

ESOR 2019 – POSTER SESSION

- P-1 KINETIC STUDY ON THE THERMAL Z-E ISOMERIZATION OF PHOTOSWITCHABLE N-ACYLHYDRAZONES**
Ho Yin Chan, [Mónica Barra](#)
- P-2 SIZE-DEPENDENT RATE ACCELERATION IN THE SILYLATION OF SECONDARY ALCOHOLS: THE BIGGER THE FASTER**
Marta Marin-Luna, [Benjamin Pölloth](#), Fabian Zott, Hendrik Zipse
- P-3 SOLVENTS EFFECTS IN THE FRAGMENTATION OF LIGNOCELLULOSIC BIOMASS**
[Daniela Millan](#), Josei Perez Recabarren, Ingrid Soledad Vidaurre
- P-4 SYNTHESIS AND CHARACTERIZATION OF NEW AROMATIC AZODIOXY AND AZO POLYMERS**
[Ivana Biljan](#), Ivan Kodrin, Mateja Pisačić, Petar Štrbac, Hrvoj Vančik
- P-5 OPPOSING HOST BEHAVIOUR OF TWO ISOSTRUCTURAL APOHOST MATERIALS IN THE PRESENCE OF SELECTED HETEROCYCLIC GUESTS – CRYSTAL DIFFRACTION AND MOLECULAR MODELLING CONSIDERATIONS**
Benita Barton, Mino R. Caira, [Lize de Jager \[Greyling\]](#), Eric C. Hostena, Cedric W. McClelland
- P-6 SOLVOLYTIC BEHAVIOUR OF BENZYL HALIDES IN AQUEOUS ETHANOL**
[Mirela Matić](#), Bernard Denegri
- P-7 ELECTROFUGALITIES AND SOLVOLYTIC BEHAVIOR OF SOME FERROCENYLPHENYLMETHYL CATIONS**
[Sandra Jurić](#), Marijan Marijan, Olga Kronja
- P-8 RADICAL-INDUCED DAMAGE OF PEPTIDES: MECHANISTIC INSIGHTS FROM STUDIES INVOLVING ENVIRONMENTAL OXIDANTS**
J. Nathanael, J. Cui, L. Gamon, [U. Wille](#)
- P-9 4-(DIMETHYLAMINO)DIPHENYLCARBENE: MATRIX ISOLATION STUDIES OF A MAGNETICALLY BISTABLE CARBENE**
[Tobias Thomanek](#), Wolfram Sander
- P-10 SIZE, SHAPE AND SURFACE STRUCTURE AFFECT INTERACTION OF METALLIC NANOPARTICLES WITH TRANSPORT PROTEINS**
Ivona Capjak, Rinea Barbir, Darija Domazet Jurašin, Željko Debeljak, Goran Šinko, Maja Dutour Sikirić, [Ivana Vinković Vrček](#)
- P-11 STABILIZATION OF TRIPLET NITRENES IN NAFION POLYMER BEYOND CRYOGENIC CONDITIONS**
[Adrian Portela-Gonzalez](#), Nesli Özkan, Wolfram Sander
- P-12 DIRECT OBSERVATION OF HEMITHIOINDIGO-MOTOR UNIDIRECTIONALITY**
[K. Hoffmann](#), L. A. Huber, S. Thumser, N. Böcher, P. Mayer, H. Dube
- P-13 ACCELERATION OF A TUNNELING REACTION VIA INTERACTION WITH LEWIS ACIDS**
[Melania Prado-Merini](#), Stefan Henkel, Enrique Méndez-Vega, Wolfram Sander
- P-14 NATURE OF CHALCOGEN BONDS: A QUANTITATIVE KOHN-SHAM MO INVESTIGATION**
[Lucas A. Santos](#), Stephanie van der Lubbe, Trevor A. Hamlin, Teodorico C. Ramalho, F. Matthias Bickelhaupt
- P-15 TRIPLET STATE ANTIAROMATICITY OF SUBSTITUTED BENZENES: A COMPUTATIONAL INVESTIGATION**
[Anup Rana](#), Henrik Ottosson
- P-16 RADICAL CHEMISTRY NEAR BORONIC ESTERS: ELUCIDATING MECHANISM AND REACTIVITY WITH DFT**
A. Studer, [C. Mück-Lichtenfeld](#)
- P-17 PREDICTING REACTIVITY WITH A SUPRAMOLECULAR ELECTROSTATIC SOLVATION MODEL**
[Matthew J. Watson](#), Nicholas H. Williams
- P-18 BOROHYDRIDE REDUCTION OF 2-HALOCYCLOHEXANONES: DFT ANALYSIS OF REACTIVITY AND STEREOSELECTIVITY**
[Daniela Rodrigues Silva](#), Trevor A. Hamlin, Pascal Vermeeren, Matheus P. Freitas, Célia Fonseca Guerra

- P-19 ACTIVATION STRAIN ANALYSES OF ARYLIC VERSUS ALIPHATIC C–X BOND ACTIVATION BY PALLADIUM CATALYST**
Pascal Vermeeren, Xiaobo Sun, F. Matthias Bickelhaupt
- P-20 SIMULATION-BASED EVALUATION OF NON-EQUILIBRIUM SOLVATION FREE ENERGY IN ORGANIC SOLUTION REACTION**
Yasuhiro Shigemitsu, Yasushi Ohga
- P-21 CALCULATION OF REDOX POTENTIAL IN FERROCENE DERIVATIVES. WHY HYBRID DFT METHODS FAIL?**
Mateja Toma, Tea Kuvek, Senka Djaković, Jasmina Lapić, Davor Šakić, Valerije Vrček
- P-22 SOLUBILITY AND SOLVATION PHENOMENON IN WATER ORGANIC MIXTURES AT THE MOLECULAR LEVEL**
Henry Vider, Siim Salmar
- P-23 IRREVERSIBLE INHIBITION OF THE MAO B ENZYME. A COMPUTATIONAL INSIGHT INTO THE INACTIVATION MECHANISM**
Tana Tandarić, Robert Vianello
- P-24 COMPUTATIONAL INSIGHT INTO THE METAL-FREE CLEAVAGE OF THE CARBON-CARBON TRIPLE BOND IN ALKYNES**
Lucija Hok, Robert Vianello
- P-25 BIARYL CROSS-COUPPLING INVOLVING ANIONIC REDUCED FORMS OF CYANOARENES IN LIQUID AMMONIA**
R. Peshkov, E. Panteleeva, C. Wang, Z. Yu, E. Tretyakov, V. Shteingarts
- P-26 CHEMOSELECTIVITY IN ESTERIFICATION REACTIONS – SIZE MATTERS AFTER ALL**
Julian Helberg, Marta Marin-Luna, Hendrik Zipse
- P-27 SIZE-DEPENDENT INVERSION OF SELECTIVITY IN ESTERIFICATION REACTIONS**
Stefanie Mayr, Marta Marin-Luna, Hendrik Zipse
- P-28 EXPERIMENTAL AND COMPUTATIONAL STUDY OF THE REACTION BETWEEN FERROCENYL LITHIUM AND N-PHENYL PHTHALIMIDE**
Davor Šakić, Martin Grumbt, Dieter Schaarschmidt, Valerije Vrček, Alexander Hildebrandt
- P-29 MECHANISM AND STEREOSELECTIVITY OF DECARBOXYLATIVE ELIMINATION OF DIBROMOCARBOXYLIC ACIDS IN DMF**
Petr K. Sazonov, Elnara E. Vezirova, Irina P. Beletskaya
- P-30 HALOGENOPHILIC REACTIONS OF $[\text{Re}(\text{CO})_5]^-$ AND $[\text{Mn}(\text{CO})_5]^-$ ANIONS WITH DIODOACETYLENE PRODUCING SQUARIC ACID ANION COMPLEX**
Petr K. Sazonov, Victor N. Khrustalev, Irina P. Beletskaya
- P-31 ORIENTED EXTERNAL ELECTRIC FIELDS AFFECT RATE AND STEREOSELECTIVITY OF ELECTROCYCLIC REACTIONS. A COMPUTATIONAL DFT STUDY**
Edoardo Jun Mattioli, Andrea Bottoni, Matteo Calvaresi
- P-32 SOLVENT EFFECTS ON THE IN-CAGE REACTIONS IN THE PHOTOSOLVOLYSIS OF 2-OCH₂PH-3-OME-NAPHTHALENE**
Satoshi Usui, Ayaka Ohkura, Chihiro Kinugawa, Haruka Fujita, Takahiro Murohashi
- P-33 KINETICS OF RING-OPENING REACTIONS OF ELECTROPHILIC CYCLOPROPANES**
Patrick Jüstel, Herbert Mayra, Armin R. Ofial
- P-34 AMBIPHILIC REACTIVITY OF DIMETHYL DIAZOMALONATE**
Le Li, Armin R. Ofial, Herbert Mayr
- P-35 GEM-DIFLUORINATION OF TERMINAL ALKYNES USING ELECTRO-GENERATED ACID**
Kouichi Matsumoto, Mizuki Yamaguchi, Shigenori Kashimura
- P-36 REACTION ROUTE FOR ALLYLIC ARYLATION IN WATER CATALYZED BY METAL NANOPARTICLES**
Atsushi Ohtaka, Misa Kawase, Go Hamasaka, Yasuhiro Uozumi, Tsutomu Shinagawa, Osamu Shimomura, Ryôki Nomura

- P-37 THE ENHANCEMENT OF THE ANTITUMOR EFFECT OF TEMOZOLOMIDE ON GLIOBLASTOMA CELLS BY NOVEL DEHYDROABIETYLAMINE DERIVATIVES**
Kseniya Kovaleva, Olga Oleshko, Evgeniya Mamontova, Olga Yarovaya, Olga Zakharova, Alexandra Zakharenko, Alena Kononova, Nadezhda Dyrkheeva, Sergey Cheresiz, Andrey Pokrovsky, Olga Lavrik, Nariman Salakhutdinov
- P-38 SYNTHESIS OF (+)-CAMPHOR-10-SULFONIC ACID AND (+)-CAMPHORIC ACID DERIVATIVES AS POTENTIAL ANTIVIRAL AGENTS**
D. V. Baranova, A. S. Sokolova, N. F. Salakhutdinov
- P-39 COMPARATIVE STUDY OF SI-DOPED GRAPHENE AND FULLERENE IN OXYGEN REDUCTION REACTION (ORR). A QUANTUM CHEMICAL INSIGHT**
Anton V. Kuzmin, Bagrat A. Shainyan
- P-40 CONFORMATIONAL SPIN SWITCHING AND SPIN-SELECTIVE HYDROGENATION OF A MAGNETICALLY BISTABLE CARBENE**
Enrique Mendez-Vega, Iris Trosien, Tobias Thomanek, Wolfram Sander
- P-41 PHOTOCHEMISTRY OF 2-IODOTHIAZOLE IN INERT GAS MATRICES**
Anjali Mahadevan, Amandeep Singh, Sugumar Venkataramani
- P-42 MAKING CARBON–PHOSPHORUS BONDS WITH VISIBLE LIGHT: CHALLENGES AND OPPORTUNITIES**
Sami Lakhdar
- P-43 ELECTRON TRANSFER REACTIONS AT CRYOGENIC TEMPERATURE**
Ankit Somani, Wolfram Sander
- P-44 CATALYSIS BY PURE GRAPHENE - FROM SUPPORTING ACTOR TO PROTAGONIST THROUGH π - π INTERACTIONS**
Asia A. Kroeger, Amir Karton
- P-45 ACTIVATION OF AMMONIA BY TRIPLET ARYL CARBENES**
M. Maehara, W. Sander
- P-46 NON-IDEALITY IN IONIC LIQUID MIXTURES AND THE POTENTIAL FOR RATIONAL CONTROL OF REACTION OUTCOME**
Matthew D. Taylor, Jason B. Harper
- P-47 KINETIC ANALYSES TO DRIVE SOLVENT CHOICE – SELECTING AN IONIC LIQUID TO GET THE DESIRED SYNTHETIC OUTCOME**
Karin S. Schaffarczyk McHale, Ronald S. Haines, Jason B. Harper