Monday

**Physical Foundations of Organic Reactivity**

**Session 1a**

IL1 - **Henrik Ottosson**, Relating the Triplet State Baird-Aromaticity of the Macrocycle to that of the Monocycle

O1 - **Yoshimitsu Itoh**, Ring Inversion Kinetics of Photoexcited Chiral [4n]Annulene Derivatives: Energetic Impact of Baird Aromaticity

O2 - **Goetz Bucher**, Quenching of Triplet and Singlet Excited States by Carbon Dioxide

O3 - **Gavin Jones**, Theoretical Studies on Ring-opening Polymerizations by Alkoxides and (Thio)ureas

O4 - **Renana Gershoni-Poranne**, Aromatic Additivity in Three Dimensions

Coffee Break

**Session 1b**

O5 - **Anat Milo**, Physical Organic Principles for Controlling the Secondary Sphere in Organocatalysis


O7 - **Leonor Cruzeiro**, A Kinetic Pathway for Protein Folding in vivo

O8 - **Artur Mardyukov**, Unravelling Lawessons’s Reagent – The Structure of Monomeric (4-Methoxyphenyl)phosphine Disulfide

O9 - **Kazuhide Nakata**, Computational Study of Substituent Effects on Gas-Phase Stabilities of Amino(phenylboranyl)methyl Anions

**Reaction mechanisms and Catalysis**

**Session 2a**

IL2 - **Herbert Mayr**, Nucleophilicity and Electrophilicity Parameters for the Analysis of Cycloaddition Reactions

O10 - **Michael Page**, Kinetics and mechanisms of organo-iridium catalyzed reactions

O11 - **Igor V. Alabugin**, Coupling N-H deprotonation, C-H activation and oxidation: metal-free C(sp^{3})-H aminations with unprotected anilines

O12 - **Xin Li**, Modeling Structure-Stereoselectivity Relationship Using Steric and Electronic Parameters for Chiral Bifunctional Tertiary-amine Thioureas Catalysis

O13 - **Eduardo Humeres**, Desulfurization route of carbons modified with SO_{2}. Polymerization of the sulfur allotropes intermediates

Coffee Break
Session 2b

O14 - **Einar Uggerud**, C–C bond formation of Mg and Zn activated carbon dioxide

O15 - **Daisuke Kaneno**, Regioselectivity and Reaction Mechanism on Tricyanovinylation of Pyrrole Derivatives

O16 - **Joaquim Faria**, Chemical Modification of g-C₃N₄ by beta-Cyclodextrin for Enhanced H₂ Photocatalytic Generation

O17 - **Alexey Ignatchenko**, Beta keto acids: structure, reactivity, and formation as elusive intermediates in heterogeneous catalysis

O18 - **Niklaas J. Buurma**, Predicting Racemisation Risk to Avoid Pointless Stereoselective Syntheses

Supramolecular and Systems Chemistry

Session 3a

IL3 - **Shuichi Hiraoka**, Nanocube: Hyperthermostable Discrete Self-Assemblies in Water

O19 - **Sota Sato**, Chiral Intertwined Spirals and Chiroptical Properties Dictated by Cylinder Helicity

O20 - **Thierry Brotin**, Molecular Recognition of Cations by Enantiopure Cryptophanes

O21 - **Hrvoj Vančik**, Reaction mechanisms in crystalline molecular solids and their general importance in physical organic chemistry: a case study

O22 - **Tatiana Nekipelova**, Aggregation-induced Chemical Reaction: Annulation of Acetylenes with Mixed Phosphonium-Iodonium Ylides

Coffee Break

Session 3b

O23 - **Philippe Lainé**, From single-electron processes to multielectron handling and storage at the molecular level: designing super-electrophores for the next generation of prototypes of photochemical molecular devices for man-made photosynthesis?

O24 - **Nuno Basílio**, Stimuli-Responsive Supramolecular Systems Based on Bio-Inspired Molecular Switches

O25 - **Laura Salonen**, A Supramolecular Strategy to High-Quality Covalent Organic Frameworks

O26 - **Samuel Guieu**, Organic fluorophores in confined environment: properties and applications

O27 - **Ofer Reany**, Hetero-Bambusurils
Tuesday

Physical Foundations of Organic Reactivity

Session 1c

IL4 - Robert McMahon, Astrochemistry: A Perspective from Physical-Organic Chemistry
O28 - Ian Williams, Influence of Dielectric Environment upon Isotope Effects on Glycoside heterolysis: computational evaluation and atomic hessian analysis
O29 - John Wallis, New Studies of Interactions and Bond Formation in Peri-Naphthalenes
O30 - Jiří Váňa, On the way from understanding of basic principles to rational design of reaction conditions for palladium catalysed C–H activation reactions
O31 - Luís Duarte, Interaction of Formic Acid with Nitrous Oxide and Carbon Monoxide
O32 - Igor Reva, Spontaneous and Photochemically Induced Reactions of Triplet 2-Formyl-Phenylnitrene in Low-Temperature Matrix

SESSÃO 2 - Reaction mechanisms and Catalysis

Session 2c

IL5 - Halina Szatylowicz, Physical Interpretation of the Substituent Effect – the Quantum Chemistry Approach
O33 - Hendrik Zipse, Size-Induced Chemoselectivity in Esterification Reactions
O34 - Victor Chechik, A new approach to detect short-lived radicals: application to atmospherically-relevant radicals
O35 - Dasan M. Thamattoor, Generation and Trapping of 3-Thiacyclohexyne
O36 - Moisés Canle, In search for truly green photocatalysts
O37 - Luis Viegas, Reactivity of the atmospherically important hydrofluoropolyethers towards OH: a cost-effective implementation of multiconformer transition state theory

Supramolecular and Systems Chemistry

Session 3c

IL6 - Sanzhong Luo, Stereo-ionic Interaction of Protonated Amines in Asymmetric Catalysis
O38 - Ryo Sekiya, Chemical Functionalization of Nanographene
O39 - Florian Auras, Solvatochromic donor-acceptor covalent organic frameworks
O40 - Dirk Kurth, Metallo-supramolecular polyelectrolytes: From growth kinetics to electrochromic properties
O41 - Anna McConnell, Metal-Organic Cages: Expanding the Toolbox of Stimuli-Responsive Behaviour
O42 - Bruno Medronho, Advances in cellulose dissolution and regeneration: From scattering and rheology to a new NMR approach (with some controversial thoughts in between)
Thursday

Physical Foundations of Organic Reactivity

Session 1d

IL8 - Uta Wille, Position matters: Amide neighbouring group participation facilitates the rate of phenylalanine oxidation in peptides

O43 - Bagrat Shainyan, Structural, Electronic and Mechanistic Features of Unsaturated Triflamides

O44 - Hans-Ullrich Siehl, The Conundrum of the C₄H₇⁺ Cation. Dedicated to George A. Olah

O45 - Oliver Maguire, How to cope with change? The effects of dynamic environments on out-of-equilibrium chemical reaction networks: behaviour diversification and early warning signals

O46 - Igor Khmelinskii, ADH1A - catalysed ATP hydrolysis is coupled to ethanol dehydrogenation by energy transfer

Reaction mechanisms and Catalysis

Session 2d

IL9 - María Paz Muñoz, Precious metal catalysis in Allene chemistry: from divergent systems to heterobimetallic catalysis

O47 - Satoshi Usui, In-Cage Reaction of Intermediates Generated in the Photosolvolysis of 3-Substituted-2-benzlyoxy-naphthalene

O48 - Luis Frija, Broad-spectrum Azole-based Molecules: From Strong Ligands in Coordination Chemistry to Organocatalysts

O49 - Luis Branco, Task-Specific Ionic Liquids for CO₂ Capture and Catalytic Conversion in fuels

O50 - Bruno S. Souza, Aminolysis of 1,8-Naphthalic Anhydrides in Aprotic Solvents Involves Two Reaction Paths

Supramolecular and Systems Chemistry

Session 3d

IL10 - Adriana Gerola, Reactive and Selective Supramolecular Artificial Enzymes for Phosphate Transfer Reactions

O51 - Wataru Setaka, Thiophenediyi-bridged Macrocages as Crystalline Molecular Dipolar Rotors

O52 - Uwe Pischel, Light-induced Release of Guests from Host-Guest Complexes in Water

O53 - Sean Ryan, Light-controlled molecular encapsulation

O54 - Carlos Baleizão, Tuning particle diameter and morphology of hybrid mesoporous silica nanoparticles and application to controlled drug release
Session 3e

IL11 - Shmaryahu Hoz, A New Reaction Mechanism Diagnostic Tool for the Reaction of SmI2
O55 - Carlos Lima, Influence of Molecular Symmetry on the Entropy of Pure Phases
O56 - Ricardo Simões, Development of novel autoreactive and ecological monocomponent adhesives
O57 - Manuel Aureliano, Recent insights into the biological activities of polyoxometalates
O58 - Francisco José Ostos, Influence of the surfactant degree of oligomerization on the formation of cyclodextrin:surfactant inclusion complexes