

MEMORABLE DATES

Essay

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Z.M. Muldakhmetov — a Creator of the Scientific School of Quantum Chemistry in Kazakhstan

This year, the famous scientist and organizer of science and education in Kazakhstan, Academician of the National Academy of Sciences of the Republic of Kazakhstan Z.M. Muldakhmetov turns 90 years old. His scientific activity is closely connected with such branches of the theory of the structure of matter as molecular spectroscopy and quantum chemistry. His path in science reflects the history of the development of these scientific disciplines. The article gives a brief description of the creation of a scientific school of quantum chemistry in Kazakhstan with the direct participation of Z.M. Muldakhmetov.



One of the significant merits of Zainulla Muldakhmetovich Muldakhmetov is the introduction and development of quantum-chemical research in Kazakhstan. The rapid development of the ideas of quantum mechanics and quantum chemistry during the formative years of Z.M. Muldakhmetov as a scientist and understanding of their role in creating the foundations of the theory of the structure of matter led him to the desire to continue his spectroscopic research using the methods of quantum chemistry.

Zainulla Muldakhmetovich was born on August 3, 1933 in the village of Oktyabr, Presnovsky district, North Kazakhstan region. In 1952, he finished Chistov secondary school and entered the Faculty of Physics and Mathematics of the Alma-Ata Pedagogical Institute named after Abay. After graduation from the Institute Z.M. Muldakhmetov worked as a physics teacher in a rural school for three years. In 1959, he entered the graduate school of the Moscow Institute of Fine Chemical Technology named after M.V. Lomonosov.

In graduate school under the guidance of Professor M.M. Sushchinsky, the young scientist studied second-order lines in the vibrational spectra of molecules [1–3]. A comprehensive study of the second-order lines in the Raman spectra (RS) and infrared (IR) absorption spectra of a number of polyatomic molecules was conducted: benzene, hexadeuterobenzene, chloroform, deuteriochloroform, deuterocyclohexane, etc. The spectra of the last two deuteroderivatives were studied for the first time. For these compounds, quantitative data were obtained on frequencies, intensities, and the degree of depolarization of the observed lines, and the vibration anharmonicity coefficients were calculated. Based on the studies of second-order lines and comparison of the obtained results with the literature data, some fundamental frequencies were refined. In 1963 Z.M. Muldakhmetov successfully defended his dissertation for a candidate degree in physical and mathematical sciences.

Spectroscopic studies of polyatomic molecules Z.M. Muldakhmetov could continue in 1965 after a short teaching career at the Kazakh State University named after S.M. Kirov and work as Vice-Rector of the

Tselinograd Pedagogical Institute. He was appointed head of the Laboratory of spectroscopy of the Chemical and Metallurgical Institute of the Academy of Sciences of the Kazakh SSR and worked in this position for almost ten years. It was when Z.M. Muldakhmetov and his collaborators began research on the study of the structure of organic molecules using quantum chemistry methods. During these years, the laboratory was equipped with modern equipment necessary for research: two German IR spectrophotometers, UV, NMR and Raman spectrometers. An important acquisition at that time was the electronic computer “Minsk-22” (Photo 1). The research objects of the laboratory were numerous new compounds synthesized in other laboratories of the Institute, but the main attention was paid to ethylene oxide and a number of its derivatives, including epichlorohydrin, divinyl oxide, styrene oxide, esters of glycidic acids, acetylenic and nitrile derivatives, etc. The influence of substituents, temperature, the reaction medium for their preparation on vibrational spectra, conjugation of chemical bonds, and the appearance of rotational isomers of various α -oxide compounds were studied [4–6]. The studies were carried out both by the methods of IR, Raman, NMR spectroscopy, and by semi-empirical methods of quantum chemistry (EHM (Extended Hückel method), then CNDO/2, INDO). The calculations were carried out on the Minsk-22 computer, as well as BECM-3M (Big electronic calculating machine-3M). According to the results of these studies, Z.M. Muldakhmetov and co-workers wrote the fundamental monograph “The Structure of Ethylene Oxide Derivatives” [7], which became the basis of the Z.M. Muldakhmetov’s doctoral thesis “Study of structural features of α -oxide compounds molecules”, which was defended in 1972.



Photo 1. Employees of the Laboratory of spectroscopy at work on the computer “Minsk-22”:
S.Kh. Fazylov, I.S. Irgibaeva, N.S. Kupriyanov, and K.A. Akhmetkarimov

From 1974 to 1980, toward the Ministry of Higher and Specialized Secondary Education of the Kazakh SSR, Z.M. Muldakhmetov first worked as a Vice-Rector for scientific work at Karaganda State University (KarSU), then as a Rector of the Kazakh Chemical Technology Institute (KazChTI) in Chimkent. He paid great attention to the training of highly qualified young specialists, improving the quality of the teaching staff, construction of new educational buildings and re-equipping laboratories with the newest facilities. Zainulla Muldakhmetovich oversaw scientific research in several areas, but the main one was study of the electronic structure of molecules, intermolecular interactions and reaction mechanisms by spectroscopic and quantum chemical methods. In co-authorship with his colleagues in ongoing research, a number of articles have been published [8-11].

In the same period, a meeting occurred between Z.M. Muldakhmetov with future well-known scientists in the field of quantum chemistry — candidates of physical and mathematical sciences Boris Filippovich Minaev and Sergey Aleksandrovich Beznosyuk, who are graduates of different years of Tomsk State University. Deeply understanding the spectroscopic subtleties of the structure of molecules, Zainulla Muldakhmetovich immediately recognized in them high-level specialists and huge scientific potential in this field, and for many years provided them with comprehensive support. B.F. Minaev in 1974 was hired at

KarSU, first at the Faculty of Physics, and then he headed the Chair of Physical Chemistry at the Chemical Faculty. S.A. Beznosyuk, having arrived in 1979 on vacation from Tomsk to Chimkent, looked, in his words “from the street”, to the Rector of KazChTI to know what they were doing in this Institute. Here is how he recalled this meeting: “The Rector showed great interest in my scientific direction — the quantum theory of the structure of matter. He was especially interested in a new theoretical approach at that time — the density functional method. Without hesitation Zainulla Muldakhmetovich suggested me to move to Chimkent and join his scientific team dealing with the problems of quantum chemistry. So, our long-term cooperation in the field of theoretical chemistry began” [12].

In 1980, in order to better know the scientists of Kazakhstan new achievements in the field of quantum chemistry, as well as to present Kazakhstan theoretical developments, Z.M. Muldakhmetov organized the All-Union School of Quantum Chemistry based on KazChTI. The leading scientists of quantum chemistry N.D. Sokolov, I.G. Kaplan, and many others took part in it. The classes were held in the most beautiful place — the Mashat gorge near Chimkent, and in general, according to the opinions of the school participants, it was organized very excellent.

In 1980, Z.M. Muldakhmetov was appointed Rector of the KarSU and remained in this post until 1988. During the work as a rector of this University Z.M. Muldakhmetov proved to be an experienced and skillful leader, administrator, scientist and teacher. During this period, educational buildings of the biological and physical faculties, student dormitories, a sanatorium and other facilities of the University were built. There was a computer center in which regular visitors were employees of the Chair of Physical Chemistry, who carried our quantum chemical calculations on the ES-2030 computer machine.

With his great employment, Zainulla Muldakhmetovich continued to pay much attention to the development of quantum chemical research and molecular spectroscopy at KarSU. In 1982, he organized the All-Union Conference on Theoretical Chemistry, which was also held for a week in one of the most beautiful places in Kazakhstan — Karkaralinsk. With great gratitude, Professor A.S. Masalimov, who was directly involved in this conference and who was also invited by Z.M. Muldakhmetov in 1980 still a young Candidate of sciences to work at KarSU as a specialist in the field of EPR spectroscopy, spoke in detail about this event [12]. The forum turned out to be grandiose. Well-known soviet scientists not only in the field of chemistry, but also physics, mathematics and metallurgy delivered lectures, whole discussions flared up on the fundamental problems of physical chemistry. Z.M. Muldakhmetov’s followers-colleagues also made presentations: B.F. Minaev, G.A. Ketsle, S.A. Beznosyuk, I.S. Irgibaeva, V.V. Bryukhanov — the future doctors of sciences and professors. The holding of such scientific forums, when well-known scientists from all over the Soviet Union came, gave impetus to the implementation of the own research, and also contributed to the creation of friendly relations with the leading scientific centers of the country.

Z.M. Muldakhmetov with great desire attended scientific seminars of the Chair of Physical Chemistry, headed by B.F. Minaev, participated in discussions on the problems of the influence of spin-orbit interaction (SOI) on the spectral characteristics of molecules and the mechanisms of chemical reactions. We (including the author of this article, N.M. Ivanova) carried out quantum-chemical calculations mainly using the MINDO/3 method, taking into account the configurational interaction and SOI. At the same time, the members of the Chair and with the participation of the physicist-programmer I.M. Danilovich created the software package MINDO/3 + CI-2, which makes it possible to carry out calculations of molecular systems, taking into account singly and doubly excited configurations. Based on the results of calculations, several articles were published on the manifestations of SOI in molecules and its role in chemical reactions, among which are articles [13–15], as well as the fundamental monograph “Optical and magnetic properties of the triplet state” [16]. In this monograph the methods for research of triplet state of molecules are described, the calculations of the electronic structure and spectra of a number of molecules are given, the mechanisms of the occurrence of SOI in oxygen molecule and its effect on singlet-triplet transitions in organic molecules are explained, etc.

In 1984, another important event initiated by Z.M. Muldakhmetov took place for the KarSU: the second Chair of Quantum Chemistry after the Leningrad State University in the USSR was opened, which until 1989 was headed by Doctor of chemical sciences B.F. Minaev. It was the recognition of the results of research in the field of quantum chemistry, conducted by a group of scientists headed by Z.M. Muldakhmetov. In 1985, Candidate of Chemical Sciences S.A. Beznosyuk and his wife were invited to work at the Chair, A.E. Buketova and G.I. Kobzev also were hired. Photo 2 shows the members of the Chair of Quantum Chemistry. The teachers of Physics Faculty of the KarSU Yu.A. Serebrennikov, R. Mukhin and others, closely interacted with the staff of Quantum Chemistry chair. It was a very fruitful period for all members of

the Chair of Quantum Chemistry headed by Z.M. Muldakhmetov. In 1984, the Republican scientific-theoretical conference on photochemistry and photophysics of singlet oxygen was held based on KarSU. The monograph "Quantum Electrochemistry of Alkaloids" (1986) [17] was published as a result of quantum chemistry and electrochemistry chair's staff collaboration using the example of alkaloids. On the development of new approaches to the density functional theory, the theory of quantum density topology, the republican publishing house also released a monograph "Electronic theory of the structure of molecules. New Aspects" (1988) [18].



Photo 2. Employees of the Department of Quantum Chemistry: in the first row — N.M. Ivanova, I.S. Irgibaeva, E.P. Sim, in the second row — Yu.A. Kazantsev, S.A. Beznosyuk, B.F. Minaev, G.D. Rempel

In 1988 Z.M. Muldakhmetov was elected as Academician-secretary of the Central Kazakhstan Branch of the Academy of Sciences of the KazSSR and came to grips with coordinating the activities of all academic institutions in this region. In 1989 Z.M. Muldakhmetov was elected an Academician of the Academy of Sciences of the KazSSR in physical chemistry.

In the same year, the Chair of Quantum Chemistry at KarSU was headed by Dr. Chem. Sc. S.A. Beznosyuk after leaving of Professor B.F. Minaev for Ukraine to continue his research in the field of quantum chemistry at the Cherkasy State Technological University, then at the Bohdan Khmelnytsky National University of Cherkasy, where he still works, having trained a whole pleiad of students. Boris Filippovich repeatedly came to Kazakhstan, to Karaganda, lectured University students, participated in conferences and met with Z.M. Muldakhmetov. After one of these visits, Boris Filippovich sent a letter of thanks to Zainulla Muldakhmetovich, in which he wrote: "Time flies, but the warmth of human friendship remains between us. Your friendship and the years that we worked together at KarSU are especially dear to me. I have always appreciated it, you were that person who gave me the impetus not to stop, helped me to overcome difficult phases in life, and taught me to fight for my goals."

From 1991 to the present, Z.M. Muldakhmetov is the Director of the Institute of Organic Synthesis and Coal Chemistry of the National Academy of Sciences of the Republic of Kazakhstan (today LLP "IOSCCh RK"). After his arrival at the Institute Zainulla Muldahmetovich again took up the creation of the Laboratory of spectroscopy and the organization of quantum chemical studies of the structure of organic molecules and the mechanisms of their reactions. At IOSCCh at that time, the methods of quantum chemistry were already being used in the Laboratory of catalytic synthesis and, in particular, by L.K. Abulyaissova, whose scientific and pedagogical activity is still connected with quantum chemistry at the Chair of Physical and Analytical Chemistry in the E.A. Buketov Karaganda University. At the beginning of the 90s, honored chemists worked at IOSCCh, including Doctors of Chemical Sciences I.V. Kirilyus, K.A. Ayapbergenov, A.M. Gazaliyev, S.M. Adekenov, Professor A.V. Shchelkunov, and young scientists were also taken on the Chair: Candidates of Physical and Mathematical Sciences K.M. Turdybekov and M.E. Agelmenev, Candidates of Chemical Sciences A.T. Edrisov, G.D. Rempel and N.M. Ivanova, united by a common direction of research into the

structure of matter under the guidance of Z.M. Muldakhmetov, but developing their own narrow research topics [19–23]. Despite the difficult financial situation in science, and throughout sovereign Kazakhstan in the 90s, personal computers began to be purchased at IOSCC, which together with the ready-made software packages for semi-empirical calculation methods (MOPAC, AMPAC), then non-empirical methods (GAMESS, GAUSSIAN, QChem and others) contributed to the incredibly rapid spread and development of quantum chemical research in chemistry and physics.

In 1993 Z.M. Muldakhmetov was awarded the Honorary title “Honored Science Worker of the Republic of Kazakhstan”.

In 1998, on the initiative of Academician Z.M. Muldakhmetov, the Russian-Kazakhstan Modern Humanitarian University was opened, later renamed the Kazakh-Russian University, with branches in many cities of Kazakhstan, which implemented an innovative opportunity to receive education remotely.

In September 2004, based on LLP “IOSCC RK”, an International scientific and theoretical conference “Molecular spectroscopy and quantum chemistry of organic compounds” was organized. Z.M. Muldakhmetov presented a review report “Quantum Chemistry and Molecular Spectroscopy in Kazakhstan” [24]. Active participation in the conference was also taken by former colleagues and students of Z.M. Muldakhmetov — B.F. Minaev, V.V. Bryukhanov, A.S. Masalimov, I.S. Irgibaeva, N.A. Mazhenov and others.

Z.M. Muldakhmetov received many awards both during the existence of the Soviet Union and in 30 years of independent Kazakhstan for his great contribution to the development of science and high technology education. And he can be proud of the achievements of his followers in scientific research, confirming the D.I. Mendeleev’s well-known expression: “**All the pride of the teacher is in the students, in the growth of the seeds sown by him.**” Z.M. Muldakhmetov was the supervisor and scientific consultant of dissertations at 9 Doctors of Sciences and 25 Candidates of Sciences. His followers and collaborators share their knowledge with students and young scientists not only in Kazakhstan, but also in Russia, Ukraine, and Germany.

The IOSCC RK collective cordially congratulates You on Your magnificent 90th anniversary and wishes You further creative success, good health for many years, the joy of communicating with grandchildren and great-grandchildren, warmth and home comfort!

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