

Poster presentations

Physical Foundations of Organic Reactivity

PP1	Antony J. Stasyuk	Reliable charge assessment on encapsulated fragment for endohedral systems
PP2	Aicha Hassani	Biological activities and phytochemical study of <i>Cistus Salviifolius</i>
PP3	André K. Eckhardt	Spectroscopic evidence for aminomethylene ($\text{H}-\ddot{\text{C}}-\text{NH}_2$) - The simplest amino carbene
PP4	Amin Ismael	Insights into the photochemistry of 5-aminotetrazole derivatives; effect of the saccharyl moiety on the photostability
PP5	Bernard Denegri	Different solvolytic behavior of aryl/alkyl carbonates, carboxylates and phenolates
PP6	Carolina Rio	The termolecular reaction $\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}$
PP7	Charles Perrin	Polynomial coefficients. Application to spin-spin splitting by N equivalent nuclei of spin $I > 1/2$
PP8	Cláudio Nunes	Cyclization of triplet 2-formyl-phenylnitrene to 2,1-benzisoxazole: A new heavy-atom tunneling event?
PP9	Davide Corinti	Structural insights into non-covalent halide adducts with tyrosine and 3-nitrotyrosine using ion-spectroscopy
PP10	Elisa M. Brás	The structure and properties of a novel sulphanyl-bridged thiadiazolyl-saccharinate ligand
PP11	Ephrath Solel	Fulvalene: computationally tuning aromaticity and tunneling
PP12	Fynn Röhricht	Anisotropy of the current induced density (ACID) - a new method for prediction and explanation of Diels-Alder reactions
PP13	James Scotson	Effects of binary solvent mixtures on reactivity
PP14	Jan M. Schümann	A synthetical approach to 1,4-di-substituted-cyclooctatetraene based dispersion balances
PP15	Jesús Sanjosé-Orduna	Road to a full understanding of the C-H Activation using $\text{Cp}^*\text{Co(III)}$ metal complexes
PP16	Jin-Dong Yang	iBonD: a databank of measured pKa and BDE values
PP17	Kazuhide Nakata	Computational study of the through-resonance effect operating on (phenylamino)methyl cations
PP18	Lijuan Song	Understanding and utilizing the role of London dispersion interactions in catalysis
PP19	Luuk Kortekaas	Protonation of spiropyrans: revising acidochromism and electrochromism
PP20	Mika Maehara	Interaction of 3,6-dimethylfluorenylidene with ammonia and water at cryogenic temperatures
PP21	Mirela Matic	Solvolytic Reactivity Of Organophosphates And Organophosphinates
PP22	Moisés Canle	Photochemistry of thiazolidines in solution
PP23	Morten Peters	Development of a contrast agent based on Fe^{III} -recordplayer

PP24	Nadezhda Danilenko	Quantum chemical calculation of SuFEx reaction thermodynamics
PP25	Neshat Rozatian	Kinetics of fluorination of 1,3-dicarbonyls
PP26	Ouassila Ferroukhi	Influence of alkyl spacer on the physical behaviors of novel mesogenic bioactive phases for GC
PP27	Pengju Ji	Homolytic bond dissociation enthalpies in room temperature ionic liquids
PP28	Potlaki Tseki	The chemical behaviour of nitromethane in inert solvents examined through spectroscopic techniques
PP29	Rikuo Akisaka	Kinetic stabilization of singlet-2,2-dialkoxy-1,3-diradical by introducing bulky substituents
PP30	Rui M. Borges dos Santos	Thermochemistry of peroxy radicals: a combined photoacoustic calorimetry, quantum chemistry, and molecular dynamics study
PP31	Jorn D. Steen	Proton dependent redox chemistry of spiropyrans
PP32	Sayaka Hatano	Development of a photo-induced fast spin-state switching molecule
PP33	Gulce Ogruç-Ildiz	Structural Aspects and Reactivity of 5-Methylhydantoin
PP34	Zoe Dominguez	Chiroptical properties of azabora[5]helicene architectures
PP35	Yusuke Inagaki	Rotation of the π -system rotor in crystalline molecular gyrotops
PP36	Zoran Glasovac	The role of intramolecular hydrogen bonds in construction of model donor-acceptor salt bridged crystals

Reaction mechanisms and Catalysis

PP37	Uta Wille	Decoding the mechanism of environmental radical polyester degradation
PP38	Xiuling Cui	Alkynone-based synthesis of heterocycles
PP39	Alba Pereira Vilar	Formation of pillar[5]arene based stable rotaxane with azobenzene
PP40	Alyssa Gilbert	Investigation of the effects of ionic liquids as solvents on a unimolecular substitution process
PP41	Anastasiia Kovrizhina	Methods for the preparation of new 11 <i>H</i> -indeno[1,2- <i>b</i>]quinoxalin-11-one oxime analogs as promising JNK inhibitors
PP42	André D. Lopes	Catalytic performance of pyridyl-benzimidazole oxidomolybdenum(vi) complex in olefin epoxidation
PP43	Anna Rovaletti	Theoretical investigation on the effect of ligand bulkiness on the reactivity of organometallic complexes
PP44	Thomas Dent	Investigation of the caesium effect in palladium catalysed coupling reactions
PP45	Barbara Ticconi	Oxidation of aliphatic and aromatic amino acids with H ₂ O ₂ catalyzed by a nonheme imine based iron complex
PP46	Christina McCulley	A mechanistic examination of the influence of alkene substitution on rates of biomimetic platinum-promoted polyene polycyclization

PP47	Christof Jaeger	Thermodynamic reaction control in radical enzymes and the role of orientated electric fields
PP48	Elisa M. Brás	UV-induced photolysis of a dispiro-1,2,4-trioxolane with antiparasitic activity
PP49	Gabriel J. Reyes-Rodríguez	Evans enolates: lithium hexamethyldisilazide-mediated enolization of acylated oxazolidinones
PP50	Hidetoshi Noda	On the mechanism of direct amidation catalyzed by the B ₃ NO ₂ heterocycle
PP51	Inmaculada Moreno	Oxidation of Desmetryn by Peroxynitrous Acid
PP52	Ivana Biljan	Self-assembly and dimerization of aromatic dinitroso derivatives on gold surface
PP53	Jessica J. Sánchez García	Bis-cations with two (2,3-diferrocenylcyclopropenium) fragments stabilized with diamino-alkanes: synthesis and reactivity
PP54	Jiayun Zhu	Towards an organocatalytic route for the d ¹ -deuterated of aldehydes
PP55	Ana R. Garcia	Chemistry of model catalytic systems at very low pressure: studies by RAIRS
PP56	Jiri Hanusek	Kinetics and mechanism of Cu(I)-catalyzed [3+2]cycloaddition between phenyl sydnone and phenylacetylenes
PP57	João Lourenço	Catalytic conversion of glycerol to value-added products
PP58	Joel Le Bars	Kinetic investigation of methyl bromide reaction with ethanolamine
PP59	Julian Helberg	The phosphane-catalyzed oligomerization of isocyanates – mechanistic study and identification of a transient intermediate
PP60	Karin Schaffarczyk McHale	Interactions of the components of ionic liquids with species along the reaction coordinate of substitution processes
PP61	Kevin O. Maduka	Synthetic and kinetic evaluation of triazolyl mimics of thiamine pyrophosphate (TPP) for biocatalysis
PP62	Lídia Cavaca	Oleuropein: a valuable chiral building block
PP63	Long Zhang	The enantiocontrol in primary amine catalysis
PP64	Patrick Jüstel	Concurrent S _N 1 and S _N 2 mechanisms in solvolysis reactions
PP65	Paulina Pavez	Dual function of amino acids ionic liquids (AAILs) on the degradation of organophosphate pesticide, Paraoxón®
PP66	Pedro Horta	Synthesis and Structure of a novel O-linked diazirine-quinolone conjugate
PP67	Markus Schaueremann	NMR evidence for the aromatic, thiamine-like Breslow-Intermediate
PP68	Miroslav Ludwig	Push-Pull dicyanoimidazoles in photoredox catalysis
PP69	Nelaine Mora-Diez	Modelling the Repair of Damaged Proteins by Antioxidants
PP70	Rafael Gomes	Mechanistic studies on the formation of novel cyclopentenones from activated furans
PP71	Raquel Fernandes	Photocatalytic synthesis of benzaldehyde derivatives

PP72	Rebecca Hawker	Rational selection of the components of an ionic liquid solvent to control the reaction outcome of some organic processes
PP73	Roberto Colunga	A Radical twist in the mechanism of lithium-halogen exchange
PP74	Roberto Figueroa	Synthesis of amino acid ionic liquids (AAILs) and their effect in the reactivity of thiol-Michael addition reaction
PP75	Rodrigo Montecinos	Synthesis and characterization of pillar[5]arene functionalized with hydroxy-L-proline. Searching an asymmetric organocatalyst
PP76	Ricardo Ferreira Affeldt	Experimental and theoretical evidence of intramolecular bifunctional catalysis in amide cleavage
PP77	Roland Löw	Relaxation time measurements of azo functionalized TATA platforms
PP78	Romain Lepage	Computational study of the mechanism of glycosylation of L-idose derivatives
PP79	Tainah Dorina Marforio	A mechanistic insight into CNT-catalyzed oxidative dehydrogenation of ethylbenzene to styrene. A DFT computational study
PP80	Tatiana Nekipelova	Mechanism of the annulation of 4-ethynylanisole with mixed phosphonium-iodonium ylide

Supramolecular and Systems Chemistry

PP81	Sebastian Hamer	Dipolar molecular rotors in surface-anchored metal organic frameworks
PP82	Rui Fausto	The role of perchlorate anion on dimerization of a macrocyclic binuclear Cu(II) complex: comparison with a mononuclear Ni(II) macrocyclic complex
PP83	Silvia Hristova	Theoretical design and spectral investigations of tautomeric rotary switches
PP84	Agustin Morales	Use of photolabile Ru(II) complexes for supramolecular release
PP85	Alexandra Filipe	A brief survey on diffusion wave spectroscopy in soft matter systems
PP86	Alexandre Miranda	Synthesis and anion recognition by dinitrophenylurea-dihomooxalix[4]arene receptor
PP87	Alvaro Cañete	Synthesis and spectroscopic characterization of 4-(diethylamino)salicylaldehyde bearing at coumarin derivative. Effect of Cucurbit[7]uril encapsulation on its spectral properties
PP88	Andreas H. Heindl	Tuning the switching properties of macrocyclic azobenzenes by ring strain
PP89	Angel Acuña Barros	Nitric Oxide release from a cucurbituril encapsulated NO-donor
PP90	Baya Berka-Zougali	Comparison of the chemical composition and biological activities of essential oils obtained by classical steam distillation (SD), Instant Controlled Pressure Drop (DIC) and Ultrasound Assisted Extraction (UAE) from Myrtle Leaves Growing Spontaneously In Algeria
PP91	Davor Margetic	Self-Assembly of aromatic donor-acceptor systems by guanidine-carboxylate binding
PP92	Rubén Martín	Encryption of chemical information in a supramolecular assembly

PP93	Guntram Schwarz	Electrochromic properties of metallo-supramolecular polyelectrolytes (Mepes)
PP94	Joana Cristo	How does cholesterol affect the fluidity of model lipid bilayers at the molecular level?
PP95	João Ravasco	New double functionalizable trans-cyclooctenes for enhanced spatial and temporal resolution study of biological systems
PP96	Jackson Alcazar	Reactivity of carbonates and thiocarbonates derivatives toward hydrolysis reaction in the presence of calixarene
PP97	J.C. Mejuto	Stability of iprodione in AOT-based reverse micelles under alkaline conditions
PP98	Jorge Martins	Measuring dielectric constants of lipid bilayers: excluding experimental artifacts from pyrene fluorescence in liposomes
PP99	José G. Santos	Hydrolysis reactions of carbonates and thiocarbonates derivatives. Supramolecular catalysis by cucurbit[7]uril
PP100	Kajetan Dąbrowa	Dynamic control of ion-pair binding by photo-tunable azobenzene-derived hosts
PP101	Koki Ikemoto	Synthesis and structures of nanometer-sized geodesic phenylene bowl
PP102	Leandro Scorsin	A kinetic study with neutral and cationic dioxolanes catalyzed by CB7
PP103	Marcella S. H. Queiroz	Study of phase solubility of bioactive naphthoquinones
PP104	Margarita E. Aliaga	Cucurbit[7]uril encapsulation effect on tautomerism equilibrium in aza-coumarin and quinoxalinone scaffolds. Experimental and molecular modeling studies
PP105	Matthew Watson	Predicting reactivity in binary solvent mixtures using a supramolecular solvation model
PP106	Miguel A. Romero	Binding of terpenes by cucurbituril macrocycles
PP107	Nelaine Mora-Diez	Macroscopic pKa prediction of polyprotic acids from DFT calculations: the case of acetohydroxamic acid
PP108	Niklaas Jan Buurma	I2CITC : modular deconvolution of ITC data for complex equilibrium systems
PP109	Olimpo García-Beltrán	Synthesis and characterization of a new coumarin-derivative chemosensor to detect mercuric ions
PP110	Orlando Oliveira	Towards catalytic metalated covalent organic frameworks through supramolecular strategies
PP111	Patricia Remón	Chemical communication in a supramolecular cascade
PP112	Pravat Mondal	<i>Thio</i> -Bambusurils
PP113	Rubén Martín	Encryption of chemical information in a supramolecular assembly
PP114	R. J. Mayer	From peroxides to hypohalites: towards a general understanding of the reactivities of anionic oxygen nucleophiles