How to Cite: Irgibaeva, I.S., Minaeva, V.A. (2023). Professor Boris Filippovich Minaev: More than Half a Century of Scientific Activity and the 80th Anniversary of His Birth. *Eurasian Journal of Chemistry, 111(3), 13-20.* https://doi.org/10.31489/2959-0663/3-23-2

Essay Received: 25 May 2023 | Published online: 28 July 2023

UDC 539.19+544.1 https://doi.org/10.31489/2959-0663/3-23-2

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Professor Boris Filippovich Minaev: More than Half a Century of Scientific Activity and the 80th Anniversary of His Birth

The article highlights the main periods of life, scientific and pedagogical activity of Boris Filippovich 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. The article reflects Minaev's great contribution to scientific research and informs about his achievements in the field of physical organic chemistry and molecular electronics. At the end of this article an overview of his most important scientific papers is presented.

The former Head of the Department of Chemistry and Nanomaterials Science at the Bohdan Khmelnytsky National University, Professor Boris Minaev celebrates the 80th anniversary in this year. At the same time, we mark another remarkable date — 55 years of his scientific activity.

B.F. Minaev was born on September 21, 1943 in Sverdlovsk (now Yekaterinburg) in a family of employees. After the war, his father, Filip Prokopovich, supervised the Novgorod and Semipalatinsk Regional Executive Committee, the Ministry of Building Materials Industry in Kazakhstan Republic, therefore the family often moved from one end of the Soviet Union to another. In 1962, B. Minaev graduated from secondary school No. 3 in Karaganda and entered the Faculty of Physics of the Tomsk State University named after V. V. Kuibyshev (TSU). His first scientific research was devoted to the calculations of nitro compounds by the Hückel method. He began this study in his third year at the University. In 1967, Boris Minaev graduated from the University and entered the post-graduate school at the Optics and Spectroscopy Department of TSU. 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]. At the beginning of 1973 he defended his PhD thesis 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”.

From 1974 to 1988, Boris Minaev worked first as a docent 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 [2–9]. In the upper atmosphere, these weak transitions have a purely magnetic nature and occur due to a very specific Spin-Orbit Coupling (SOC) in the O_2 molecule. In 1978, Minaev showed that the well-known red Fraunhofer line of the sunlight absorbed by the atmosphere actually borrows 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 for first-time discovered in molecular spectroscopy [2]. Two years later, following the same principles, Minaev explained the specific luminescence enhancement of the singlet ($a^1\Delta_g$) oxygen in solutions.

In 1984, B. Minaev defended his doctoral thesis in the specialty 02.00.04–Physical Chemistry. Subject of doctoral dissertation: “Theoretical Analysis and Prognostication of Spin-Orbit Coupling Effects in Molecular Spectroscopy and Chemical Kinetics”. In a letter to the rector of Karaganda State University professor Z.M. Muldakhmetov, signed by the head of the Expert Council of the Suprim Appraisal Commission of the USSR Academician V.A. Legasov, B. Minaev was allowed to apply for the degree of Doctor of Chemical Sciences on the basis of defending an abstract without writing an entire dissertation on the totality of scientific articles. The defense took place in the *N.N. Semenov Institute of Chemical Physics* of the USSR Academy of Sciences in Moscow and aroused a great interest in the scientific community. The Dissertation Council of the Institute had a group of leading scientists from the USSR Academy of Sciences (among them two Nobel laureates).

In the same year, Boris Minaev headed a newly created Quantum Chemistry Department at the Karaganda State University (Photo 1) which was the second one in the former Soviet Union. During that time he educated six PhD candidates, five of them later became professors and defended doctoral dissertations (Photo 2).

Photo 1. B.F. Minaev in the Quantum Chemistry Laboratory (Karaganda, 1985)

Photo 2. Boris Minaev with colleagues and PhD students
of the Quantum Chemistry Department (Karaganda, 1980)

That time Minaev and Muldakhmetov'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 an actual at that time 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 [2–5]. 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 performed its direct verification based on the impulse experiments.

Growing chaos as a result of perestroika and the collapse of the USSR forced B. Minaev to leave Kazakhstan. He was invited to the post of the head of the department of chemistry at the branch of the Kyiv

Polytechnic Institute in Cherkassy (Ukraine). Since February 1988, he worked in this branch, which was later transformed into the Cherkasy State Technological University (ChSTU). During his work in ChSTU, B. Minaev prepared four candidates of chemical sciences, one of them subsequently defended his doctoral dissertation in chemistry.

At the same time, Professor Minaev gave lectures on quantum chemistry at the National University named after Bohdan Khmelnytsky in Cherkasy (ChNU). In 2007, he was appointed the head of the Department of Organic Chemistry of ChNU, and then (2016) — the head of the Department of Chemistry and Nanomaterials Science of ChNU.

Thus, for the 35-year period of intense work on the electronic structure, spectra, and chemical reactivity of molecules with the account of spin-orbit coupling initiated by Professor B. Minaev, the Cherkasy School of theoretical chemistry and weak magnetic perturbations became the world-known one. In addition to the traditional approach in magnetochemistry, when magnetic perturbations are taken into account for the calculation of the hyperfine structure in EPR spectra of radicals or in a Nuclear Magnetic Resonance (NMR) of diamagnetic molecules [6–25], 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. B. Minaev with colleagues carried out numerous calculations of the electronic mechanisms for the photochemical and biochemical reactions taking into account SOC, in particular, for the T-S transitions rate in intermediate biradicals and radical pairs [26–39].

Together with colleagues from the Stockholm University, B.F. Minaev carried out quantum chemical calculations of the electronic structure for a number of flavoprotein enzymes and copper containing aminoxidases. In reaction with oxygen these enzymes formed superoxide ion O_2^- by electron transfer; the same happend upon spontaneous oxidation of hemoglobin, ferredoxin and adrenaline [29–32]. Minaev was the first who paid attention to a specific electronic open shell of the superoxide ion, its great SOC effect and explained how the magnetic torque in O_2^- induces the T-S spin inversion in radical pairs of enzyme active centers in oxidases [29, 30], mono- and di-oxygenases [31] including cofactor-free enzymes [32].

B. Minaev pays much attention to the problems of ecology [20–26, 29–35]. It is well known that the singlet $^1\Delta_g$ oxygen participates in the smog formation over smoky cities. In the upper atmosphere there is a permanent O_2 photodissociation into atoms and their reverse recombination with formation of the oxygen metastable forms, including the quintet $O_2(^5\Pi_g)$ state [35]

Recently, Minaev's group carried out quantum chemical calculations to determine intensity of the new oxygen and nitrogen singlet-triplet bands [20–25]. 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) [35]. B.F. Minaev has also predicted the spin-orbit effects in photo-decay of the chloric HClO and bromic HBrO acids [34], 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 conclusion about the possible effect of external magnetic fields on the ozone layer.

In recent years B.F. Minaev pays much attention to the application of quantum chemistry in nanotechnology [36-47]. Currently, nanoclusters can be assembled “manually”, which allows them to be embedded in semiconductor structures, used as memory elements, molecular conductors, etc. The unique properties of fullerenes, metal-organic frameworks, and nanotubes allow them to be used in electronics, quantum computers, DNA testing, genetic engineering and medicine [47]. This is a new branch of nanomaterial science — spintronics. These studies are closely related to the problem of spin catalysis, which B. Minaev has been studying for many years [7, 26, 29–40].

In 1993, at a seminar of the Department of Molecular Electronics in Linköping (Sweden), B. Minaev focused attention for the first time on the important spin-orbit coupling effects in Organic Light-Emitting Diodes (OLEDs) because the singlet-triplet transitions increased three-fold efficiency of recombination of electrons and holed during electroluminescence. In 1999, in the United States, this idea was implemented in the use of heavy ion complexes of Iridium. That time B. Minaev was the first who applied 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 [16]. In the future, the papers devoted to the study of Ir(III) complexes for OLED applications laid the foundation for new directions in the development of molecular electronics, being fixed in cooperation with the Electronics Department, Lviv Polytechnic National University [38, 39]. These OLED studies are summarized in the reviews [21, 38] which were cited 855 times according to Scopus.

An important direction in the development of the ChNU chemistry department was founded in 2011 [40] and was associated with research of circulenes, a new class of organic molecules. These materials have attracted the attention of Boris Minaev due to their high symmetry and their use as promising materials for OLED applications [36–47]. A lot of DFT calculations of the electronic structure, IR and UV-Vis spectra of tetraoxa[8]circulenes, their magnetic and aromatic properties were 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 [41]. 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 [41] (Photo 3). Quite recently this and other ChNU predicted two-dimensional nano-polymers [47] were synthesized; thus, the "Cherkasit" material becomes reality.

Photo 3. Cover of the "Chemical Physics Letters" journal (Elsevier)
with novel graphene allotropes proposed in Ref. [41]

B. Minaev pays a great attention to work with young students. His lectures on biochemistry, ecology and quantum chemistry do not leave the youth indifferent. They 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. Working with graduate students B. Minaev is very demanding and at the same time very generous; he permanently shares his findings, gives ideas and helps a lot in this hard work on the calculation of the electronic structure of molecules. Under the supervision of Prof. Minaev 17 theses for the PhD degree in chemistry were defended.

Scientific Achievements of B. Minaev

B.F. Minaev's scientific potential has more than 600 papers in the high-ranking international journals in the field of quantum chemistry and six monographs. Three of them were published in 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) [36] and "Handbook of Computational Chemistry" (2017). The Linköping University published a voluminous book "Spin Catalysis" for five years of B. Minaev's work in Sweden. 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.

B.F. Minaev was a coordinator of NATO project in terms of the REHE program (Relativistic Effects in Heavy Elements) 1998–1999 together with Prof. Pekka Pyyko, and headed the Organizing Committee of the International Conference "Relativistic Effects in Chemical Reactions" in Torun (Poland) in January 1999. He is constantly invited for oral presentations and gives talks at the International Conferences (Sweden, Japan, Finland, USA, Spain, China, Poland, Norway, France, etc.) (Photo 4).

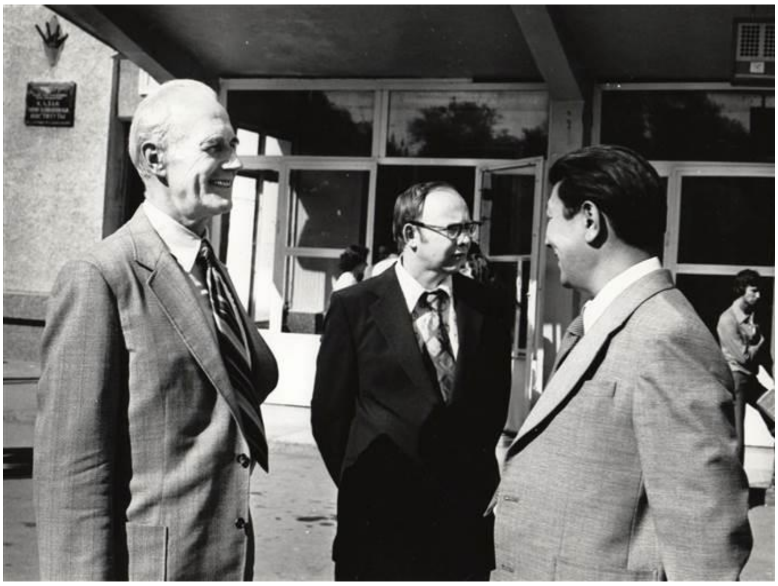

Photo 4. B.F. Minaev (in the center) at the Quantum Chemistry Conference in Shimkent (Kazakhstan).
On the left — Professor N.D. Sokolov (ICP, Moscow),
right — Rector of KazHTI Academic Z.M. Muldakhmetov, 1976

Minaev headed a number of scientific grants: the INTAS (1993–1996) project "Spin Catalysis"; together with Professor Tom Slanger the Joint Ukrainian-American grant CRDF (UKC1-2819-CK-06) "Spin-Forbidden Transitions of Molecular Oxygen and New Emission Bands from the Upper Atmosphere" (2006–2007); the Joint Ukrainian-Romanian grant "Design of Novel Sensitizing Dyes for Nanocrystalline TiO_2 Solar Cells on the Basis of Their Electronic Structure Calculations" (with Professor Mihai Girtu, Ovidius University in Konstanca) (2008–2009); headed together with Professor Hans Agren (KTH) Swedish-Ukrainian grant Visby "Organic Light Emitting Diodes Theory" (2008–2011); a number of projects (five) in organic synthesis and electronic structure calculations for development of OLED technology (2008–2022) governed by the Ministry of Education and Science in Ukraine. The late one is: "Interface Architecture and Electronic Mechanisms of Excitons and Excimers Formation in the Multilayer Organic Light-Emitting Diodes and Transistors".

He 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). 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 Branch of the National Academy of Sciences of the Republic of Kazakhstan" for the merits in development of chemical science in the Republic of Kazakhstan (2010), and honorary title "Honoured Worker of Science and Technology of Ukraine" (2011). Recently he received the prestigious "Scopus Award Ukraine" (2016), medal of the Ukrainian Cabinet of Ministers (2017), Order of the Government of Ukraine: "Za zaslugi" 3rd class (2021).

The scientific works of Professor B.F. Minaev 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 B.F. Minaev is equal IH = 46 (Google Scholar IH =55), and Professor B.F. Minaev ranks among the best chemists in Ukrainian universities.

A prominent scientist in the field of quantum chemistry, 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, Professor Boris Minaev has devoted more than 55 years of his life to science and education. The personal and leadership qualities of Professor Minaev are unambiguous. On behalf of numerous colleagues, scientific followers, grateful students, we sincerely congratulate Profes-

sor B.F. Minaev on his 80th anniversary and wish great energy, health, new achievements in the scientific field and all the best!

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