Key Salikhov

Chemical Reactions and Spin Dynamics

Born in 1936 in Bashkiria, USSR, studied physics at Kazan State University (Diploma 1959) and the Institute of High Molecular Compounds of the USSR (Ph. D. 1962). After working as a researcher at the Institute of Chemical Kinetics and Combustion in Novosibirsk, professor of physics in 1979 at Novosibirsk State University; moved to Kazan in 1988 and became Chair of the Chemical Physics department at Kazan State University as well as director of Zavoisky Physical-Technical Institute in Kazan. Lenin Prize winner (1986); member of the scientific council of the Russian Academy of Sciences on "Magnetism", the board of directors of the International EPR Society, and Conference Chair of the 1994 AMPERE meeting; editor and founder of the journal *Applied Magnetic Resonance.* Book publications include *Spin Polarization and Magnetic Effects in Radical Reactions* (co-authored with Yu. N. Mohn, R. Z. Sagdeev, A. I. Buchachenko) and *Spin Exchange* (co-authored with Yu. N. Mohn and K. I. Zamaraev). Major areas of interest: Theory of Chemical Reactions and Spin Effects, Magnetic Resonance and its Applications to the Field of Chemical Reactions. — Address: Kazan Physical-Technical Institute, Sibirsky trakt 10/7, Kazan, 420020, Tatarstan, Russia.

I came to the Wissenschaftskolleg with the idea and hope of writing two books: one had the working title *Magnetic Isotope Effect in Radical Reactions* and the other (to be co-authored by Yu. N. Molin) was to be on chemical reactions and spin coherence. From my stay in Berlin, I not last expected a lively and fruitful exchange with my colleagues at the Freie Universität Berlin (FU) from which my book projects would highly benefit. As one tends to think at the beginning that there is plenty of time to do everything, I enthusiastically joined the seminar of the Chaos Group and took part in their discussions, presenting a talk on spin and magnetic effects in chemical reactions. This talk and further discussions with my

colleagues at the FU set off an idea with which I became quite preoccupied for part of my stay. What if spin polarization patterns in solids could be created with a spatial design?

In the simplest case, spins on one surface of a solid could be polarized in one direction while spins on the other surface would be polarized oppositely. The algorithm for such spin polarization in solids with a spatial design is as follows: First, an ensemble of spins is prepared in a state with zero Zeeman energy but non-zero energy in the reservoir of spin-spin interactions. So far no space inhomogeneity occurs. Then, a linear gradient magnetic field is switched on and the spin-spin energy is converted to a spatial non-homogeneous ordering of spins with respect to the external field. I presented this idea in talks at the Wissenschaftskolleg, the FU Berlin, Stuttgart University, Zurich University, Washington University (St. Louis), Einstein College (New York) and at the 34th Experimental Nuclear Magnetic Resonance Conference in St. Louis, MO. The resulting paper will be published in *Chemical Physics.* While all this was not part of my original plan for my stay in Berlin, it nicely demonstrates the effect of the intellectually stimulating atmosphere at the Wissenschaftskolleg.

My other "detour" involved my collaboration with Yu. N. Molin. The Rector kindly invited my co-author from Novosibirsk to spend two months at the Wissenschaftskolleg. We intended to use this time for working on our book *Chemical Reactions and Spin Coherence* but — alas - plans changed once again. Although we started on the book and have written about half of what we were hoping to achieve, it is not finished yet and will probably need several months to be completed. However, Yu. N. Molin's stay at the Kolleg was highly productive in another area. Reading about some experimental results awakened our curiosity to theoretically consider the experimental data presented. As a result, we submitted two papers for publication in *Chemical Physics Letters* and the *Journal of Physical Chemistry.*

All went as planned with my book on the Magnetic Isotope Effect (MIE). *An Introduction to the Magnetic Isotope Effect in Radical Reactions* is ready for publication. Writing this book in Berlin, I was able to receive most appreciated comments and suggestions of Professor Dietmar Stehlik (FU Berlin). During the last two decades it was shown that not only the charges and the masses of nuclei but also their magnetic moments play an important role in the course of chemical reactions. The physical model is very simple: decomposition of molecules creates radical pair or biradical intermediate states. In these intermediate states the unpaired (valent) electron spins can either be in the singlet or in the triplet state which then influences the chemical reactivity of the intermediates. The Magnetic Isotope Effect originates from the fact that the hyperfine interaction of unre-

paired electrons with the magnetic moments of the nuclei causes singlet-triplet transitions in radical pairs and biradicals. As a result, the populations of the singlet and triplet states of radical pairs and biradicals depend on the isotope composition of radicals.

MIE can be exploited as a mechanistic probe for reactions, proceeding via the radical pair or biradical formation, as well as for isotope separation. The present book is a review of the state of affairs in this field of chemical physics. In it, I discuss the physical background (both theoretical and experimental) of MIE for radical reactions in solutions and the possible applications of MIE for solving problems of chemical kinetics. The book has a broader audience as it is intended for physicists, chemists and biologists studying photophysical and photochemical processes in condensed media, researchers in related fields of chemical physics and — nonetheless — postgraduates and senior undergraduate students.

Staying at the Wissenschaftskolleg also made it possible forme to start on a cooperative project with physicists at the FU Berlin (Dr. Martin Plato) and Odense University (Professor Boiden Pedersen). This project aims to elaborate Monte Carlo simulations of the dynamics of physical and chemical processes in micellar solutions. One further matter that has been a concern of mine is the present state of science and scientists in Russia. I was able to discuss current problems and perspectives with an interested and informed audience at the Wissenschaftskolleg as well as during my visits to Denmark, Switzerland and the US.

The Tuesday Colloquia were a fascinating experience for me as here academics from the most diverse disciplines came together to present (and discuss) their research. I found the idea of holding the interest of an audience so different from the usual conference or seminar attendants very challenging, and I hope that at least the title of my colloquium ("Minor Interactions with Major Consequences in Chemical Reactions") — which was also a product of my cooperation with Professor Klaus Möbius (FU Berlin) — demonstrates how I labored over this problem.

Finally, I wish to thank all those who made my stay so enjoyable. I had wonderful assistance from Kerstin Hoge and the secretariat, Dr. Hans-Georg Lindenberg and the computer services, in fact, from the whole staff at the Wissenschaftskolleg, including Technische Dienste and Hauswirtschaft. Last but not least I wish to thank Dr. Reinhart Meyer-Kalkus, Elke Rauschecker, Kerstin Hoge, and Felix Volck for their efforts in solving my visa problems.