of Chemistry and Nanomaterials Science of ChNU.

Coworkers of the Department of Chemistry and Nanomaterials Science, 2018

Thus, for a quarter of a century initiated by Professor B. Minaev intense study of the electronic structure, spectra and chemical reactivity of molecules is carried out in Cherkasy considering the spin-orbital and other weak magnetic perturbations. In addition to the traditional approach in magnetochemistry, when magnetic perturbations are taken into account for calculation of the hyperfine structure in EPR spectra of radicals or in nuclear magnetic resonance (NMR) of diamagnetic molecules, Minaev focuses on the role of triplet states in chemistry, catalysis, molecular electronics and biochemistry based on calculations of SOC, spin-spin coupling, g-factor anisotropy and other internal magnetic interactions [11].



Russian Chemical Reviews **76** (11) 988 – 1010 (2007)

DOI 10.1070/RC2007v076n11ABEH003720

Electronic mechanisms of molecular oxygen activation

B F Minaev

Contents

Chemically stable substances that exist under normal conditions typically are diamagnetic, i.e. have a singlet ground state; due to saturation of chemical valences all electron spins are paired and full electron spin is equal to zero. The first excited state of such molecules is always a triplet (T_1) and is characterized by the presence of two unpaired electron spins [12]. The triplet states of many molecules are photochemically stable; they are well studied in the phosphorescence and EPR

spectra and by T-T energy transfer in crystals, glass and liquid solutions [12]. Since the spontaneous transition from the T_1 state to the ground singlet state (S_0) is spin-forbidden and can occur only due to a weak SOC that leads to a slight mixing of singlet and triplet states; thus, the T_1 state is metastable. It is not surprising that many photochemical reactions take place through an intermediate triplet T_1 state. B. Minaev and colleagues carried out numerous calculations of the electronic mechanisms for the photochemical reactions taking into account SOC, in particular, for the T-S transitions in intermediate biradicals [11, 13–15]. He showed that the role of triplet states is much broader and is not limited to the photochemical processes only. Boris Filipovych has long held and expressed the opinion that almost all chemistry of diamagnetic substances is encoded in the properties of unpaired electrons of the excited triplet state [12]. Upon chemical transformations the molecules pass through the activated complex stages whose electronic structure is much closer to the properties of the triplet state intermediate than to the ground S_0 state properties. This idea was obtained from the quantum chemical calculations and now it seems obvious, although its experimental verification is very complicated because all measurements in chemistry are carried out for the stable molecules and the transition state can be studied only by indirect methods of chemical kinetics. Solving the Schrödinger equation, we can calculate both an unstable molecule and any of its excited states. The calculations of the transition states of chemical reactions have shown that the spin flipping can occur during the dark (not only photochemical) transformations. Spin-orbit coupling can effectively mix the S and T states in the activated complex and induces the switching of chemical reactions channels, thus, gaining the greater excess in the exchange energy, which mainly controls the chemical bond and

reactivity. If we compare the energy consumption for overcoming the energy activation barrier of a chemical reaction with the ram, which breaks down the fortified wall, then the weak spin-orbit coupling can be compared to a small key, whose turn easily opens fortress gates. Most catalysts act by the same principle particularly the enzymes; although the role of spin in catalysis can be more complicated. In this case, an important role can be played not only by magnetic interactions, but also by spin exchange with a catalyst [11, 13–15]. For example, the oxidation of organic substances is a highly exothermic reaction that ensured the rapid evolution of aerobic life forms after the emergence of photosynthesis on the Earth (the first blue-green algae). Thus, the appearance of oxygen in the atmosphere 1.4 billion years ago started the development of new oxidase enzymes which efficiently overcome spin prohibition for the triplet O_2 reactions with organic matter. We note here that all living matter is thermodynamically unstable in the sense of possible combustion in oxygen of the air. However, the entire Earth's biosphere is quite stable which, in fact, contradicts the basic principles of thermodynamics. This paradox can be explained by the kinetic spin barriers for reactions of the triplet oxygen. Before Minaev's papers [11, 13] in biochemistry there was no clear idea of the role of these prohibitions and how they are overcome in living matter (in the respiratory chain and in the cellular oxidation of carbohydrates, fats and lipids). Oxygen is paramagnetic and most of the organic nutrients and their oxidation products are diamagnetic. By the spin prohibition of the burning of organic substances it requires initial activation by the high-temperature stage of ignition for the formation of initial radicals [14]. The radical-chain combustion process causes an uncontrolled release of energy in the form of heat and light [14, 15]. Clearly, such oxidation mechanism is unacceptable for living cells. Thanks

to metabolism the energy needs of animal cells are satisfied by the energy release upon oxidation of organic compounds with participation of molecular oxygen [11]. This energy is used by the cell to carry out all chemical syntheses of DNA and proteins, ion transport, mechanical work and brain activity.

All various metabolic processes and reactions that provide energy to the whole aerobic life are the subjects to subtle enzymatic control. Until now the question of the spin control specifics in biological oxidation processes by molecular oxygen remained open.

B. Minaev together with colleagues from the University of Stockholm have carried out quantum chemical calculations of the electronic structure for a number of enzymes of flavoproteins and copper containing aminoxidase [13]. In reaction with oxygen these enzymes form superoxide ion O_2^-, the same happens upon spontaneous oxidation of hemoglobin, ferredoxin and adrenaline [14]. B. Minaev has shown for the first time why the oxidative attack by the O_2 molecule is slow and why after the addition of the first electron to oxygen the further reduction proceeds easily [11]. It was found that the oxygen activation (as an age-old riddle of biochemistry) can be explained by a very simple spin effect which is a clear from the physical point of view; i.e. a large spin-orbit coupling between the quasi-degenerate states of the superoxide ion formed in the radical pair with the enzyme (flavoproteins) and fast spin-lattice relaxation in this radical [12]. These ideas were first presented in 2002 at the congress in Tokyo [11] but B. Minaev returned repeatedly to them as it is evidenced by the following papers [12–15]. It turned out that the manifestation of internal magnetic interactions in the spectra of O_2 is associated with the oxygen activation by the oxygenase, oxidases and other enzymes.

Dioxygen Spectra and Bioactivation

Boris F. Minaev,[a] N. Arul Murugan,[b] and Hans Ågren*[b]

Intensities of spin-forbidden transitions in electronic absorption and emission spectra of molecular oxygen are analyzed in order to understand the key mechanisms of spin-states mixing induced by spin-orbit coupling (SOC) and the ways to overcome spin prohibition for various photophysical and biochemical processes. Multireference configuration interaction calculations with SOC account are used to generalize spin-selection rules for the oxygen atmospheric and Herzberg bands in free O_2 molecule and in collision complexes. Intensity enhancement of the atmospheric $a^1\Delta_g \rightarrow X^3\Sigma_g^-$, $b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$, and Noxon $b^1\Sigma_g^+ \rightarrow a^1\Delta_g$ transitions upon bimolecular collisions are compared with those for Herzberg III transitions $A^3\Delta_u \leftarrow X^3\Sigma_g^-$. Electric quadrupole, dipole, and magnetic approximations are used for transition probability calculations. Intensity distribution in rotational lines is also considered. With this background, we propose some simple spin-selection rules for dioxygen activation in enzymatic reactions. © 2013 Wiley Periodicals, Inc.

DOI: 10.1002/qua.24390

Boris Minaev was born in Yekateriburg (Russia) in 1943. He has graduated from Tomsk State University (in Siberia) and received there his PhD in physics devoted to EPR and phosphorescence lifetime calculations. In 1974, Minaev received an assistant professor position in Karaganda State University (Kazakhstan) and the chief of physical chemistry chair (1976). He has defended habilitation work in Moscow Institute of chemical physics (1983) and created a quantum chemistry chair in Karaganda SU. Minaev moved to Ukraine just before the collapse of the Soviet Union and received a chemistry chair in Cherkassy Institute of Technology. Since 2007, he is a chief of Organic Chemistry Department and director of Scientific Institute of Physics and Chemistry of Functional Materials at Bogdan Khmelnitsky Natioanl University in Cherkasy. As a guest professor, during last decade, Minaev delivered lectures at the Royal Institute of Technology and collaborates with a group of Hans Ågren. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

N.A. Murugan was born in Paramakudi, India, in 1976. He received his master degree in general chemistry in 1998 from GRI Deemed University, Dindigul, India. He was awarded with a PhD degree from Indian Institute of Science in 2005 for his contributions in understanding temperature- and pressure-induced structural transitions in organic molecular crystals using variable shape Monte Carlo simulations. Until 2010, he had postdoctoral visits to ULB (Brussels), UPC (Barcelona), KTH (Stockholm). From 2011, he is working as a researcher at the Department of Theoretical Chemistry and Biology at the Royal Institute of Technology, Sweden. His current research is mostly devoted to understanding the structure, dynamics, and properties of molecular probes for medical diagnosis application. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Hans Ågren was born 1950 in the town of Skelleftea in northern Sweden. In 1979, he received his PhD in experimental atomic and molecular physics at the University of Uppsala under the supervision of Kai Siegbahn. After a few PostDoc years in USA, he became assistant professor in Quantum Chemistry in Uppsala in 1983. He became the first holder of the chairs in Computational Physics at Linköping University in 1991 and in Theoretical Chemistry at the Royal Institute of Technology, Stockholm, in 1998. The Department of Theoretical Chemistry and Biology at KTH, which he currently heads, houses ca 20 scientists and 40 PhD students, with research activities in theoretical modeling primarily in the areas of molecular/nano/bio photonics and electronics, in catalysis, and in X-ray science. The research is a mix of method development and problem-oriented applications in collaboration with experimentalists. Hans Ågren participates in several national and international networks in his research areas. He spends his spare moments in the summer cottage close to his home town up north, with some fishing and mountain hiking. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

ACCOUNTS of chemical research

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Singlet Oxygen Photophysics in Liquid Solvents: Converging on a Unified Picture

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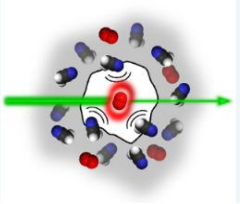
Supporting Information

CONSPECTUS: Singlet oxygen, $O_2(a^1\Delta_g)$, the lowest excited electronic state of molecular oxygen, is an omnipresent part of life on earth. It is readily formed through a variety of chemical and photochemical processes, and its unique reactions are important not just as a tool in chemical syntheses but also in processes that range from polymer degradation to signaling in biological cells. For these reasons, $O_2(a^1\Delta_g)$ has been the subject of intense activity in a broad distribution of scientific fields for the past ~50 years.

The characteristic reactions of $O_2(a^1\Delta_g)$ kinetically compete with processes that deactivate this excited state to the ground state of oxygen, $O_2(X^3\Sigma_g^-)$. Moreover, $O_2(a^1\Delta_g)$ is ideally monitored using one of these deactivation channels: $O_2(a^1\Delta_g) \rightarrow O_2(X^3\Sigma_g^-)$ phosphorescence at 1270 nm. Thus, there is ample justification to study and control these competing processes, including those mediated by solvents, and the



The spin flip in the superoxide ion is equivalent to the T-S transition in the radical ion pair $FADH_2^+...O_2^-$, after that the usual "singlet-spin chemistry" of diamagnetic substances is observed, i.e. the transfer of the hydrogen atoms with formation of the H_2O_2 peroxide and oxidized flavinadenine dinucleotide (FAD). An unusual aspect which was shown by B. Minaev concerns the spin flip during the electron transfer stage and the formation of an ion-radical pair [12, 13]. The proposed spin relaxation mechanism in superoxide ions clarified this problem. The following reactions in the singlet state of the flavoprotein-O_2 system have small activation energies and proceed rapidly [13]. Since the release of radicals into the cell volume is detrimental to the living organism, therefore the spin transition inhibits the radical channel.

Thus, the spin effects play an important role in the discovery of the deep secrets of the living matter. Spin is an exclusively quantum property of an electron. The spin flip upon the T-S transition is one of the subtlest quantum effects which have no analogs in classical physics. We can note that the specificity of the living matter is determined by quantum

effects (for instance, the respiratory chain and enzymes oxidases which use the air oxygen to oxidize glucose).

We can conclude that the most effective medicine can be one of those which directly affect the quantum transitions in the living cells. This can be arranged via microwave electromagnetic fields (EMFs) [16] and radio terahertz EMFs. It should be noted that the T-S splitting in the radical pair $FADH_2^+...O_2^-$ belongs to the microwave range and it is possible to affect the rate of spin conversion and enzyme work by EMF. One should note that microwave fields have long been used in the treatment and diagnostics (nuclear tomography is based on NMR spectra, i.e. transitions between nuclear spin sublevels).

Another example of quantum medicine is the use of visible range lasers for cancer therapy. A dye molecule is supplied to the diseased cell and then it is transferred to an excited state using a laser and a light-guide fiber. The dye transfers its electronic excitation energy to the ground triplet molecular oxygen, which is always present in the cell solutions; thus, a new active form of singlet oxygen in the $^1\Delta_g$ state ($^1O_2$) is obtained [17, 18]. There is no spin inhibition for singlet oxygen in reactions with diamagnetic substances and the $^1O_2$ is very reactive. This oxygen kills the diseased tumor cells. More than a hundred papers by Minaev together with his PhD students are dedicated to the theoretical studies of singlet oxygen. The doctoral and eight candidate theses on this topic are defended.

B. Minaev has explained for the first time the mechanism of singlet $^1\Delta_g$ and $^1\Sigma_g^+$ oxygen emission in a gas phase without collisions (at zero pressure) and in solutions. He has also explained the O_2 ($^1\Delta_g$) quenching, calculated the oxygen effect on the singlet-triplet transitions in molecular crystals and predicted several cooperative effects in the oxygen collisions complexes with diamagnetic and paramagnetic molecules. A reach experience acquired through studying the spin effects

in oxygen has certainly helped Minaev in the development of the enzymatic spin-catalysis theory. For example, the SOC effect between different charge-transfer states in the theory of singlet oxygen quenching by aliphatic amines in gas phase, proposed 35 years ago [126], was recently considered to explain the spin-relaxation rate in superoxide ion for discovery of O_2 activation mechanism by various oxidases and oxygenases [11, 13].

Ukrainian Biochemical Journal, 2009, Vol. 81, N. 3

СПИН-КАТАЛИЗ В ПРОЦЕССАХ ФОТО- И БИОАКТИВАЦИИ МОЛЕКУЛЯРНОГО КИСЛОРОДА

Б. Ф. МИНАЕВ

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e-mail: bfmin@rambler.ru

Обзор посвящен анализу электронно-спиновых механизмов фотофизической и биохимической активации кислорода. Парамагнитный характер основного состояния молекулы O_2 приводит к сильным спиновым запретам на химические реакции кислорода с органическими веществами, а также на оптические триплет-синглетные (T-S)-переходы в видимой и ближней инфракрасной областях спектра. Ускорение радиационных и безызлучательных T-S-переходов в молекуле O_2 под влиянием растворителя, включая сенсибилизацию синглетного кислорода, $O_2(a^1\Delta_g)$, а также T-S-переходы в реакциях O_2 с энзимами, обьединены под термином спин-катализ. Рассмотрена структура и энергетика низших состояний кислорода, а также его комплексов с энзимами и растворителями. С учетом спин-орбитального взаимодействия (СОВ) обьяснено усиление вероятности перехода $a^1\Delta_g - X^3\Sigma^-_g$, а также его тушение в различных растворителях (Р). Отмечена роль переноса заряда $P^+ {}^3O_2^-$, приводящая к росту СОВ между T-S-состояниями. Знания физических механизмов активации и тушения синглетного $O_2(a^1\Delta_g)$ кислорода важны не только для его детектирования in vivo (фотобиология), но и для понимания энзиматических процессов окисления кислородом.

К л ю ч е в ы е с л о в а: синглетный кислород, супероксид-ион, глюкозооксидаза, медьаминоксидазы, гемоглобин, миоглобин, цитохромоксидазы, спин-орбитальное и обменное взаимодействие, фотодинамическая терапия.

B. Minaev pays much attention to the problems of ecology [18–28]. It is well known that singlet $^1\Delta_g$ oxygen participates in the smog formation over smoky cities. In the upper atmosphere there is a constant O_2 photodissociation into atoms and their reverse recombination with formation of the oxygen metastable forms. The O_2 molecule absorbs almost all solar radiation in the ultraviolet region due to absorption in the Schumann-Runge band. The question of the longer-wavelength oxygen absorption is extremely important for the atmospheric photochemistry simulation and the ozone layer problem. All electronic transitions in the spectrum of O_2 molecule in the

long-wave region (200–1300 nm) are spin-forbidden or parity-forbidden. Therefore, it is very difficult to determine the intensity of these weak transitions, although worldwide attempts are being made to measure the intensity of new oxygen bands using the modern experimental methods.

Recently, Minaev's group has carried out quantum chemical calculations to determine intensity of the new oxygen singlet-triplet bands. The absorption spectra of the singlet oxygen $b^1\Sigma_g^+ \rightarrow B^3\Sigma_u^-$ were calculated for the first time. It was found that the $a^1\Delta_g \rightarrow c^1\Sigma_u^-$ transition is comparatively intense. This fact was confirmed by the researchers from NASA (USA).

Absorption of the stratospheric ozone in the near-UV region saves life on the Earth from harmful Sun radiation [19]. B. Minaev and his PhD students from CSTU for many years worked on the budget-supported topics dedicated to calculations of the ozone S-T absorption spectra and its photocatalytic decomposition with participation of halogen oxides [19, 20]. In these papers, the role of spin-orbit coupling and spin-effects in ozone decay is considered for the first time. It is shown that the weak ozone absorption in the region 1000 nm (the Wulf band) is a triplet-singlet transition [19]. The upper T-excited state of this bands system is metastable; its energy is just above the dissociative limit and is separated by an insignificant potential barrier. Since these states can be formed by recombination of atom and oxygen molecule in the lower stratosphere, where the pressure of extraneous gases is still high, then there is no need for triple collisions for the ozone formation from metastable T-states. This fact is extremely important for photochemistry of the ozone layer and the greenhouse effect.

B. F. Minaev has also predicted the spin-orbit effects in the photodecay of chloric(I) HClO and bromic(I) HBrO acids [20], which play an important role in the photochemical cycle of ozone decay. The study of the spin-selectivity of the

photolysis processes for these acids and ozone itself allows concluding about the possible effect of external magnetic fields on the ozone layer.

In recent years [21–23] B. F. Minaev pays much attention to the application of quantum chemistry in nanotechnology. Now it is possible to collect nanoclusters «manually», which allows them to be embedded in semiconductor structure, to use them as memory elements, molecular conductors, etc. Unique properties of the fullerenes and nanotubes allow their application in electronics, quantum computers, DNA testing, genetic engineering and medicine. Quantum chemistry methods play an important role, since they allow to predict and understand the processes occurring at the atomic and electronic levels. In this case, the quantum theory directly intersects with the technology. Design and synthesis of novel organic polymers with high conductivity and superconductivity can be planned based on quantum-chemical calculations [22–27]. New OLEDs are created based on the polythiophene and other conjugated polymers and contain impurities of iridium and ruthenium complexes. The calculations of their electronic structure are the focus of many leading laboratories around the world, in particular, the USA, Japan and other countries. B. Minaev for the first time has taken into account the effects of the SOC influence on the conductivity of this type polymers and molecular conductors [23]. On this basis, the influence of the external magnetic field and microwave fields on the conductivity of polymer films was predicted [23]. The possibility of ferromagnetic spin formation in molecular systems consisting of bi- and mono-radicals has long been of interest to physicists and chemists [1]. The calculations carried out at the Department of Chemistry and Nanomaterials of the ChNU [28–30] consider not only exchange interactions but also SOC effects. In particular, the calculation of the zero-field splitting and the spin-selectivity for the reactions of the

synthesis of magnetic polymers can be very significant for obtaining these materials. This represents a new branch of nanomaterialology – spintronics. These studies are closely related to the spin-catalysis problem, which B. Minaev has been engaged in for many years [1, 3, 16, 17, 24–40].

It is known that about 90% of all processes in the chemical industry and almost all biochemical reactions are catalytic. The enzymes are significantly superior to industrial catalysts due to their high activity and chemical specificity. As noted above, the spin effects play a central role in the work for some enzymes, such as FAD-based oxidases. It is not surprising that the general catalysis theory should take them into consideration. The production of ammonia, sulfate and nitric acids, oil-cracking and synthesis of polymers are large scale manufacturing depending on the catalysts activity [25, 36]. B. Minaev has proposed catalysis models in which the main attention is paid to spin-dependent electronic activation mechanisms. For example, the methane activation by platinum and palladium clusters is reduced to the addition of a triplet-excited state of methane to the triplet states of metals [25–27]. This double-triplet state [28–30] has zero total spin, like the initial reagents, while methane molecule in triplet state dissociate spontaneously into the radicals $CH_3 + H$; but methane decomposition in the ground singlet state requires high activation energy [24]. The catalyst makes it possible to involve the triplet state of methane in the process of the C–H bond breaking. It was found an important catalyst characteristic which relates to the establishment of the position its triplet level [24]. Previously, this catalyst parameter was not considered. Spin-splitting on the activated chemical bond can occur under the catalyst action without changing of the total spin for the whole system (exchange mechanism) or due to the spin-orbit coupling with a spin flip. Spin-catalysis concept was applied to the adsorption of acetylene, ethylene and benzene on

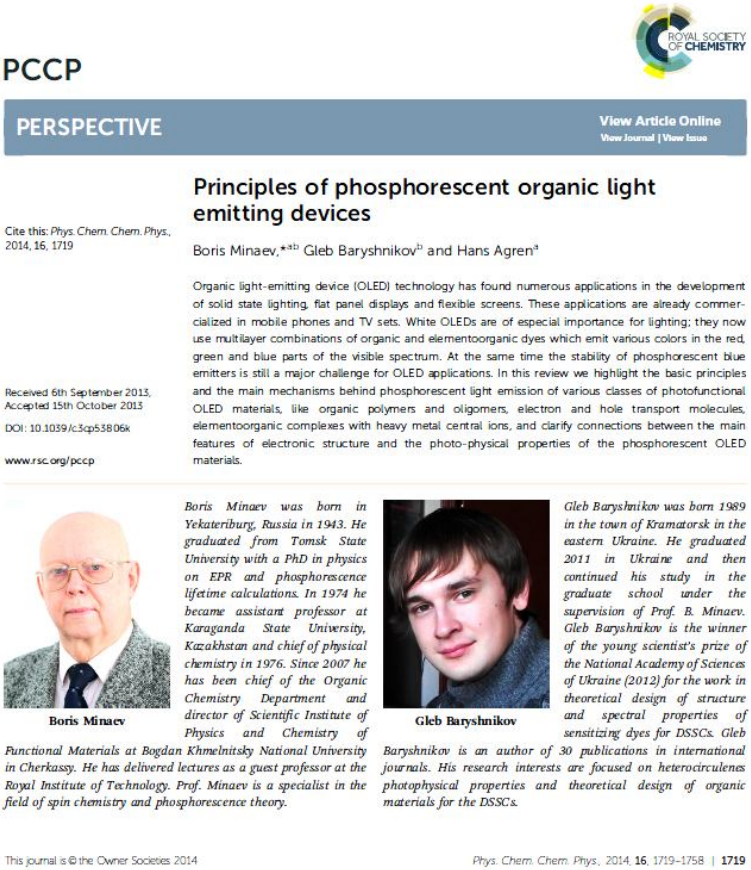
the surface for a number of metals [25–27]. It is shown that adsorbed molecules have a shape that almost coincides with the structure of triplet-excited molecules wherein the cluster that simulates a metal surface also has unpaired spins.

Coordination of alkanes with metal complexes is the initial stage for many important catalytic processes. It is interesting to note, that organometallic rhodium and iridium complexes activate methane, while similar isovalent cobalt complexes – do not. An explanation of this paradox was found in the spin-catalysis theory [27]. The cobalt complex has a triplet ground state and cannot carry out T-S transitions due to weak SOC; its catalytic activity in the methane activation is spin-blocked. Working at the Cherkasy National University, B. F. Minaev has showed that the SOC effects play an important role in many physical, chemical and biological processes [25–40]. They are important in catalysis, molecular electronics, atmospheric chemistry, combustion physics, biology, cellular respiration.

In 1993, at a seminar at the Department of Molecular Electronics in Linköping (Sweden), B. Minaev focused for the first time on the important effects of spin-orbit interaction in organic light-emitting diodes (OLEDs) because the singlet-triplet transitions increase threefold efficiency of recombination of electrons and holes during electroluminescence. In 1999, in the United States, this idea was implemented in the use of heavy ion complexes of Iridium. At that time B. Minaev was the first to apply the DFT theory for calculation of the spin-orbit coupling in the Ir(III) complex with phenylpyridyllium ligands to explain the work of phosphorescent OLEDs.

In the future, the papers dedicated to the study of Ir(III) complexes for OLED applications laid the foundation for new directions in the development of molecular electronics that was fixed in cooperation with the Department of Electronic Devices, Lviv Polytechnic National University. These papers

dedicated to the OLED studies are summarized in a review published in the journal Physical Chemistry Chemical Physics (PCCP) in 2014 which according to the Scopus agency has been cited more than 200 times.



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Cite this: *Phys. Chem. Chem. Phys.*, 2014, 16, 1719

Principles of phosphorescent organic light emitting devices

Boris Minaev,*[ab] Gleb Baryshnikov[b] and Hans Agren[a]

Organic light-emitting device (OLED) technology has found numerous applications in the development of solid state lighting, flat panel displays and flexible screens. These applications are already commercialized in mobile phones and TV sets. White OLEDs are of especial importance for lighting; they now use multilayer combinations of organic and elementoorganic dyes which emit various colors in the red, green and blue parts of the visible spectrum. At the same time the stability of phosphorescent blue emitters is still a major challenge for OLED applications. In this review we highlight the basic principles and the main mechanisms behind phosphorescent light emission of various classes of photofunctional OLED materials, like organic polymers and oligomers, electron and hole transport molecules, elementoorganic complexes with heavy metal central ions, and clarify connections between the main features of electronic structure and the photo-physical properties of the phosphorescent OLED materials.

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Accepted 15th October 2013

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www.rsc.org/pccp

Boris Minaev

Boris Minaev was born in Yekateriburg, Russia in 1943. He graduated from Tomsk State University with a PhD in physics on EPR and phosphorescence lifetime calculations. In 1974 he became assistant professor at Karaganda State University, Kazakhstan and chief of physical chemistry in 1976. Since 2007 he has been chief of the Organic Chemistry Department and director of Scientific Institute of Physics and Chemistry of Functional Materials at Bogdan Khmelnitsky National University in Cherkassy. He has delivered lectures as a guest professor at the Royal Institute of Technology. Prof. Minaev is a specialist in the field of spin chemistry and phosphorescence theory.

Gleb Baryshnikov

Gleb Baryshnikov was born 1989 in the town of Kramatorsk in the eastern Ukraine. He graduated 2011 in Ukraine and then continued his study in the graduate school under the supervision of Prof. B. Minaev. Gleb Baryshnikov is the winner of the young scientist's prize of the National Academy of Sciences of Ukraine (2012) for the work in theoretical design of structure and spectral properties of sensitizing dyes for DSSCs. Gleb Baryshnikov is an author of 30 publications in international journals. His research interests are focused on heterocirculenes photophysical properties and theoretical design of organic materials for the DSSCs.

A new direction in the development of our department was founded in 2011 and is associated with research of circulenes. These materials have attracted the attention of Boris Minaev due to their high symmetry and their use as promising materials for OLED applications. A lot of DFT calculations of the electronic structure, IR and UV-Vis spectra of tetraoxa[8]circulenes, their magnetic and aromatic properties

was performed at the Department of Chemistry and Nanomaterials Science of the ChNU. This served as an impetus to strengthening solid-state DFT calculations of two-dimensional nanopolymers based on [8]circulenes, as well as modeling of novel nitrogen-containing high-energy materials. Novel graphene allotropes were proposed. This paper was published in the «Chemical Physics Letters» journal (Elsevier) and was placed on the cover of this journal for the editor's choice as the most significant article in this issue.

Chemical Physics Letters 612 (2014) 229–233

Contents lists available at ScienceDirect

Chemical Physics Letters

journal homepage: www.elsevier.com/locate/cplett

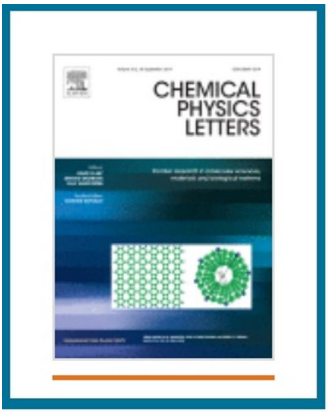
DFT characterization of a new possible graphene allotrope

Nataliya N. Karaush[a,*], Gleb V. Baryshnikov[a], Boris F. Minaev[a,b]

[a] Bohdan Khmelnytsky National University, 18031 Cherkasy, Ukraine

Abstract

In the present work we have studied the electronic and magnetic properties of the new one- and two-dimensional π-conjugated materials containing biphenylene (Bp)-monomer on the basis of DFT calculations including the periodic boundary condition for the infinite structures. Thus, we have predicted a new planar and stable graphene allotrope composed of a combination of the four-, six- and eight-membered rings of the (4, 6, 6, 8) topology, which resembles the classical graphene. These novel materials are predicted to demonstrate the promising hole/electron mobility values which are typical for the ambipolar organic semiconductors. Furthermore, the growth of π-conjugated Bp-based 2D sheets leads to the material with the band-gap being significantly smaller than that for the 1D polymer ribbons containing the same number of the Bp-units. The Bp-based nanotubes are also designed and are predicted to be promising candidates for miniaturizing electronics.



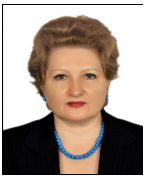
B. Minaev pays much attention to working with young people [41–95]. His lectures on biochemistry, ecology and quantum chemistry do not leave students indifferent. The lectures combine high professionalism, scientific depth and emotional tension. The information about atoms and quanta is always reported interestingly with additions from personal research experience and with humor.

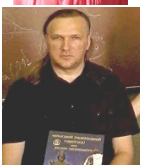
Boris F. Minaev with students, 2013

Working with graduate students B. Minaev is very demanding and at the same time very generous; he constantly shares his findings, gives ideas and, in general, helps a lot in this hard work on the calculation of the electronic srtucture of molecules.

Under the supervision of Prof. Minaev sixteen theses for the PhD degree in chemistry were defended and five theses for the Doctor of Science (Dr.Sc.) degree.

Doctors and Candidates (PhD) of Sciences which came out of the B. F. Minaev's group

1	Irgibaeva I. S. PhD in Physical and Mathematical Sciences, Dr. Sc. in Chemistry	Professor of the L. M. Gumilev Eurasian National University, Astana, Kazakhstan	
2	Dausheev J. K. PhD in Chemistry	Assistant Professor of the Kazakh Chemical Technology University, Shymkent, Kazakhstan	
3	Mukhin R. R. PhD in Chemistry Dr.Sc.in Physics and Mathematics	Professor of the Starooskol Institute of Technology, Stary Oskol, Russia	
4	Buketova A. E. PhD in Chemistry Dr.Sc. in Technical Sciences	Assistant Professor at the Department of Chemical Engineering, Kazakhstan-British Technical University, Almaty, Kazakhstan	
5	Ivanova N. M. PhD in Chemistry Dr.Sc. in Chemistry	Head of Electrocatalysis Laboratory, Institute of Organic Synthesis and Coal Chemistry, Karaganda, Kazakhstan	

6	Kukueva V. V. PhD in Chemistry	Doctoral position of the State Institution «Institute of Environmental Geochemistry of National Academy of Sciences of Ukraine», Kyiv, Ukraine	
7	Khomenko O. M. PhD in Chemistry	Professor, Head of the Department of Ecology Cherkasy State Technological University, Cherkasy, Ukraine	
8	Kobzev G. I. PhD in Chemistry Dr.Sc. in Chemistry	Professor of the Department of Chemistry, Orenburg State University, Russia	
9	Loboda O. A. PhD in Chemistry	Research associate of the Institute of Chemistry, Karl Franz Graz University, Graz, Austria	
10	Shevchenko O. P. PhD in Chemistry	Assistant Professor at the Department of Chemistry and Nanomaterials Science, Bohdan Khmelnytsky National University of Cherkasy, Ukraine	
11	Yashchuk L. B. PhD in Chemistry	Assistant Professor at the Department of Ecology, Cherkasy State Technological University, Cherkasy, Ukraine	
12	Sathya Perumal PhD in Chemistry	Indian Institute of Science, Department of Structural Chemistry, Bangalore, India	

13 Litvin V. A.
PhD in Chemistry
Assistant Professor at the Department of Chemistry and Nanomaterials Science, Bohdan Khmelnytsky National University of Cherkasy, Ukraine

14 Filonenko S. M.
PhD in Chemistry
Research associate of the Department of Porous Materials and Sorbents, L. V. Pisarzhevsky Institute of Physical Chemistry of the National Academy of Sciences, Kyiv, Ukraine

15 Baryshnikov G. V.
PhD in Chemistry
Assistant Professor at the Department of Chemistry and Nanomaterials Science, Bohdan Khmelnytsky National University of Cherkasy, Ukraine

16 Bondarchuk S. V.
PhD in Chemistry
Senior Lecturer at the Department of Quality, Standardization and Project Management, Bohdan Khmelnytsky National University of Cherkasy, Ukraine

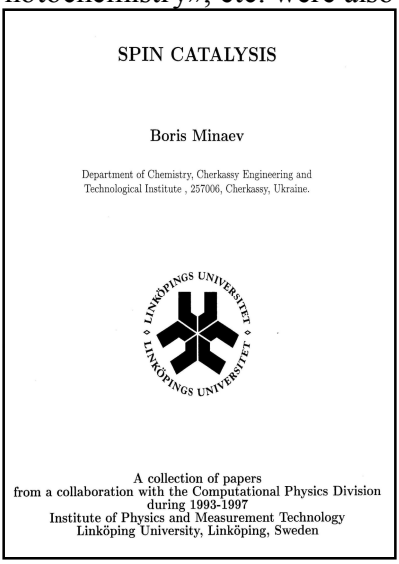
17 Karaush-Karmazin N. N.
PhD in Chemistry
PhD researcher of the Quantum Chemistry Laboratory, Bohdan Khmelnytsky National University of Cherkasy, Ukraine

All these years, his wife, Valentina A. Minaeva, (PhD in Chemistry, Assistant Professor) works together with Boris F. Minaev. She is his science and life partner. They have prepared over a hundred of their joint scientific papers. Their works are dedicated to decoding the IR and UV spectra of organic and organoelemental dyes, steroid hormones, hemoglobin and other compounds.

B. F. Minaev with his wife at the internship at the Department of Theoretical Chemistry and Biology at the Royal Technological University (Stockholm, Sweden, 2002)

Scientific Achievements of B. Minaev

B. F. Minaev's scientific achievements include more than 600 papers in the high-ranking international journals in the field of quantum chemistry, as well as six monographs. Three of them were published by the USSR «Science» publishing house: «The theory of electronic structure of molecules» (1988), «Quantum electrochemistry of alkaloids» (1986), «Optical and magnetic properties of the triplet state» (1983). The textbook «Organic Electronics» (2014) was published at the Lviv Polytechnic National University, and the monograph «Electronic structure and spectral properties of heterocirculenes» (2017) was published by the ChNU publishing house. Two great sections were published in the monographs «Organic Light Emitting Diode – Material, Process and Devices» (2011) and «Handbook of Computational Chemistry» (2017). The Linköping University (Sweden) has published a voluminous book «Spin Catalysis» covering five years of B. Minaev's work. The lecture courses «Quantum Chemistry», «Spectral Research Methods», «Physics and Chemistry of Nanomaterials», «Theoretical Foundations of Organic Chemistry», «Fundamentals of Photochemistry», etc. were also developed.

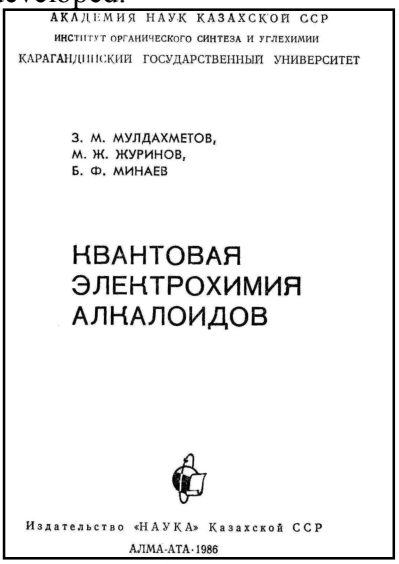

SPIN CATALYSIS

Boris Minaev

Department of Chemistry, Cherkassy Engineering and Technological Institute , 257006, Cherkassy, Ukraine.

LINKÖPINGS UNIVERSITET

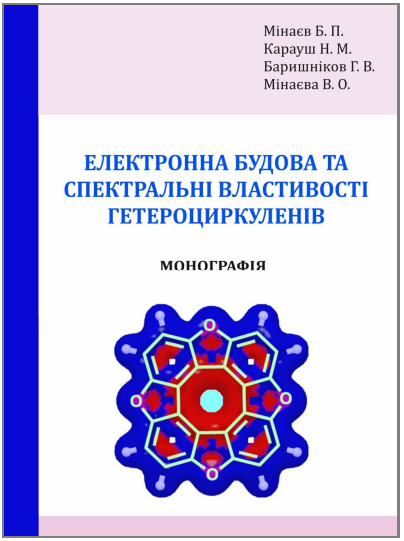
A collection of papers
from a collaboration with the Computational Physics Division
during 1993-1997
Institute of Physics and Measurement Technology
Linköping University, Linköping, Sweden

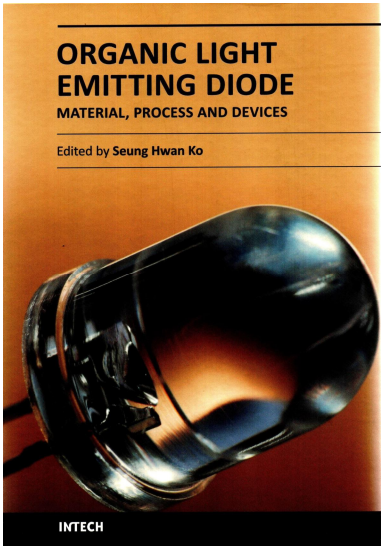

АКАДЕМИЯ НАУК КАЗАХСКОЙ ССР
ИНСТИТУТ ОРГАНИЧЕСКОГО СИНТЕЗА И УГЛЕХИМИИ
КАРАГАНДИНСКИЙ ГОСУДАРСТВЕННЫЙ УНИВЕРСИТЕТ

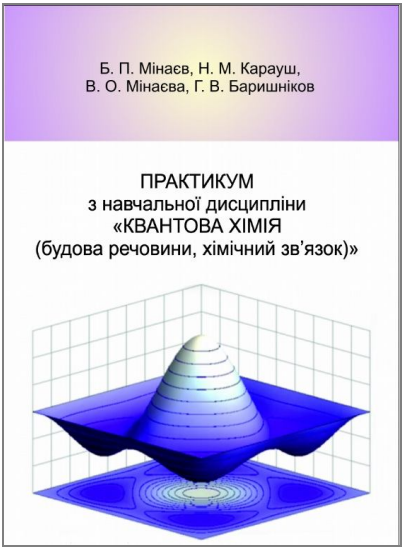
З. М. МУЛДАХМЕТОВ,
М. Ж. ЖУРИНОВ,
Б. Ф. МИНАЕВ

КВАНТОВАЯ ЭЛЕКТРОХИМИЯ АЛКАЛОИДОВ

Издательство «НАУКА» Казахской ССР
АЛМА-АТА·1986







B. Minaev headed a number of scientific grants: INTAS (1993–1996) «Spin Catalysis», a joint Ukrainian-American grant CRDF (UKC1-2819-CK-06) «Theoretical study of new spectral bands of the oxygen molecule and the processes

induced by collisions in the nightglow of the atmosphere» (2006–2008), a joint Ukrainian-Romanian grant «Design of novel sensitizing dyes for nanocrystalline TiO_2 solar cells on the basis of their electronic structure calculations» (2008–2009), Swedish-Ukrainian grant Visby «Theoretical design of solar cell dyes» (2008–2011). He has received the title of «Soros Professor» (1997), and a personal grant from the Chinese Academy of Sciences (CAS) in the framework of the international initiative of the President of CAS of the People's Republic of China for invited scientists (Institute of Chemistry of the Chinese Academy of Sciences, Beijing, 2015). Now he heads the scientific research of the Department of Chemistry and Nanomaterials Science within the state budget framework. B. Minaev is the winner of the World Prize «World Lifetime Achievement Award ABI-USA-1999», awarded with a medal «25 years for the Central-Kazakhstan Brahch of the National Academy of Sciences of the Kazakhstan Republic» for the merits in development of chemical science in Kazakhstan Republic (2010), and honorary title «Honoured Worker of Science and Technology of Ukraine» (2011). Recently he received the prestigious «Scopus Award Ukraine» (2016), and a medal of the Ukrainian Cabinet of Ministers (2017).

Awarding «Scopus Award Ukraine» by the British representative of the «Elsevier», 2016

In June 18, 2016, B. F. Minaev was elected as an Academician of the Ukrainian Higher School Academy of Sciences.


ДИПЛОМ

АКАДЕМІКА АКАДЕМІЇ НАУК ВИЩОЇ ШКОЛИ УКРАЇНИ

№ 279

м. Київ

АКАДЕМІЯ НАУК ВИЩОЇ ШКОЛИ УКРАЇНИ

на підставі свого Статуту обрала

Мінаєва Бориса Филиповича

академіком

по відділенню хімії

збори затверджене загальними зборами

"16" 06 2016 р.

Президент АН ВШ України О.Г. Наконечний

Головний вчений секретар І.В. Бейко

Minaev B. F. is included in the list «Top 100 Scientists» of Ukraine according to the Vernadsky National Library rating (he occupies the 27th position). His Scopus h-index is 35.

Minaev B. F. is constantly invited for oral presentations and gives talks at the International Conferences (Sweden, Japan, Finland, USA, Spain, China, Poland, Norway, France, etc.).

Minaev B. F. (in the center) at the Conference in Shimkent. On the left – Professor Sokolov N. D. (ICP, Moscow), right – Rector of KazHTI Academic Muldametov Z. M., 1976

In 1999, Minaev B. F. has organized and held an International Conference in Torun (Poland) within the REHE program of the European Union, and also organized International Conferences in Cherkasy (2010), Linköping (1997) and Stockholm (2003).

Minaev B. F. (in the centre) at the conference «Relativistic Effects in Chemistry», Torun, 1999

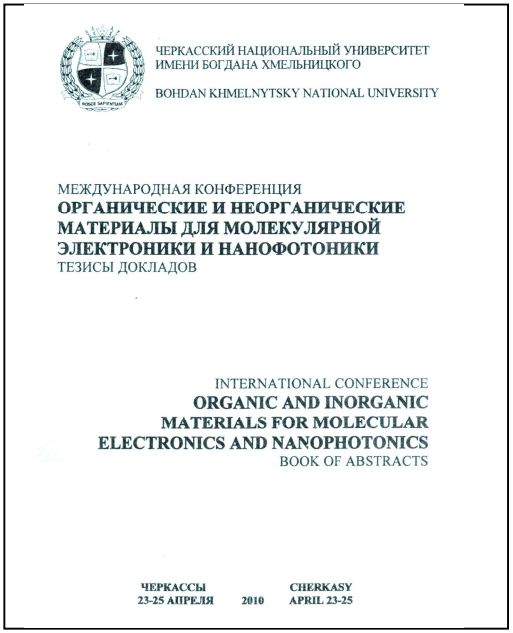
B. F. Minaev with Professor Ulrich Steiner (Germany)
At the conference «Spin chemistry and magnetic spin effects», Switzerland, Alps, 1999

Meeting after 20 years with the former postgraduate students (Professors N. M. Ivanova and I. S. Irgibaeva) at the International Congress of Quantum Chemistry, Helsinki, Finland, 2009.

8th European Conference on Computational Chemistry

25-28 August 2010, Lund, Sweden

Satellite meeting to 3rd EuCheMS Chemistry Congress in Nürnberg



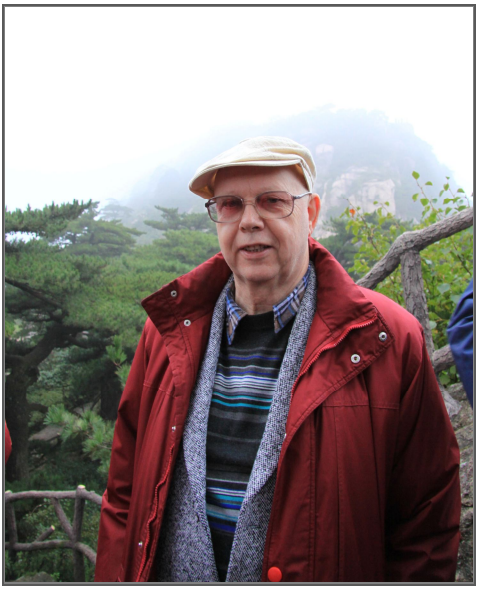
Cherkasy, 2010

At the conference «Correspondence Between Concepts in Chemistry and Quantum Chemistry», Valadalen, Sweden, 2010. From left to right: Professors Hans-Georg Jensen (Denmark), Per Siegbahn (Sweden), Boris Minaev (Ukraine), Fahmi Himo (Sweden), Hans Ågren (Sweden), Wenjian Liu (China)

中国-北欧分子生物及纳米科学会议（合肥，2010）
Nordic-China Symposium on Molecular Bio- and Nanoscience
Hefei, China, Sep. 20-25, 2010

Professor Minaev B. F. with a plenary report "Relativistic Effects in Biochemistry"

"Nordic-China Simposium on molecular Bio- and Nanoscience Sep. 20-25, 2010, Hefei, China"



On the tour during the conference «Relativistic Effects in Heavy Elements», Beijing (China), September 25–29, 2010

At the conference «European Advanced Materials Congress», August 22–24, 2015, Stockholm, Sweden

Announcements about the plenary report at the seminar of the Institute of Chemistry of the Chinese Academy of Sciences «Photo- and bio-activation of dioxygen», Beijing, 2015

分子动态与稳态结构国家重点实验室
State Key Laboratory for Structural Chemistry of Unstable and Stable Species

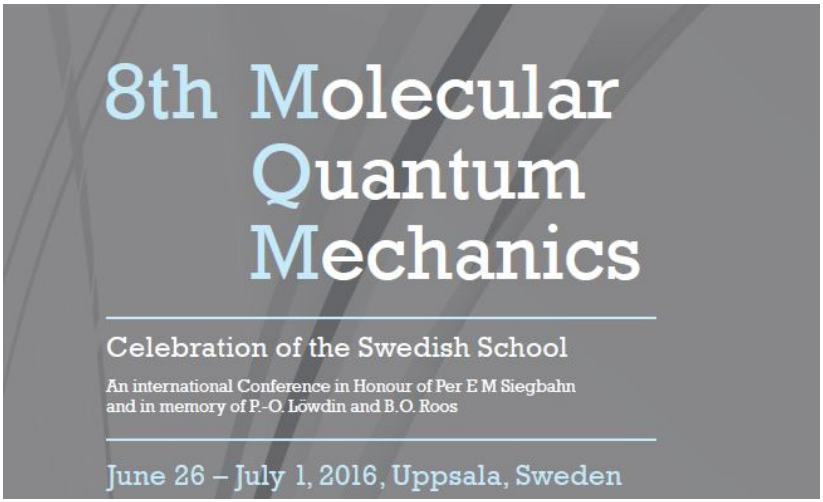
学术报告

Photo- and bio-activation of dioxygen

报告人：Professor Boris F. Minaev
Head of Organic Chemistry Department, National University in Cherkasy, Ukraine; Professor emeritus, Division of Theoretical Chemistry& Biology, Royal Institute of Technology, Sweden
报告地点：3号楼101会议室
报告时间：2015年11月5日（星期四）下午14:00

Research interests: Quantum chemistry, spin-orbit coupling effects in molecular spectra and in chemical reactivity; Phosphorescence spectra of molecules including the zero field splitting properties; New mechanisms of CIDEP and magnetic field effects on photophysical and photochemical properties of triplet molecules; Optical and chemical properties of molecular oxygen.

Vita: 1967, BS and MS in Physics, Tomsk State University; 1974, PhD in Physics and Mathematics, Tomsk State University; 1984, Dr. Sci. Degree by the USSR Attestation Committee.
1974, Assistant professor, Theoretical Physics Department in Karaganda State University (KarSU); 1976-1984, Head of Physical Chemistry Department at Chemical Faculty of KarSU; 1984-1989, Head of Quantum Chemistry Department at Chemical Faculty of KarSU; 1989-2007, Head of the General Chemistry Department at Cherkasy State University of Technology, Cherkasy, Ukraine; 2007-present: Head of Organic Chemistry Department at Cherkasy State University by B. Khmelnitskij, Cherkasy, Ukraine.
Visiting professorship: Linkoping University, Sweden; Royal Institute of Technology, Sweden; ICCAS.



Participation in the conference «European Advanced Materials Congress» with a plenary report «Tetraoxa[8]circulenes and heterocirculenes expedient synthesis for OLED: Excited state engineering of these conjugated organic materials by the oxygen and chain-group substitution», August 22–24, 2017, Stockholm, Sweden.

List of selected papers

1. Минаев Б. Ф. Спин-орбитальное взаимодействие в комплексах с переносом заряда / Б. Ф. Минаев, А. Ф. Терпугова // Изв. вузов. Физика. – 1969. – № 10. – С. 30–36.

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Boris Minaev with his son Alexander, 1979

Son Alexander with his wife and daughter Polina, 2007

Grandchildren Polina and Yan are growing up, 2018

Celebrating the New Year in a friendly family, 2006

Walking around a blueberry with his wife in Stockholm suburb (Sweden, 2010)

On the way to the Stockholm archipelago, 2002

Annotation. Scientist, Teacher, Enthusiast. **Professor Boris Filipovych Minaev: On the 75th anniversary.** *The main periods of life, scientific and pedagogic activity of the Doctor of Chemical Sciences, the Honoured Scientist of Ukraine, Professor Boris Filippovich Minaev are described in this book and a short review of his scientific researchs is presented.*

A significant contribution of the scientist and his achievements in the field of physical organic chemistry and molecular electronics are represented in the review. The material informs the reader on the range of scientific interests of B. F. Minaev which include spin-orbit coupling effects in molecules and their influence on spectra, photochemistry, luminescence and chemical reactivity. Boris Filippovich is an author of spin-catalysis theory and of its applications in enzymatic, homogeneous and heterogeneous catalysis. For the first time he has calculated the atmospheric oxygen bands intensity, indicated the role of spin-orbit coupling in the oxygen magnetic phosphorescence phenomena, has developed the quantum theory of phosphorescence for unsaturated hydrocarbons and dyes, spin splitting in zero magnetic field, hyperfine structure in the triplet state and the solvent effects on these EPR parameters.

The scientific works of Professor Minaev B. F. are well-known in the world; they are published in the leading international journals and are widely cited in the scientific literature. According to Scopus agency the Hirsch index of Minaev B. F. equals h = 35 and professor Minaev B. F. is one of the five best chemists in all Ukrainian universities.

Анотація. Учений, учитель, ентузіаст. Борис Пилипович Мінаєв. До 75-го дня народження. *У книзі висвітлено основні періоди життя, наукової та педагогічної діяльності доктора хімічних наук, професора,*

заслуженого діяча науки і техніки України Бориса Пилиповича Мінаєва, а також наведено короткий огляд вибраних наукових праць ученого. Книга відображає вагомі досягнення Б. П. Мінаєва в науково-дослідній діяльності та інформує наукову спільноту про досягнення вченого в галузі фізичної органічної хімії і молекулярної електроніки. Матеріали книги знайомлять читача з напрямами наукових інтересів Мінаєва Б. П., до яких відносяться ефекти спін-орбітальної взаємодії в молекулах і їх вплив на спектри, фотохімію, люмінесценцію, провідність, магнітні та хімічні властивості молекул. Борис Пилипович є автором концепції спін-каталізу та її застосування у ферментативному, гомогенному і гетерогенному каталізі. Він вперше розрахував інтенсивності атмосферних смуг молекулярного кисню, показав роль спін-орбітальної взаємодії у формуванні магнітної фосфоресценції кисню, розробив квантову теорію фосфоресценції ненасичених вуглеводнів і барвників, спінового розщеплення в нульовому магнітному полі, надтонкої структури у триплетному стані та впливу розчинника на ці параметри електронного парамагнітного резонансу.

Роботи професора Мінаєва Б. П. добре відомі у світі, опубліковані у провідних міжнародних наукових журналах і широко цитуються у світовій науковій літературі. На сьогоднішній день за даними всесвітньої агенції «Scopus» Мінаєв Б. П. має рейтинг Хірша h = 35.

Valentina A. Litvin,
Valentina A. Minaeva,
Nataliya N. Karaush-Karmazin,
Glib V. Baryshnikov

Scientist, Teacher, Enthusiast
Boris Filipovych Minaev

On the 75th anniversary

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