

## Conference Program



### Monday, March 27, 2017

<b>15:00-16:00</b>	<b>Registration</b>
<b>16:00 -16:15</b>	<b>Opening session</b>
16:00	<b>Opening (Sándor Kunsági-Máté, Iwata Koichi, Piotr Wieczorek, Teobald Kupka)</b>
<b>16:15-18:15</b>	<b>(S1) Session. Invited talks (chair Sándor Kunsági-Máté)</b>
16:15    I-1	<b>Anne-Marie Kelterer</b> ( <i>TU Graz, Austria</i> ), Intermolecular Interactions In The Binary System Water-Methanol.
16:45    I-2	<b>Hans Heinrich Limbach</b> ( <i>Freie Universität Berlin, Berlin, Germany</i> ), <sup>15</sup> N Labeled Pyrazoles And Imidazoles: Molecular NMR Probes Of Complex Environments.
17:15    I-3	<b>Stephan Sauer</b> ( <i>University of Copenhagen, Copenhagen, Denmark</i> ), Weak molecular interactions and NMR parameters: Some calculated examples.
17:45    I-4	<b>Pavel Hobza</b> ( <i>CAS Prague, Czech Republic</i> ), Quantum mechanical computations on host – guest and protein – ligand complexes.
<b>18:30- 20:30</b>	<b>Dinner</b>

### Tuesday, March 28, 2017

<b>8:00 - 9:00</b>	<b>Registration</b>
<b>9:00-11:15</b>	<b>(S2) Session. Invited talks (chair Joanna Sadlej)</b>
9:00    I-5	<b>Frank Jensen</b> ( <i>Aarhus Universitet, Aarhus, Denmark</i> ), Developing Improved Force Fields.
9:30    I-6	<b>Tatsuyuki Yamamoto</b> ( <i>Shimane University, Matsue, Japan</i> ), A Raman Imaging Study on the Molecular Distributions.
10:00   I-7	<b>Miklós Kellermayer</b> ( <i>Semmelweis University, Budapest, Hungary</i> ), Weak Biomolecular Interactions Explored with Single-Molecule Manipulation.

10:30	I-8	<b>Szczepan Roszak</b> ( <i>Wrocław Technical University, Wrocław, Poland</i> ), The Beryllium Doping – Carbon Material Functionalization for the Hydrogen Storage.
11:00	O-1	<b>Agnieszka Kowalczyk</b> ( <i>LOT-Quantum Design, Chorzów, Poland</i> ), Nanoscale analysis of surface, interactions and reactions.
<b>11:15-11:45</b>		<b>Coffee break</b>
<b>11:45- 14:15</b>		<b>(S3) Session. Lectures (chair Anne-Marie Kelterer)</b>
11:45	I-9	<b>Radek Marek</b> ( <i>Masaryk University, Brno, Czech Republic</i> ), Covalence in Supramolecular Interactions.
12:15	I-10	<b>Henryk Kozłowski</b> ( <i>University of Wrocław, Poland</i> ), Strong and Weak Interactions in Metalloproteins.
12:45	I-11	<b>Andrzej Eilmes</b> ( <i>Jagiellonian University, Kraków, Poland</i> ), Hydrogen Bonding in EMIM-TFSI Ionic Liquid Studied via <i>ab initio</i> Molecular Dynamics.
13:15	I-12	<b>Michal Straka</b> ( <i>CAS Prague, Czech Republic</i> ), Endohedral Fullerene as Room-Temperature Single-Molecule Switch.
13:45	I-13	<b>Jakub Kaminský</b> ( <i>CAS Prague, Czech Republic</i> ), Structure and Interactions of Saccharides Probed by Raman Optical Activity.
<b>14:15-15:15</b>		<b>Lunch</b>
<b>15:15-17:15</b>		<b>(S4) Session. Lectures (chair Koichi Iwata)</b>
15:15	I-14	<b>Jacek Korchowiec</b> ( <i>Jagiellonian University, Kraków, Poland</i> ), Inclusion Phenomena from Reactant Perspective.
15:45	I-15	<b>Marcin Palusiak</b> ( <i>Łódź University, Łódź, Poland</i> ), Halogen Atoms in View of Many-Body Interaction Theory.
16:15	I-16	<b>Tatiana Korona</b> ( <i>Warsaw University, Warsaw, Poland</i> ), Intermolecular Interactions from the Point of View of a Computational Chemist: How Far Can We Go with Interaction Partitioning?
16:45	I-17	<b>Poul Erik Hansen</b> ( <i>Roskilde University, Denmark</i> ), Weak Interactions and Solvent Effects.
17:15	O-2	<b>Klemens Noga</b> ( <i>ACK Cyfronet Kraków, Poland</i> ), Molecular Electrocatalysis Controlled by Noncovalent Interactions.
<b>17:30-18:30</b>		<b>(S5) Poster session and tee break:</b>
	<b>P-1</b>	<b><u>Justyna Kozłowska</u>, <u>Agnieszka Roztoczyńska</u>, <u>Wojciech Bartkowiak</u></b> , About the Electric Properties of Spatially Confined Molecular Systems.

- P-2** Aneta Buczek, Małgorzata A. Broda, Manuel K. Strauss, Sandor Kunsági-Máté, Teobald Kupka and Anne-Marie Kelterer, Anharmonic Description of the Fundamental Modes in Water and Methanol Dimers.
- P-3** Łukasz Kołodziej, Joanna Nackiewicz, Małgorzata Broda, New Aspects of Drug Pollution Removal from the Environment by Phtalocyanine Complexes. Theoretical Study.
- P-4** K. Wolnica, M. Dulski, E. Kamińska, A. Cecotka, M. Tarnacka, R. Wrzalik, K. Kamiński and M. Paluch, Monitoring the Mutarotation Phenomenon in D-Fructose in Wide Temperature Range by Means of Experimental Spectroscopic Methods (FTIR, BDS).
- P-5** S.A. Berger, E. Perlt, B. Kirchner, A.-M. Kelterer, Intermolecular Vibrations in the System Water-HCl. How Much Anharmonicity is Needed?
- P-6** Manuel K. Strauss, Romina Brasca, Maria Julia Culzoni, Anne-Marie Kelterer, pKa-Calculation of Three Photoacidic Compounds.
- P-7** Kinga Wzgarda-Raj, Agnieszka Rybarczyk-Pirek, Marcin Palusiak, Halogen Bonding in Crystal Structures of Selected 14 and 15 Group Elements.
- P-8** G. Boda, P.W. Needs, P.A. Kroon, M. Poór, Displacement of Racemic Warfarin from Human Serum Albumin by Different Polyphenols.
- P-9** O. Fedorova, R. Petrina, N. Zayarnyuk, R. Konechna, V. Novikov, Obtaining Compositions "Polymeric Microsphere - Bioligand" for Use in Immunological of Diagnostics Systems.
- P-10** A. J. Rybarczyk-Pirek, M. Palusiak, M. Małecka, K. Wzgarda-Raj, QTAIM Corrections for Hydrogen Atom Locations in X-Ray Diffraction Based Studies.
- P-11** H. Mohamed Ameen, S. Kunsági-Máté, B. Lemli, The Effect of pH on the Interaction Between Sulfamethazine and  $\beta$ -Cyclodextrin.
- P-12** B. Lemli, D. Kovács, S. Kunsági-Máté, Studies on the Non-Covalent Interaction Between Tilmicosin and Bovin Serum Albumin.
- P-13** B. Lemli, D. Derdák, S. Kunsági-Máté, Effect of Amphotericin B Antibiotic on the Thermodynamics of the Conformation Transitions of Some Serum Albumins.
- P-14** M. Poór, A. Zand, L. Szente, Interaction of the Cell Viability Dye Resorufin with  $\beta$ -Cyclodextrins.
- P-15** B. Lemli, M. Poór, S. Kunsági-Máté, Non-Covalent Interactions of Some Mycotoxin and Antibiotic Molecules with a Series of Mammalian Serum Albumins.
- P-16** B. Lemli, D. Szerencsés, S. Kunsági-Máté, Effect of the Ionic Strength

	on the Interaction of Zearalenone Mycotoxin with Bovin Serum Albumin.
<b>P-17</b>	<b>Jacek Kitowski, Kazimierz Wiatr, Łukasz Dutka, Tomasz Szepieniec, Mariusz Sterzel, Katarzyna Zaczek, Magdalena Kruszlenicka, Robert Pająk and <u>Klemens Noga</u></b> PLGrid Infrastructure as a Tool for Open Science.
<b>P-18</b>	<b><u>A. Lutyńska</u>, M. Domagała, M. Palusiak</b> , The Cooperativity of Halogen-, Hydrogen- and Chalcogen- Bonds: Sulphur Atom as a Center of Noncovalent Interactions in Dimeric and Trimeric Complexes.
<b>P-19</b>	<b><u>A. Lutyńska</u>, M. Domagała, M. Palusiak</b> , The Halogen Bond, Hydrogen Bond – Noncovalent Interactions in the Cl-, Br-Complexes.
<b>P-20</b>	<b>B. Sobetov, <u>N. Zayarnyuk</u>, A. Krychrovska, O. Fedorova, S. Popel, <u>V. Novikov</u></b> , Biodistribution of Injecting Prolongs of Disulfiram.
<b>P-21</b>	<b><u>Monika Porada</u>, Dawid Siodłak, Anna Kusakiewicz-Dawid</b> , Pyrazole Amino Acids: Hydrogen Bonding Directed Conformations of 3-amino-1H-pyrazole-5-carboxylic Acid Residue.
<b>P-22</b>	<b><u>Ania Chudoba</u>, Zygmunt Flisak, <u>Szczepan Roszak</u></b> , Ionization Energies for Precursors of Conducting Polymers.
<b>P-23</b>	<b><u>Łukasz Gajda</u>, Małgorzata A. Broda, Monika Ignasiak</b> Interaction of Zinc Phthalocyanine with Water Molecule. DFT Study.
<b>18:30- 19:30</b>	<b>Easter eggs, Opole china pottery decoration show</b>
<b>19:30-21:30</b>	<b>Conference dinner</b>
<b>Wednesday, March 29, 2017</b>	
<b>9:00 - 11:15</b>	<b>(S6) Session. Lectures (<i>chair Poul Erik Hansen</i>).</b>
9:00	<b>I-18</b> <b>Koichi Iwata</b> ( <i>Gakushuin University, Tokyo, Japan</i> ), Properties of Liposome Lipid Bilayer Membranes Examined by Time-Resolved Raman and Fluorescence Spectroscopies.
9:30	<b>O-3</b> <b>Marijana Marković</b> ( <i>TU Graz, Austria</i> ), Weak Intramolecular Interactions in Bis(L-Threoninato)Copper(II) Compared to Bis(L-Allo-Threoninato) Copper(II).
9:45	<b>I-19</b> <b>Todor Dudev</b> ( <i>Sofia University, Bulgaria</i> ), $\alpha$ -Cyclodextrin: How Effectively Can Its Hydrophobic Cavity be Hydrated?
10:15	<b>I-20</b> <b>Tadeusz Andruniów</b> ( <i>Wrocław Technical University, Wrocław, Poland</i> ), Photoisomerization of Structurally Modified Chromophores in Rhodopsin Protein.
10:45	<b>I-21</b> <b>Sándor Kunsági-Máté</b> ( <i>University of Pécs, Hungary</i> ), Competitive Interaction of Fe(III) and Cu(II) Ions with a Multidentate Cavitand

	Derivative.
<b>11:15 -11:45</b>	<b>Coffee break</b>
<b>11:45-12:45</b>	<b>(S5) Session. Lectures (chair Andrzej Elimes).</b>
11:45 I-22	<b>Volodymir Novikov</b> ( <i>Lviv Polytechnic National University, Ukraine</i> ), Main Directions of the Investigations of the Department of Technology of Biologically Active Substances, Pharmacy and Biotechnology.
12:15 O-4	<b>Erik Donovan Hedegård</b> ( <i>Lund University, Sweden</i> ), The Enigmatic Permanganate Ion, and Its Heavier Congeners: Is the Solvent-Solute Interaction Weaker Than Relativistic and Multireference Effects?
12:30 O-5	<b>Justyna Dominikowska</b> ( <i>University of Łódź, Poland</i> ), Cooperativity in Halogen-Bonded Tetramers.
12:45 O-6	<b>Andrzej Kałamarz, Arkadiusz Wiewiórski, Cezary Kluszczyk, Teobald Kupka</b> ( <i>ECO-TECH, Warsaw, University of Opole</i> ), From strong and weak intermolecular interactions to clean environment.
<b>13:00-13:45</b>	<b>(S6) Session. Young scientists session (chair Dawid Siodłak)</b>
13:00 Y-1	<b>Wiktor Beker</b> ( <i>Wrocław Technical University, Wrocław, Poland</i> ), Understanding Kemp Eliminase KE07 Mutants with Differential Transition State Stabilization Theory.
13:15 Y-2	<b>Monika Staś</b> ( <i>University of Opole, Poland</i> ), Weak Interactions Between Oxazole/Isoxazole and Argon.
13:30 Y-3	<b>Tomasz Płowucha</b> ( <i>University of Opole, Poland</i> ), Theoretical study on 5-fluorouracil (5-FU) and its $\beta$ -cyclodextrin inclusion complex.
13:45	<b>Conference closing</b>
<b>14:00-15:00</b>	<b>Lunch</b>

