

XVII

2019  
ESOR

# European Symposium on Organic Reactivity

September 8–13, 2019, Dubrovnik, Croatia

## PROGRAMME



University of Zagreb, Faculty of Science,  
Department of Chemistry



Croatian Chemical Society



Inter-University Centre - Dubrovnik



# European Symposium on Organic Reactivity

September 8–13, 2019, Dubrovnik, Croatia

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## ORGANISERS

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University of Zagreb, Faculty of Science,  
Department of Chemistry



Croatian Chemical Society



Inter-University Centre Dubrovnik

## PARTNER IN ORGANISATION

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Dear Participants,

On behalf of the Organising Committee, we welcome you to the **17<sup>th</sup> European Symposium on Organic Reactivity (ESOR 2019)**. The symposium is organised by the Department of Chemistry (Faculty of Science, University of Zagreb), the Croatian Chemical Society, and in cooperation with Inter-University Centre Dubrovnik.

The meeting will be held in the beautiful Croatian city of Dubrovnik on the Adriatic coast between 8 and 13 September 2019.

The ESOR series has a long and proud history, with meetings being held in Paris (1987), Padova, Italy (1989), Göteborg, Sweden (1991), Newcastle, UK (1993), Santiago de Compostela, Spain (1995), Louvain la Neuve, Belgium (1997), Ulm, Germany (1999), Cavtat (Dubrovnik), Croatia (2001), Oslo, Norway (2003), Rome, Italy (2005), Faro, Portugal (2007), Haifa, Israel, (2009), Tartu, Estonia (2011), Prague, Czech Republic (2013), Kiel, Germany (2015), and Durham, UK (2017).

The meeting will cover all areas of Physical Organic Chemistry, including all aspects of mechanism, structure and binding in organic systems. This also encompasses a wider range of areas from biology to materials using both theoretical and experimental approaches.

There will be a mixture of plenary and invited lectures plus submitted oral and poster presentations.

We very much look forward to welcoming you to Dubrovnik!



**Hrvoj Vančik**

*Local Organising Committee*

# International Standing Committee of ESOR Conferences

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**Rainer Herges**, President

(Christiana Albertina University of Kiel, Germany)

**Hans-Ullrich Siehl**

(Ulm University, Germany)

**Moisés Canle López**

(University of A Coruña, Spain)

**Hrvoj Vančik**

(University of Zagreb, Croatia)

**AnnMarie O'Donoghue**

(Durham University, United Kingdom)

**Jana Roithová**

(Radboud University, The Netherlands)

**Koop Lammertsma**

(Vrije Universiteit Amsterdam, The Netherlands)

**Amnon Stanger**

(Technion - Israel Institute of Technology, Israel)

**Einar Uggerud**

(University of Oslo, Norway)

**Maria de Lurdes dos Santos Cristiano**

(The Centre of Marine Sciences – CCMAR, Portugal)

## Local Organiser of ESOR 2019

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**Hrvoj Vančik**

(University of Zagreb, Croatia)

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## PLENARY LECTURERS

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**Josef Michl (University of Colorado, USA)**

*Porphene – a Regular Heterocyclic Two-dimensional Polymer*



**Henry Dube (Ludwig-Maximilians-Universität München, DE)**

*From Indigoid Photoswitches To Molecular Machines*



**Eric Vauthey (University of Geneva, CH)**

*Photoinduced Symmetry-breaking Charge-transfer*



**Massimo Bietti (Università "Tor Vergata", IT)**

*Reactivity and Selectivity Patterns in Hydrogen Atom Transfer from Aliphatic C-H Bonds*



**Stefan Grimme (University Bonn, DE)**

*New Tight-binding Quantum Chemistry Methods for the Exploration of Chemical Space*



**Leonard J. Prins (University of Padova, IT)**

*Energy Consumption in Chemical-fuel Driven Self-assembly*



**Sason S. Shaik (Hebrew University, IL)**

*Oriented External Electric Fields as Effectors in Chemistry*



**Johan Åquist (Uppsala University, SE)**

*Entropy and Enzyme Adaptation*



**Lyle Isaacs (University of Maryland, US)**

*Cucurbit[n]uril Molecular Containers: from Basic Science to Biomedical Applications*



**Harry L. Anderson (University of Oxford, UK)**

*Global Aromaticity at the Nanoscale*



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## INVITED LECTURERS

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**Jirí Kaleta (Institute of Organic Chemistry and Biochemistry, CAS, CZ)**  
*Regular 2-D Assemblies of Molecular Machines*



**J. Chris Slootweg (University of Amsterdam, NL)**  
*Circular Chemistry, Steric Attraction and Photoinduced Single-electron Transfer: New Adventures in Main-group Chemistry*



**F. Matthias Bickelhaupt (Vrije Universiteit Amsterdam, NL)**  
*Chemical Reactivity*



**Amnon Stanger (Technion – Israel Institute of Technology, IL)**  
*Surprises in NICS Studies and a New NICS-based Criterion for Aromaticity*



**Yitzhak Apeloig (Technion – Israel Institute of Technology, IL)**  
*Isomerization Mechanisms Around  $E=E'$  ( $E, E'=C, Si, Ge$ ) Bonds- Double Bonds, Anions, Radicals. Experiment and Theory*



**Nikola Basarić (Ruđer Bošković Institute, HR)**  
*Photochemical Elimination of Nitrogen from Diazirines and Diazo Compounds*



**Ruth M. Gschwind (University of Regensburg, DE)**  
*NMR in Catalysis and Photocatalysis Pushing the Frontiers*



**Davor Margetić (Ruđer Bošković Institute, HR)**  
*Guanidine-carboxylate Bonding Motif in Self-assembly of Aromatic Donor-acceptor Systems*



**Marcin Stępień (Uniwersytet Wrocławski, PL)**  
*Open-shell Nanographenoids*

# SCHEDULE

## SUNDAY, 8 SEPTEMBER

<b>14:00-20:00</b>	<b>Registration</b>	
<b>17:30</b>	<b>Introduction, Hrvoj Vančik</b>	
<b>18:00</b>	<b>PL-1</b>	<b>Opening Lecture, Josef Michl (University of Colorado, USA)</b> <i>Porphene – a Regular Heterocyclic Two-dimensional Polymer</i>
<b>19:00</b>	<b>Welcome Party, IUC</b>	

## MONDAY, 9 SEPTEMBER

<b>9:00 – 9:50</b>	<b>PL-2</b>	<b>Henry Dube (Ludwig-Maximilians-Universität München, DE)</b> <i>From Indigoid Photoswitches To Molecular Machines</i>
<b>9:50 – 10:20</b>	<b>IN-1</b>	<b>Jirí Kaleta (Institute of Organic Chemistry and Biochemistry of the CAS, CZ)</b> <i>Regular 2-D Assemblies of Molecular Machines</i>
<b>10:20 – 10:40</b>	<b>OP-1</b>	<b>Michael Schmittel (University of Siegen, DE)</b> <i>Multicomponent Catalytic Machinery: How the Machine Speed Impacts Catalytic Activity</i>
<b>10:40 – 11:10</b>	<b>Coffee Break</b>	
<b>11:10 – 11:30</b>	<b>OP-2</b>	<b>Henrik Ottosson (Uppsala University, SE)</b> <i>Exploring Photoreactions Potentially Triggered by Excited State Antiaromaticity Relief</i>
<b>11:30 – 11:50</b>	<b>OP-3</b>	<b>Moisés Canle (Universidade da A Coruña, ES)</b> <i>Short-lived Intermediates Derived from Sym-triazines: Structure, Thermodynamic Properties and Reactivity</i>
<b>11:50 – 12:10</b>	<b>OP-4</b>	<b>Shigeru Yamago (Kyoto University, JP)</b> <i>Synthesis and Properties of Novel Cyclic <math>\pi</math>-conjugated Molecules</i>
<b>12:30 – 14:00</b>	<b>Lunch Break</b>	
<b>14:00 – 14:50</b>	<b>PL-3</b>	<b>Eric Vauthey (University of Geneva, CH)</b> <i>Photoinduced Symmetry-breaking Charge-transfer</i>
<b>14:50 – 15:20</b>	<b>IN-2</b>	<b>J. Chris Slootweg (University of Amsterdam, NL)</b> <i>Circular Chemistry, Steric Attraction and Photoinduced Single-electron Transfer: New Adventures in Main-group Chemistry</i>
<b>15:20 – 15:40</b>	<b>OP-5</b>	<b>Eva Blokker (Vrije Universiteit Amsterdam, NL)</b> <i>Hydride Affinities of Cationic Main Group-element Hydrides</i>
<b>15:40 – 16:10</b>	<b>Coffee Break</b>	
<b>16:10 – 16:30</b>	<b>OP-6</b>	<b>Trevor Hamlin (Vrije Universiteit Amsterdam, NL)</b> <i>1,3-dipolar Cycloaddition Reactivity of Alkynes</i>
<b>16:30 – 16:50</b>	<b>OP-7</b>	<b>Uta Wille (The University of Melbourne, AU)</b> <i>Decoding the Mechanism of Environmental Polymer Degradation: a Mass Spectrometric Approach</i>
<b>16:50 – 17:10</b>	<b>OP-8</b>	<b>Hendrik Zipse (Ludwig-Maximilians-Universität München, DE)</b> <i>Molecule-induced Radical Formation With Peroxides</i>
<b>17:10 – 17:30</b>	<b>OP-9</b>	<b>Götz Bucher (University of Glasgow, UK)</b> <i>Bay Quinones – Electronic Properties and Stability</i>

## TUESDAY, 10 SEPTEMBER

9:00 – 9:50	PL-4	<b>Massimo Bietti (Università "Tor Vergata", IT)</b> <i>Reactivity and Selectivity Patterns in Hydrogen Atom Transfer from Aliphatic C-H Bonds</i>
9:50 – 10:40	PL-5	<b>Stefan Grimme (University Bonn, DE)</b> <i>New Tight-binding Quantum Chemistry Methods for the Exploration of Chemical Space</i>
10:40 – 11:10	<b>Coffee Break</b>	
11:10 – 12:00	PL-6	<b>Leonard J. Prins (University of Padova, IT)</b> <i>Energy Consumption in Chemical-fuel Driven Self-assembly</i>
12:00 – 12:30	IN-3	<b>F. Matthias Bickelhaupt (Vrije Universiteit Amsterdam, NL)</b> <i>Chemical Reactivity</i>
13:30	<b>CONFERENCE TRIP</b>	

## WEDNESDAY, 11 SEPTEMBER

9:30 – 10:20	PL-7	<b>Sason S. Shaik (Hebrew University, IL)</b> <i>Oriented External Electric Fields as Effectors in Chemistry</i>
10:20 – 10:50	IN-4	<b>Amnon Stanger (Technion – Israel Institute of Technology, IL)</b> <i>Surprises in NICS Studies and a New NICS-based Criterion for Aromaticity</i>
10:50 – 11:10	OP-10	<b>Hans-Ullrich Siehl (Ulm University, DE)</b> <i>1,3-H-shift – a New Route to Static Bicyclobutonium Ions Further Answers to the Conundrum of the Structure of C<sub>4</sub>H<sub>7</sub><sup>+</sup> Cations</i>
11:10 – 11:40	<b>Coffee Break</b>	
11:40 – 12:00	OP-11	<b>Sujan K. Sarkar (Hiroshima University, JP)</b> <i>Heavy Atom Tunneling, Matrix Effect, and Wavelength Effect in the Photoreaction of 2,3-diazabicyclo[2.2.1]hept-2-ene</i>
12:00 – 12:20	OP-12	<b>Neil Griffin (Syngenta, UK)</b> <i>Applying Physical Organic Processes To Formulation Chemical Stability</i>
12:30 – 14:00	<b>Lunch Break</b>	
14:00 – 14:30	IN-5	<b>Yitzhak Apeloig (Technion – Israel Institute of Technology, IL)</b> <i>Isomerization Mechanisms Around E=E' (E, E'=C, Si, Ge) Bonds- Double Bonds, Anions, Radicals. Experiment and Theory</i>
14:30 – 15:00	IN-6	<b>Nikola Basarić (Ruđer Bošković Institute, HR)</b> <i>Photochemical Elimination of Nitrogen from Diazirines and Diazo Compounds</i>
15:00 – 15:15	<b>In Memory of Prof. Brian G. Gowenlock (H. Vančik)</b>	
15:15 – 15:30	<b>Coffee Break</b>	
16:00 – 18:30	<b><u>POSTER SESSION</u></b>	
20:00	<b>CONFERENCE DINNER</b>	

**THURSDAY, 12 SEPTEMBER**

9:00 – 9:50	PL-8	<b>Johan Åquist (Uppsala University, SE)</b> <i>Entropy and Enzyme Adaptation</i>
9:50 – 10:20	IN-7	<b>Ruth M. Gschwind (University of Regensburg, DE)</b> <i>NMR in Catalysis and Photocatalysis Pushing the Frontiers</i>
10:20 – 10:40	OP-13	<b>David R. W. Hodgson (Durham University, UK)</b> <i>Chemo-enzymatic Preparation of Nucleoside Triphosphates from Diphosphates Using Feedstock Chemicals</i>
10:40 – 11:10	Coffee Break	
11:10 – 11:30	OP-14	<b>Marina Šekutor (Ruđer Bošković Institute, HR)</b> <i>Application of Adamantyl Aminoguanidines in Functional Self-assembled Nanovesicles</i>
11:30 – 11:50	OP-15	<b>Veronika V. Semionova (Voevodsky Institute of Chemical Kinetics and Combustion, RAS, RU)</b> <i>Supramolecular Compounds Formed by Organic Photochromes and Metal-organic Coordination Polymer</i>
11:50 – 12:10	OP-16	<b>Benita Barton (Nelson Mandela University, ZA)</b> <i>Host Behaviour of N,N'-bis(9-phenyl-9-thioxanthenyl)ethylenediamine in the Presence of Aromatic and Aliphatic Five-membered Heterocyclic Guest Compounds</i>
12:30 – 14:00	Lunch Break	
14:00 – 14:50	PL-9	<b>Lyle Isaacs (University of Maryland, US)</b> <i>Cucurbit[n]uril Molecular Containers: from Basic Science to Biomedical Applications</i>
14:50 – 15:20	IN-8	<b>Davor Margetić (Ruđer Bošković Institute, HR)</b> <i>Guanidine-carboxylate Bonding Motif in Self-assembly of Aromatic Donor-acceptor Systems</i>
15:20 – 15:50	Coffee Break	
15:50 – 16:10	OP-17	<b>Maria L. S. Cristiano (University of Algarve, PT)</b> <i>Substituent Effects On the Photochemistry of 5-aminotetrazoles</i>
16:10 – 16:30	OP-18	<b>Armin R. Ofial (Ludwig-Maximilians-Universität München, DE)</b> <i>Reactivities of Electrophilic Alkynes and Allenes</i>
16:30 – 16:50	OP-19	<b>Bagrat A. Shainyan (A. E. Favorsky Irkutsk Institute of Chemistry, RU)</b> <i>Silacyclohexanes: Conformational Preferences in Gas and Solution</i>
16:50 – 17:10	OP-20	<b>Robert J. Mayer (Ludwig-Maximilians-Universität München, DE)</b> <i>Ambident Reactivity of Phenolate Anions Revisited: a Quantitative Approach To Phenolate Reactivities</i>

## FRIDAY, 13 SEPTEMBER

9:00 – 9:50	PL-10	<b>Harry L. Anderson (University of Oxford, UK)</b> <i>Global Aromaticity at the Nanoscale</i>
9:50 – 10:20	IN-9	<b>Marcin Stępień (Uniwersytet Wrocławski, PL)</b> <i>Open-shell Nanographeneoids</i>
10:20 – 10:40	OP-21	<b>Ian Williams (University of Bath, UK)</b> <i>Computational Simulation of Energy Landscapes and Isotope Effects for Glycosidic Reactivity</i>
10:40 – 11:00	OP-22	<b>Kazuhide Nakata (Hosei University, JP)</b> <i>Computational Study of Substituent Effects on Gas-phase Stabilities of 1-phenylcyclobutane-1,3-diyliums</i>
11:00 – 11:20	OP-23	<b>Tatiana Nekipelova (Emanuel Institute of Biochemical Physics, RAS, RU)</b> <i>Structure–reactivity Correlation in the Reaction of Mixed Phosphonium-iodonium Ylides With Acetylenes</i>
11:20 – 11:40	OP-24	<b>Rebecca Hawker (University of Sheffield, UK)</b> <i>Predicting the Effects of Solvent Mixtures on the Kemp Reactions</i>
11:40 – 12:00	OP-25	<b>Cedric W. McClelland (Nelson Mandela University, ZA)</b> <i>A DFT Comparative Study of Substituent Effects in Radicals, Cations and Radical Cations</i>
12:00 – 12:20	OP-26	<b>Eduardo Humeres (Universidade Federal de Santa Catarina, BR)</b> <i>Mechanism of Reduction of Air Pollutants on Carbons: Sulfur Dioxide and Ozone</i>
12:20	Closing Ceremony	

**LEGEND:**

PLENARY LECTURES\*

INVITED LECTURES

ORAL PRESENTATIONS

\* Plenary lectures will be held at the nearby auditorium of the **University of Dubrovnik**.

# POSTER PRESENTATIONS

- 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 Millán](#), 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 Vanič
- 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 Thomaneck](#), 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 [Re(CO)<sub>5</sub>]<sup>-</sup> AND [Mn(CO)<sub>5</sub>]<sup>-</sup> 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-OCH<sub>2</sub>PH-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 Somanj](#), Wolfram Sander
- P-44** **CATALYSIS BY PURE GRAPHENE - FROM SUPPORTING ACTOR TO PROTAGONIST THROUGH  $\pi$ - $\pi$  INTERACTIONS**  
[Asja 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](#)

## SOCIAL EVENTS

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- On Sunday, September 8, at 19:00, a **welcome cocktail party** will be held at the Inter-University Centre Dubrovnik.
- **Optional excursion** will be organized on Tuesday, September 9. The trip will consist of a visit to the **Arboretum Trsteno**, and a boat tour of the **Élaphites Islands: Šipan and Lopud**.
- **Conference Dinner** will be held on Wednesday, September 11 at 20:00 at the Sunset Beach Restaurant.



Image by Flickr user Gregor Noczinski and used under the Creative Commons licence 2.0

*Arboretum Trsteno*

## VENUE & ACCESS

**17<sup>th</sup> European Symposium on Organic Reactivity** will be held in Dubrovnik, Croatia, 8–13 June 2019 at the **Inter-University Centre (IUC) Dubrovnik**. IUC is located in the vicinity of the Dubrovnik historical centre, at the address **Don Frana Bulića 4**.



The position of the Inter-University Centre (IUC) Dubrovnik

**Dubrovnik is excellently accessible by all means of transportation.**

### Arriving to Dubrovnik by plane

Once you arrive to Čilipi airport you can reach the city by taxi (the price is approximately 250 HRK or approximately 35 EUR for one direction) or you can take a shuttle bus which is linked with each plane landing. The bus will first drive you to **Pile** area which is the location of the IUC and of the Dormitory. If your accommodation is elsewhere you can take the local bus or a taxi to take you to your desired address. The next stop of the shuttle bus is the main bus station in **Gruž** area. The bus ticket from the airport is 40 HRK or app. 5 EUR in one direction.

### Arriving to Dubrovnik by bus

Once you reach the main bus station in Gruž area you can get a taxi to take you to your desired destination or you can wait for a local bus (1A and 1B) to take you to Pile area (where IUC is located).

### Arriving to Dubrovnik by car

If you are coming with your own car make sure that your accommodation also offers a free parking service since parking in all Dubrovnik streets is charged and free parking is very hard to find. It is recommended that in Dubrovnik you use public transportation.

### Public transportation in Dubrovnik

Dubrovnik is rather small town so majority of distances can be overcome by foot. However, there are many buses that cover all parts of the city. The map of bus lines and the time table can be found at the end of this booklet.

If you pay a ticket entering the bus the price is 15 HRK. You can also buy a ticket at the news-stand and the price is than 12 HRK.

**DUBROVNIK** is one of the most prominent tourist and conference destinations in the Mediterranean. In 1979, the city of Dubrovnik joined the UNESCO list of World Heritage Sites. Unique for its impressive medieval forts, churches, monuments and palaces, Dubrovnik is often called the “pearl of the Adriatic”. George Bernard Shaw, visited the city in 1929 and said: “If you want to see heaven on earth, come to Dubrovnik”. Dubrovnik is among the several best preserved medieval walled cities in the world – its walls run almost 2 km around the city. The system of turrets and towers were intended to protect the city. The walls of Dubrovnik have also been a popular filming site for HBO’s Game Of Thrones and of the new episode of the 'Star Wars'. Because of a magnificent view on the mediaeval Dubrovnik, a walk along the city walls is exceptional experience. One of the reasons for visiting Dubrovnik besides its profound beauty and historic magic are warm, mild climate and Mediterranean gastronomic delight.



## ATTRACTIONS

**City walls**, symbol of the town and the most important feature of Dubrovnik. Impressive Middle Age construction with corner towers of Minceta, Revelin, Bokar and Sveti Ivan protected Dubrovnik throughout its history.

**The Rector's palace** was the most important public building in Dubrovnik, the centre of government in the old Dubrovnik Republica. Famous inscription “Obliti privatorum publica curate” or “Forget your private business, concern yourself with public affairs” can be found above the entrance of the Rector’s Palace.

**Stradun (Placa)** is the main “artery” of the city, stretched between the two town gates, the gate of Pile and Ploce. Placa or Stradun street is the most favored promenade and gathering place of Dubrovnik.



**The Sponza Palace**, also known as Divona (from dogana, customs), was built in 1520 in a mixed late gothic and renaissance style. It served a variety of public functions, including as a customs office. Now it is the State Archive where the most important documents about Dubrovnik’s history are kept.

**Franciscan monastery** is a wonderful work of Dubrovnik architecture and one of the most prominent Dubrovnik attractions. It contains the third oldest pharmacy in the whole world (founded in 1317), continuously functioning until present day, and a very rich library with large number of preserved manuscripts of invaluable cultural and historical value.

**The Church of St. Blaise** (Crkva Sv. Vlaha) is an 18th-century baroque church on Luza Square dedicated to the patron saint and protector of Dubrovnik. This church is located at the intersection of two main thoroughfares, ‘Placa’ and Pred dvorom’.

**Orlando's column**, the symbol of Dubrovnik’s independence and freedom, is located at the eastern end of Placa (Stradun) street.



# GRADSKI VOZNI RED - CITY TIMETABLE

## 1A

**MOKOŠICA - PILE**

**POLASCI RADNIM DANOM DEPARTURES - WORKING DAYS**

MOKOŠICA	PILE
04:50 09:40 10:50 20:20	04:25 10:30 15:30 21:15
05:20 10:00 15:20 21:00	04:50 10:50 16:10 21:30
06:00 10:20 15:40 21:00	05:25 11:10 16:30 21:55
06:10 10:40 16:00 21:25	06:05 11:30 16:50 22:20
06:25 11:00 16:20 21:50	06:35 11:50 17:10 22:45
06:50 11:20 16:40 22:15	06:55 12:10 17:30 23:10
07:00 11:40 17:00 22:40	07:20 12:30 17:50 23:35
07:15 12:00 17:20 23:05	07:30 12:50 18:10 00:00
07:35 12:20 17:40 23:25	07:45 12:55 18:30 00:25
07:45 12:40 18:00 23:55	08:15 13:30 18:50 00:50
08:00 13:00 18:20 00:20	08:30 13:50 19:10 01:15
08:10 13:20 18:40 00:45	08:50 14:10 19:30 01:45
08:20 13:40 19:00 01:15	09:10 14:30 19:50 02:15
08:40 14:00 19:20 01:45	09:30 14:50 20:10
09:00 14:20 19:40	09:50 15:10 20:30
09:20 14:40 20:00	10:10 15:30 20:50

**POLASCI SUBOTIM, NEDELJOM I PRAZNIKOM DEPARTURES - SATURDAYS, SUNDAYS AND HOLIDAYS**

MOKOŠICA	PILE
04:50 09:45 15:35 21:25	04:25 10:40 16:30 22:20
05:20 10:10 16:00 21:50	04:50 11:05 16:55 22:45
06:00 10:35 16:25 22:15	05:25 11:30 17:20 23:10
06:10 11:00 16:50 22:40	06:05 11:55 17:45 23:35
06:25 11:25 17:15 23:05	06:35 12:20 18:10 00:00
06:50 11:50 17:40 23:30	06:55 12:45 18:35 00:25
07:15 12:15 18:05 23:55	07:20 13:10 19:00 00:50
07:35 12:40 18:30 00:20	07:45 13:35 19:25 01:15
07:45 13:05 18:55 00:45	08:15 14:00 19:50 01:45
08:00 13:20 19:10 01:15	08:30 14:25 20:15 02:15
08:10 13:55 19:45 01:45	09:00 14:50 20:40
08:30 14:20 20:10	09:25 15:15 21:05
08:55 14:45 20:35	09:50 15:40 21:30
09:20 15:10 21:00	10:15 16:05 21:55

## 2

**GORICA - PILE**

**POLASCI DEPARTURES**

GORICA	PILE
06:40 10:50 15:30 +20:00	07:30 11:50 16:10 +20:45
08:10 12:50 +17:15	08:50 13:30 +18:10
09:50 14:45 +19:00	

**POLASCI DEPARTURES** Prvi pol.: Zadnji pol.:  
First dep.: Last dep.:  
07:00 +21:00

**PILE** Prvi pol.: Zadnji pol.:  
First dep.: Last dep.:  
07:00 +21:00

**+** Ne prometaju do Opće bolnice.  
Not running to General Hospital.

**POLASCI SA STANICE PILE cca +15 min DEPARTURES FROM PILE STATION**

## 4

**HOTEL PALACE - PILE**

**POLASCI DEPARTURES**

HOTEL PALACE	PILE
05:40 11:00 15:15 19:30 00:20	06:20 11:30 15:30 19:45 00:40
06:40 11:10 15:45 20:00 01:00	07:00 11:45 16:00 20:15 01:20
07:20 12:00 16:15 20:30 01:40	07:40 12:15 16:30 20:45 02:00
08:00 12:30 16:45 21:00	08:20 12:45 17:00 21:15
08:40 13:00 17:15 21:30	09:00 13:15 17:30 21:45
09:20 13:30 17:45 22:00	09:30 13:45 18:00 22:20
09:45 14:00 18:15 22:40	10:00 14:15 18:30 23:00
10:15 14:45 18:45 23:20	10:30 14:45 19:00 23:40
10:45 15:00 19:15 00:00	

**POLASCI DEPARTURES** Prvi pol.: Zadnji pol.:  
First dep.: Last dep.:  
05:40 02:15

**POLASCI SA STANICE PILE cca +15 min DEPARTURES FROM PILE STATION**

## 7

**KANTAFIĆ - BABIN KUK**

**POLASCI DEPARTURES**

KANTAFIĆ	BABIN KUK
06:30 11:40 16:40	07:05 12:10 17:10
07:35 12:40 17:40	08:10 13:10 18:10
08:40 13:40 18:40	09:10 14:10 19:15
09:40 14:40 +19:40	10:10 15:00 +20:10
10:40 15:40	11:10 16:10

**+** Ne prometuje do Opće bolnice.  
Not running to General Hospital.

## 2A

**GLAVICA B.K. - SOLITUDO - PILE**

**POLASCI DEPARTURES**

GLAVICA B.K.	PILE
06:30 10:20 14:10 17:25	07:20 11:20 14:55 18:15
08:20 12:20 15:55 19:05	09:20 13:20 16:40 20:00

**POLASCI DEPARTURES** Prvi pol.: Zadnji pol.:  
First dep.: Last dep.:  
06:45 20:15

**POLASCI SA STANICE PILE cca +15 min DEPARTURES FROM PILE STATION**

## 3

**NUNCIJATA - PILE**

**POLASCI DEPARTURES**

NUNCIJATA	PILE
05:30 10:15 13:45 17:15 20:45	06:20 10:45 14:15 17:45 21:15
07:20 11:15 14:45 18:15 21:45	08:10 11:45 15:15 18:45 22:15
08:15 12:45 16:15 19:15 23:10	09:45 13:15 16:45 20:15 00:55

**+** Ne prometuje do Opće bolnice.  
Not running to General Hospital.

## 5

**VIKTORIJA - BABIN KUK**

**POLASCI DEPARTURES**

VIKTORIJA	BABIN KUK
06:35 11:00 15:45 +20:35	07:30 12:15 16:50
08:35 13:25 18:00	09:50 14:45 +19:15

**+** Ne prometuje do Opće bolnice.  
Not running to General Hospital.

## 8

**VIKTORIJA - GRUZ**

**POLASCI DEPARTURES**

VIKTORIJA	GRUZ
05:40 11:10 16:40 22:10	06:05 11:40 17:10 22:40
06:40 12:10 17:40 23:10	07:10 12:40 18:10 23:40
07:40 13:10 18:40 00:10	08:10 13:40 19:10 00:30
08:40 14:10 19:40 01:00	09:10 14:20 20:10
09:40 15:10 20:40	10:10 15:40 21:10
10:40 16:10 21:40	

## 1B

**MOKOŠICA - PILE**

**POLASCI RADNIM DANOM DEPARTURES - WORKING DAYS**

MOKOŠICA	PILE
05:30 10:30 15:30 20:40	05:10 10:40 15:40 20:40
05:45 10:50 15:50 20:50	06:00 11:00 16:00 21:00
06:10 11:10 16:10 21:10	06:15 11:20 16:20 21:20
06:35 11:30 16:30 21:35	06:40 11:40 16:40 21:40
07:00 11:50 16:50 22:00	07:05 12:00 17:00 22:05
07:15 12:10 17:10 22:25	07:30 12:20 17:20 22:30
07:35 12:30 17:30 22:50	07:55 12:40 17:40 22:55
07:50 12:50 17:50 23:15	08:10 13:00 18:00 23:20
08:10 13:10 18:10 23:40	08:20 13:20 18:20 23:45
08:30 13:30 18:30 00:05	08:40 13:40 18:40 00:10
08:50 13:50 18:50 00:30	09:00 14:00 19:00 00:35
09:10 14:10 19:10 01:00	09:20 14:20 19:20 01:00
09:30 14:30 19:30 01:30	09:40 14:40 19:40 01:30
09:50 14:50 19:50	10:00 15:00 20:00 02:00
10:10 15:10 20:10	10:20 15:20 20:20

**POLASCI SUBOTIM, NEDELJOM I PRAZNIKOM DEPARTURES - SATURDAYS, SUNDAYS AND HOLIDAYS**

MOKOŠICA	PILE
05:30 10:20 15:45 21:10	05:10 10:50 16:15 21:40
05:45 10:45 16:10 21:35	06:00 11:15 16:40 22:05
06:10 11:10 16:35 22:00	06:15 11:40 17:05 22:30
06:35 11:35 17:00 22:25	06:40 12:05 17:30 22:55
07:00 12:00 17:25 23:00	07:05 12:30 17:55 23:20
07:15 12:25 17:50 23:15	07:30 12:55 18:20 23:45
07:35 12:50 18:15 23:40	07:55 13:20 18:45 00:10
07:50 13:15 18:40 00:35	08:20 13:45 19:10 00:35
08:15 13:40 19:05 00:30	08:45 14:10 19:35 01:00
08:40 14:05 19:30 01:00	09:10 14:35 20:00 01:30
09:10 14:30 19:55 01:30	09:35 15:00 20:25 02:00
09:30 14:55 20:10	10:00 15:25 20:50
09:55 15:20 20:45	10:25 15:50 21:15

## 3A

**NUNCIJATA - PILE**

**POLASCI DEPARTURES**

NUNCIJATA	PILE
07:35 10:30 13:30 16:30 19:30	08:30 11:30 14:30 17:30 20:30
09:30 12:30 15:30 18:30 21:30	

**POLASCI DEPARTURES** Prvi pol.: Zadnji pol.:  
First dep.: Last dep.:  
07:50 21:40

**POLASCI SA STANICE PILE cca +10 min DEPARTURES FROM PILE STATION**

Linja ne prometuje nedjeljom i blagdanom.  
Not running on Sundays and holidays.

## 6

**BABIN KUK - PILE**

**POLASCI DEPARTURES**

BABIN KUK	PILE
05:30 10:10 13:40 17:10 20:40 00:10	06:45 11:00 14:30 18:00 21:30 01:00
06:45 11:00 14:30 18:00 21:30 01:00	07:00 11:10 14:40 18:10 21:40 01:15
07:15 11:20 14:50 18:20 21:50 01:30	07:30 11:30 15:00 18:30 22:00 01:45
07:45 11:40 15:10 18:40 22:10 02:00	08:00 11:50 15:20 18:50 22:20
08:15 12:00 15:30 19:00 22:30	08:30 12:10 15:40 19:10 22:40
08:45 12:20 15:50 19:20 22:50	09:00 12:30 16:00 19:30 23:00
09:00 12:40 16:20 19:40 23:10	09:15 12:40 16:10 19:40 23:10
09:20 12:50 16:30 19:50 23:20	09:30 13:00 16:30 20:00 23:30
09:40 13:10 16:40 20:10 23:40	09:50 13:20 16:50 20:20 23:50
10:00 13:30 17:00 20:30 00:00	

**POLASCI DEPARTURES** Prvi pol.: Zadnji pol.:  
First dep.: Last dep.:  
05:30 02:15

**POLASCI SA STANICE PILE cca +15 min DEPARTURES FROM PILE STATION**

## 17

**BOSANKA - PILE**

**POLASCI DEPARTURES**

BOSANKA	PILE
07:15 12:05 15:20 20:00	09:45 13:05 17:10 21:00
11:55 14:05 19:00 22:00	

**POLASCI DEPARTURES** Prvi pol.: Zadnji pol.:  
First dep.: Last dep.:  
09:15 23:35

## 1c

**MOKOŠICA - O. BOLNICA - B. KUK**

**MOKOŠICA DEPARTURES** 05:15 07:10 08:10  
Ne prometuje subotom, nedjeljom i blagdanom.  
Not running on Saturdays, Sundays and holidays.

**POLASCI DEPARTURES** Prvi pol.: Zadnji pol.:  
First dep.: Last dep.:  
06:20 07:15 08:10 07:40

**EXPRESS**  
PILESKI OBLASCI - SUSTEPAN - MOKOŠICA  
**POLASCI DEPARTURES**  
PILE 14:10 15:10 16:10  
Ne prometuje subotom, nedjeljom i blagdanom.  
Not running on Saturdays, Sundays and holidays.

VOZNI RED JE PODLOŽAN PROMJENAMA  
BEZ PRETHODNE NAJAVE!  
TIMETABLE IS SUBJECT TO CHANGE WITHOUT  
PRIOR NOTICE!

**POLASCI DEPARTURES** Prvi pol.: Zadnji pol.:  
First dep.: Last dep.:  
05:30 02:15

**POLASCI SA STANICE PILE cca +15 min DEPARTURES FROM PILE STATION**

**LIBERTAS - DUBROVNIK d.o.o.**  
Ogarić 12, 20230 Mokošica  
Tel/Phone +385(0)20 441 444  
E-mail libertas@libertas-dubrovnik.com  
[www.libertasdubrovnik.hr](http://www.libertasdubrovnik.hr)  
od valid from  
**12.08.2019.**





2019  
ESOR

# European Symposium on Organic Reactivity

September 8–13, 2019, Dubrovnik, Croatia

