

# Program 14 European Symposium on Gas Electron Diffraction Moscow, 2011 June 24-28

## Day 1

## June 24

9:40-9:50 Opening of the Symposium

9:50-10:30 Lecture 1

Prof. Istvan Hargittai, Hungarian Academy of Sciences, Hungary

Gas-phase Electron Diffraction: A History of Ideas

10:30-11:00 Lecture 2

Prof. Trygve Ulf Helgaker, University of Oslo, Norway

Molecules in strong magnetic fields.

11:00-11:30 Break

11:30-12:00 Lecture 3

Prof. Heinz Oberhammer, Institute of Physical and Theoretical Chemistry, University of Tübingen, Germany

Structures and Conformations of Disilacyclohexanes

12:00-12:30 Lecture 4

Prof. Ingvar Arnason, University of Iceland, Iceland

Energetics and Potential Energy Surfaces of Disilacyclohexanes

12:30-13:00 Lecture 5

Prof. Igor Godunov, Chemistry Department, MSU, Russia

The Structure and Conformational Dynamics of the Molecules in the Ground and Excited Electronic States as Investigated by Experimental and Theoretical Methods.

13:00-14:30 Lunch

14:30-15:00 Lecture 6

Prof. Mikhail Antipin, Institute of Organoelement Compounds, Russia Academy of Sciences, Russia

The structural chemistry of small molecules in comparative studies by the electron (gas) and X-ray (crystal) diffraction methods

15:00-15:30 Lecture 7

Dr. Yury Vishnevskiy, Bielefeld, Germany,

Some Aspects of Accuracy and Precision in GED Method

15:30-16:00 Break

16:00-16:30 Lecture 8

Prof. Jan Dillen, Stellenbosch University, South Africa

Conformational Analysis of Caprolactam. A Comparison with Cycloheptene and Caprolactone

16:30-17:00 Lecture 9

Prof. Victor Solomonik, Ivanovo State University of Chemistry and Technology, Russia

Molecular structure of d and f metal compounds: in pursuit of quantum chemistry, molecular spectroscopy, and gas electron diffraction synergy

17:00-17:20 Lecture 10

Mr. Denis Ksenafontov, Chemistry Department, MSU, GED laboratory, Russia

Molecular structure of some derivatives of 2-pyrrolidone as studied by gas electron diffraction and quantum chemical calculations

## Poster session

## Day 2

June 25

9:30-10:00 Lecture 11

Dr. Sarah Masters, University of Canterbury, New Zealand

Three phases, three conformers? A structural study of 1,2-bis(trifluoromethyl)-1,1,2,2-tetramethyldisilane.

10:00-10:30 Lecture 12

Dr. Allison Campbell, Pacific Northwest National Laboratory, USA

EMSL: High-impact Science and State-of-the-Art Capabilities at a National Scientific User Facility

10:30-11:00 Lecture 13

Prof. William Lester, University of California, Berkeley, USA

Quantum Monte Carlo for the Electron Structure of Molecular Systems

11:00-11:30 Break

11:30-12:00 Lecture 14

Dr. Raphael Berger, University of Bielefeld, Germany

Experimental improvements of GED in Bielefeld and a future perspective for GED in chemistry

12:00-12:30 Lecture 15

Prof. Debashis Mukherjee, India, Raman Center, Indian Association for the Cultivation of Science

State-specific Multi-reference Many-body Formalisms: An Overview of Recent Developments

12:30-13:00 Lecture 16

Dr. Alexander Mitin, Chemistry Department, MSU, GED laboratory, Russia

Polarization and chemical bonding in molecules

13:00-14:30 Lunch

14:30-15:00 Lecture 17

Prof. Norbert Mitzel, University of Bielefeld, Germany,

Gas phase structures of Pnictogen Compounds

15:00-15:30 Lecture 18

Prof. Mauricio Alcolea Palafox, Universidad Complutense de Madrid, Spain

Structure and conformational analysis of the anti-HIV prodrugs Nikavir and AZT 5'-aminocarbonylphosphonate using MP2 and DFT methods

15:30-16:00 Break

16:00-16:30 Lecture 19

Prof. Jochen Schirmer, Theoretical Chemistry, University of Heidelberg, Germany

Electronic excitation in molecules: From propagator theory to intermediate state representations

16:30-17:00 Lecture 20

Prof. Aldo Domenicano, University of L'Aquila, Italy

Field and resonance effects in biphenyl derivatives: a quantum chemical study based on structural variation

17:00-17:20 Lecture 21

Prof. Andrey Stolyarov, Department of Chemistry, MSU, Russia

Calculations of the thermodynamic functions of diatomic molecules at elevated temperatures

## Poster session

## Day 3

June 26

10:00 Bus excursion around Moscow, Kremlin

18:00 Banquette

## Day 4

June 27

9:00-9:50

Under clouds in the Moscow State University

9:50-10:10 Lecture 22

Mr. Maxim Abaev, Chemistry Department, MSU, GED laboratory, Russia

The Structure of 2-Methoxyfuran by Gas Electron Diffraction and Quantum-chemical Calculations

10:10-10:40 Lecture 23

Dr. Nobuhiko Kuze, Department of Materials and Life Sciences, Faculty of Science and Technology, Sophia University, Japan

The Molecular structure of camphor by gas-electron diffraction and quantum chemical calculation

10:40-11:00 Lecture 24

Dr. Vitaly Avakyan, Photochemistry Center of Russian academy of sciences, Russia

Quantum-chemical study of dye aggregation. Structure and spectral bands shifts for dimmers and tetramers of benzoazathiocarbocyanine.

11:00-11:30 Break

11:30-11:50 Lecture 25

Dr. Vadim Bataev, Chemistry Department, MSU, Russia,

Conformations of carbonyl molecules with saturated and unsaturated groups in the ground and excited electronic states

11:50-12:10 Lecture 26

Ms. Anastasia Shishkina, D.I. Mendeleev University of Chemical Technology, Russia

The electrostatic component of interactions in Van der Waals crystals

12:10-12:40 Lecture 27

Prof. Pavel D'yachkov, Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Russia.

Electronic structure of ideal and doped carbon nanotubes calculated using augmented cylindrical wave method

12:40-13:00 Lecture 28

Dr. Stanislav Dubrovensky, St-Petersburg State Institute of Technology, Russia

Quantum chemical modeling of structure and spectral properties of vanadium (V) molecular compounds

13:00-14:30 Lunch

14:30-15:00 Lecture 29

Prof. Magdolna Hargittai, Hungarian Academy of Sciences, Hungary

Special Structural Effects in Metal Halides

15:00-15:30 Lecture 30

Prof. Dines Christen, University Tubingen, Germany

Rotational spectra of Acetone,  $\text{CH}_3\text{COCH}_3$ , in the  $\nu_{17}$  torsional excited state using Microwave-Microwave-Double-Resonance techniques

15:30-16:00 Lecture 31

Prof. Lev Gorokhov, V.P. Glushko Thermocentre of RAS, Russia

Joint Institute of High Temperatures

Molecular structure and thermochemistry of  $\text{V}_m\text{O}_n$  clusters ( $m=2, n=3-5; m=4, n=8, 10$ )

16:30-

Dr. Juergen Vogt, Dr. Natalja Vogt, Chemieinformationssysteme, University of Ulm, Germany

Projects supported by Dr. Barbara Mez-Starck Foundation

Representatives of Foundation, Germany

Award of the International Dr. Barbara Mez-Starck-Prize 2011

## Day 5

June 28

9:30-9:50 Lecture 32

Dr. Aleksander Vorontsov, Chemistry Department, MSU, Russia

States and Transformations of Alkaline Metal - Water Complex Systems: Quantum Chemical Interpretation of Molecular - Beam Studies

9:50-10:10 Lecture 33

Dr. Yurii Panchenko, Chemistry Department, MSU, Russia

Secondary periodicity in the structural and vibrational characteristics of

3,3 - dimethylcyclopropes di - and mono substituted by - X (CH<sub>3</sub>)<sub>3</sub> (X=C, Si, Ge, Sn, and Pb)

10:10-10:40 Lecture 34

Prof. Georgiy Girichev, Ivanovo State University of Chemistry and Technology, Russia,

Molecular structure of macroheterocyclic compounds

10:40-11:00 Lecture 35

Ms. Dina Mukhamedzyanova, Chemistry Department, MSU, Russia

The study of unsaturated aliphatic and aromatic hydrocarbons adsorption on nanosized gold from first principles

11:00-11:30 Break

11:30-12:00 Lecture 36

Prof. Aleksander Boldyrev, Utah State University, USA,

Deciphering Delocalized Bonding in Chemistry

12:00-12:30 Lecture 37

Dr. Sergey Krasnoshchekov, Department of Chemistry, MSU, Russia

The numeric/analytic solution of the anharmonic vibrational problem for a polyatomic molecule using the high orders of canonical Van Vleck perturbation theory

12:30-13:00 Lecture 38

Prof. Julia Novakovskaya, Chemistry Department, MSU, Russia

Electronic excitation and ionization of water - based cluster systems: theoretical energy - size functional dependences and predictions

13:00 Closing of the Symposium

13:05-14:30 Lunch