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INTERNATIONAL SYMPOSIUM "SPIN CHEMISTRY AND BEYOND" DEDICATED TO PROFESSOR BORIS MINAEV'S 70TH BIRTHDAY

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The international symposium “Spin Chemistry and Beyond” in honour of our fellow-country men Professor Boris Minaev, the Head of Organic Chemistry Chair at Bohdan Khmelnitskiy National University in Cherkasy, dedicated to his 70th birthday, was held in the period of September 20-21, 2013 in Stockholm, Sweden, at the Alba Nova center. The center unites biotechnology and physics of the Royal Institute of Technology (KTH) and Stockholm University (SU). The Alba Nova is a leading scientific center in nanotechnology and molecular electronics in Sweden.

Boris Minaev collaborates with the Department of Theoretical Chemistry and Biochemistry (KTH) for 22 last years, thus the Head of the Department, Prof. Hans Agren as well as Professors Yi Luo, Olav Vahtras, Faris Gelmihanov have initiated the Organizing Committee of the symposium.

In spite of the short period of time, it was very intense and interesting Symposium. It was open by a talk of the world-wide known Prof. Peter R. Ogilby, Director of Center for Oxygen Microscopy and Imaging at Aarhus University (Denmark). In his talk “Boris Minaev’s Contributions to the Study of Radiative Transitions in Molecules” Peter R. Ogilby described a modern status of the singlet oxygen ($^1O_2$) photochemistry and photobiology. The singlet oxygen ($^1O_2$) is responsible for specific reactions that lead to the death of a biological cell, and it serves as a nice model and probe to investigate various phenomena, like diffusion or enhancement of spin forbidden processes. The study of $^1O_2$ provides a basis for development of new tools, techniques and materials, like IR imaging systems. The study of $^1O_2$ provides, particularly in photosensitized systems, a coalescence point for many topics currently at the cutting-edge of science. The speaker said that Boris Minaev has explained for the first time the magnetic nature of the singlet oxygen phosphorescence, its lifetime and the enhancement in solvents. Prof. Peter R. Ogilby stressed the role of solvent polarizability and spin-orbit coupling (SOC) inside the molecular oxygen, predicted by Boris Minaev’s theory, which was supported by his experiments.

In the next talk by Prof. Dage Sundholm (University of Helsinki, Finland) the applications of the gauge-including magnetically induced currents are discussed in connection with aromaticity problem. Boris Minaev paid attention of the speaker on recent calculation of nuclear independent chemical shifts in tetraoxa[8]circulenes and their aromaticity. During long discussion various opinions have been expressed concerning the role of magnetically induced currents and their calculations.

Prof. Antonio Rizzo (ICQEM, University of Pisa, Italy) told about recent achievements in the study of nonlinear optical mixed electric and magnetic properties. He also mentioned his long discussion with Boris Minaev which took place in train to Linkoping on magnetic properties and Kerr effect.

The great talk was represented by Prof. Per E.M. Siegbahn (SU, Swedish Academy member): “The mechanism for water oxidation in Photosystem II”. Per Siegbahn told about the structure of manganese cluster in photosynthesis; his prediction is now confirmed by series of recent experiments. Prof. Siegbahn recalled his common researches with Boris Minaev on spin catalysis in glucose oxidase.

Dr. Fabrizio Santoro, Senior Research Scientist at CNR (Pisa, Italy) made a report “Recent Developments in Methods for Computing Vibronic Spectra of Adiabatic and Nonadiabatic Systems”. Fabrizio Santoro develops models and methods for applications in the field of linear and non-linear computational electronic spectroscopy and studies the quantum dynamics of ultrafast photoinduced processes in biology and nanosystems. He mentioned a contribution of Boris Minaev to the theory of vibronic bands in free-base porphyrine.

Prof. Mats Larsson (member of Swedish Academy and of the Nobel Committee for Physics) mentioned his common work with the hero of the anniversary about the study of dissociative recombination in molecular ion

beam and told on multiionized atoms and molecules studied at the Linac Coherent Light Source (LCLS) in USA. The SLAC National Accelerator Laboratory is an Office of Science User Facility operated for the U.S. and produces pulses of X-rays more than a billion times brighter than the most powerful existing sources, the so-called synchrotron sources which are also based on large electron accelerators. The ultrafast X-ray pulses are used like flashes from a high-speed strobe light, enabling scientists to take stop-motion pictures of atoms and molecules in motion, shedding light on the fundamental processes of chemistry, technology, and life itself. Mats Larsson works at LCLS to use these highly focused, intense beams of X-rays to reveal the identity and arrangement of atoms in a wide range of materials.

Prof. Kurt Mikkelsen (Department of Chemistry, H. C. Ersted Institute, University of Copenhagen) talked about the effects of condensed phases on molecular properties and transport properties. He congratulated Boris Minaev with some presents and reminded of their common research in Ersted Institute. His younger colleague Dr. Michael Pittelkow from University of Copenhagen reported on heterocyclic circulenes studies provided together with organic chemists from Cherkasy. The similar united talk has been made by Prof. Mihai Girtu (Ovidius University in Konstanta, Rumania) about DFT study on molecular adsorption and electron transfer to titania oxide nanoclusters in application to dye-sensitized solar cells.

The next day of the Symposium was open by a talk of Prof. Chantal Daniel (CNRS, Strasbourg University, France) “Ultra-Fast Intersystem Crossing Processes in Transition Metal Complexes; a Quantum Chemical Interpretation”. The talk aims at interpretation of photochemical and photophysical experiments and complex mechanisms, involving excited states, such as inorganic photoisomerization, photophysics of iridium and rutenium metal complexes.

Kenneth Ruud, Vice-Rector for research of the University of Tromso (Norway) has told on computational studies of EPR and paramagnetic NMR using four-component relativistic DFT methods. In 2008 he was the recipient of the Dirac medal from the World Association of Theoretical and Computational Chemists. Kenneth started his talk with reminder of the paper by B. Minaev, J. Vaara, K. Ruud “Internuclear Distance Dependence of the Spin-Orbit Coupling Contributions to Proton NMR Chemical Shifts” (Chem. Phys. Lett., 1998, 295, 455) and turned to the modern NMR calculations for heavy atoms.

Presentation of Prof. Lars Pettersson (SU, Sweden) “Spin-Uncoupling and Chemical Bonding at Surface” was mainly devoted to the spin-catalysis ideas of the hero of the anniversary. Many catalytic reactions of industrial importance involve reforming of saturated hydrocarbons to more reactive species. Often the first step is C–H bond breaking, which can be activated already in the adsorbed molecular state. In paper L. Triguero, L. Pettersson, B. Minaev (J. Chem. Phys., 1998, 108, 1193) on “Spin Uncoupling in Surface Chemisorption of Hydrocarbons” the role of triplet excited state of the adsorbed molecule was stressed for the first time. Lars’s group use DFT based techniques to explain X-ray absorption and emission spectra to bring new ideas and interpretations of experimental data. Similar ideas were described in the report of Prof. Fahmi Himo (SU, Sweden) “Quantum Chemistry Applied to Biocatalysis and Homogeneous Catalysis”. Prof. Boris Dzhagarov from Institute of Physics (Minsk, Belorussia) has described the study of his laboratory on laser photolysis of meeting and parting of heme iron and O_2 in hemoglobin.

All talks were accompanied by interesting discussions; 46 participants from 11 countries took part in the Symposium.