

# *1<sup>st</sup> International Conference on Noncovalent Interactions*



## **ICNI 2019**

2 - 6 september, 2019 | Lisbon, Portugal

## **PROGRAM**

<https://icni2019.eventos.chemistry.pt/>

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# Welcome

Dear Colleagues,

Noncovalent interactions were firstly taken into consideration by van der Waals in 1873, helping to revise the equation of state for real gases. In comparison to covalent bonds, intra- and intermolecular noncovalent interactions are in general weak and exhibit much lower energy and directionality, as reflected by the term "noncovalent". Nevertheless, in many cases these interactions can collectively play a dominant role in synthesis, catalysis and design of materials.

Currently, based on the nature of the particular elements or synthons involved in the interactions, noncovalent bonds are classified into hydrogen, noble gases, halogen, chalcogen, pnictogen, tetrel and triel bonds, as well as agostic, anagostic, cation- $\pi$ , anion- $\pi$ ,  $n-\pi^*$ ,  $\pi-\pi$  stacking, metal-metal, dispersion-driven and hydrophobic interactions, etc.

As the fields of noncovalent interactions are growing intensively, several books in Wiley, Royal Society of Chemistry, Elsevier or Springer and four thematic issues on these weak forces have been published in Chemical Reviews in 1988, 1994, 2000 and 2016. The hydrogen, halogen and chalcogen bonds have already been defined by IUPAC (Recommendations 2011, 2013 and 2019, respectively), the definitions for pnictogen and tetrel bonds are under progress. Moreover, there are international conferences/symposia on Supramolecular Chemistry, and particular types of noncovalent interactions, such as The International Conference on "Horizons in Hydrogen Bond Research" (established by Prof. Lucjan Sobczyk in Poland in 1977), International Symposium on Halogen Bonding [established by Prof. Pierangelo Metrangolo and Prof. Giuseppe Resnati in Porto Cesareo (Lecce, Italy) in 2014], etc.

Thus, the chemistry of this century is expected to be largely driven by noncovalent interactions and it is timely to establish a general/regular series of **International Conferences on Noncovalent Interactions (ICNI)**, the first one to be held on 2-6 September 2019 in Lisbon.

Further editions within this series will be followed every two years, in odd number years (2021, 2023, etc.), thus avoiding competition with other major series of conferences, i.e., the ICOMC and ICCM, which are being held in even years (2014, 2016, 2018, etc.).

We are thankful to all **International Advisory Board** who are well recognized scientists in this field, representing Europe, Asia, Africa and America for their support and suggestions. Hence, on behalf of the Organizing Commission, it is our pleasure to invite you to attend the **1st International Conference on Noncovalent Interactions (ICNI)** to be held in Lisbon in 2019 (September 2-6). It is an honor for us to host the first Conference of this series in Portugal. The scientific level of the conference will be provided by its attendants and thus you are cordially invited to present your best and recent scientific work orally, by poster or by poster with a flash oral presentation. The final selection of the type of presentation will have to take into account the scientific programme and facilities layout. Not only the senior researchers are welcome, but also the younger ones, encouraging the exchange of ideas among different generations.

The conference aims to highlight the role of **Noncovalent Interactions** in Synthesis, Catalysis, Crystal engineering, Molecular recognition, Medicinal chemistry, Biology, Materials science, Electrochemical immobilization, etc. including also Theoretical aspects. All approaches will be considered, from fundamental to applied ones, including discussion of new types of noncovalent interactions (noble gases, halogen, chalcogen, pnictogen, tetrel and triel bonds) and multidisciplinary studies.

The Conference venue is in a privileged position concerning travel requirements. Lisbon is easily reachable from any place of the world, the airport and the main train stations are located inside the town itself (this is a unique case within the European capitals) and all are well served by metro. The Conference place, at the Universidade de Lisboa campus, is also in the town and with close access to public transportation, including metro. Diverse and convenient accommodation facilities are available close to the venue, including low-cost University residences.

*Attention will also be paid to the social programme, providing opportunities for mixing, visits to cultural places, excursions to sites of unique natural beauty, and for tasting the typical Portuguese cuisine and feeling the inspiration of our wines!*

*We'll be most pleased to welcome you herein and do hope you will enjoy a pleasant time along all the Conference, from both scientific and social points of view.*

*All best wishes,*

*The organizing committee*



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## Conference Medal



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Politecnico di Milano, Italy  
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CSIR-Indian Institute  
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Organische Chemie der Universität  
des Saarlandes, Germany



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University of Oxford, UK



Prof. Shinji Yamada  
Ochanomizu University, Japan  
(Tutorial Lecture)



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University of Belgrade, Serbia  
(Tutorial Lecture)

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Kansas State University, USA



Prof. Ibon Alkort  
Instituto de Química Médica, IQM-CSIC, Spain



Prof. Elangannan Arunan  
Indian Institute of Science, India  
(IUPAC Lecture)



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A. N. Nesmeyanov Institute of  
Organoelement Compounds (INEOS)  
Russian Academy of Sciences,  
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Univ Rennes, CNRS, ISCR  
(Institut des Sciences Chimiques  
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CNR-ISTM, Istituto di Scienze  
e Tecnologie Molecolari, Italy



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Prof. Yanli Zeng  
Hebei Normal University, China



<b>Monday, September 2, 2019</b>			
08.00-09.15	<b>Registration</b>		
09.15-09.45	<b>Room A</b> <i>Chair: Armando J.L. Pombeiro</i>		
	<b>Opening Ceremony</b> <b>Kamran T. Mahmudov</b> <b>Dario Braga</b> <b>Djamaladdin G. Musaev</b>		
	09.45-10.30	<b>PL1:</b> <i>Noncovalent control of spin-state in organometallic complexes</i> <b>Pavel Hobza</b> <sup>1,2</sup> <sup>1</sup> Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Czech Republic <sup>2</sup> Regional Centre of Advanced Technologies and Materials, Palacký University, Šlechtitelů, Czech Republic	
10.30-11.00	<b>COFFEE BREAK</b>		
11.00-11.45	<b>Room A</b> <i>Chair: Giuseppe Resnati</i>		
	<b>PL2:</b> <i>Quantification of noncovalent interactions-promises and problems</i> <b>Hans-Jörg Schneider</b> FR Org. Chemie der Universität des Saarlandes, Germany		
11.45-12.15	<b>Room A</b> <i>Chair: Giuseppe Resnati</i>	<b>Room B</b> <i>Chair: Deepak Chopra</i>	<b>Room C</b> <i>Chair: Antonio Frontera</i>
	<b>KL1:</b> <i>From molecular dating to functional materials</i> <b>Christer Aakeröy</b> Kansas State University, USA	<b>IL1:</b> <i>Halogen bonding influence in chloride substitution reactions</i> <b>Marta E. G. Mosquera</b> Universidad de Alcalá, Spain	<b>IL4:</b> <i>Enhancing directionality in chalcogen bonding: organic selenocyanates for anion recognition</i> <b>Marc Fourmigué</b> Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes), France
	<b>KL2:</b> <i>Tuning luminescence and photoreactivity in organic co-crystals and salts</i> <b>Fabrizia Grepioni</b> University of Bologna, Italy	<b>IL2:</b> <i>Exploring uncommon halogen bond acceptors in cocrystals of perhalogenated compounds</i> <b>Dominik Cinčić</b> University of Zagreb, Croatia	<b>IL5:</b> <i>Functional supramolecular structures assembled by chalcogen bonding</i> <b>Ignacio Vargas-Baca</b> McMaster University, Canada
	<b>KL2:</b> <i>Tuning luminescence and photoreactivity in organic co-crystals and salts</i> <b>Fabrizia Grepioni</b> University of Bologna, Italy	<b>IL3:</b> <i>The "windmill" pattern halogen bond vs the "head to tail" halogen bond</i> <b>Yanli Zeng</b> Hebei Normal University, China	<b>IL6:</b> <i>Chalcogen interactions in neutral radical gold dithiolene complexes: from semi-conducting to metallic behavior</i> <b>Dominique Lorcy</b> Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes), France



12.45-14.15	<b>LUNCH</b>		
14.15-15.00	<p><b>Room A</b> Chair: <b>Pierre Braunstein</b></p> <p><b>PL3:</b> <i>Organic-inorganic ionic co-crystals – a surprisingly versatile new class of crystalline compounds</i> <b>Dario Braga</b> University of Bologna, Italy</p>		
15.00-15.45	<p><b>PL4:</b> <i>Noncovalent interactions: your key players in stereoselective ring-opening polymerizations</i> <b>Jean-François Carpentier</b> Université de Rennes 1, CNRS, Institut des Sciences Chimiques de Rennes, FRANCE</p>		
15.45-16.15	<p><b>Room A</b> Chair: <b>Pierre Braunstein</b></p> <p><b>KL3:</b> <i>Expanding the portfolio of noncovalent driving forces</i> <b>Werner M. Nau</b> Jacobs University Bremen, Germany</p>	<p><b>Room B</b> Chair: <b>Feihe Huang</b></p> <p><b>IL7:</b> <i>Supramolecularly directed rotary motion in a photoresponsive anion receptor</i> <b>Sander J. Wezenberg</b> Leiden University, The Netherlands</p> <p><b>IL8:</b> <i>Unique responding and synergistic molecular recognition of supramolecular systems</i> <b>Tatsuya Nabeshima</b> University of Tsukuba, Japan</p> <p><b>IL9:</b> <i>Anion selective transmembrane carriers displaying biological activity</i> <b>Roberto Quesada</b> Universidad de Burgos, Spain</p>	<p><b>Room C</b> Chair: <b>Giovanni Bistoni</b></p> <p><b>IL10:</b> <i>Critical comparison of hydrogen bond and halogen bond directionality</i> <b>Kevin E. Riley</b> Xavier University of Louisiana, USA</p> <p><b>IL11:</b> <i>Theoretical studies of various noncovalent interactions in organic, organometallic and coordination compounds using QTAIM approach and other computational techniques</i> <b>Alexander S. Novikov</b> Saint Petersburg State University, Russia</p> <p><b>IL12:</b> <i>Computational discovery of CO<sub>2</sub>-philic functional groups with quantum chemistry and machine learning</i> <b>Konstantinos D. Vogiatzis</b> University of Tennessee, USA</p>
	16.15-16.45	<p><b>KL4:</b> <i>PCG factors affecting intermolecular noncovalent interactions</i> <b>Wei Jun Jin</b> Beijing Normal University, China</p>	
16.45-17.15	<b>COFFEE BREAK</b>		



	<b>Room A</b> <i>Chair: <b>Slawomir J. Grabowski</b></i>	<b>Room B</b> <i>Chair: <b>Marta E. G. Mosquera</b></i>	<b>Room C</b> <i>Chair: <b>Marijana Đaković</b></i>
17.15-17.45	<b>KL5:</b> <i>Noncovalent interactions in inorganic Chemistry</i> <b>Lee Brammer</b> University of Sheffield, UK	<b>IL13:</b> <i>Halogen-bond catalysis with molecular iodine</i> <b>Martin Breugt</b> Universität zu Köln, Germany	<b>IL16:</b> <i>Light-responsive stimulation of supramolecular host-guest complexes in water</i> <b>Uwe Pischel</b> University of Huelva, Spain
17.45-18.15	<b>KL6:</b> <i>The advent of conceptual NCI-inclusive molecular engineering in transition metal organometallic chemistry</i> <b>Jean-Pierre Djukic</b> Université de Strasbourg, France	<b>IL14:</b> <i>How Halogen Bonding Catalyzes Michael Addition Reactions</i> <b>Israel Fernández</b> Universidad Complutense de Madrid, Spain	<b>IL17:</b> <i>Supramolecular polymeric luminescent nanoparticles</i> <b>Qing-Zheng Yang</b> Beijing Normal University, China
18.15-18.30	<b>O1:</b> <i>Aroylhydrazone complexes: noncovalent interactions in their structures and catalysis</i> <b>Manas Sutradhar</b> Universidade de Lisboa, Portugal	<b>O4:</b> <i>Interdependance of halogen and hydrogen bonds in crystal structures of meta-halogenopyridine salts and cocrystals</i> <b>Vladimir Stilinović</b> University of Zagreb, Croatia	<b>O7:</b> <i>On the uselessness of bond paths linking distant atoms and on the violation of the concept of privileged exchange channels</i> <b>Mirosław Jabłoński</b> Nicolaus Copernicus University, Poland



18.30-18.45	<b>O2:</b> <i>Continuum of covalent to intermolecular bonding in halogen-bonded complexes</i> <b>Sergiy Rosokha</b> Ball State University, USA	<b>O5:</b> <i>Guest encapsulations in non-porous crystals of fully fluorinated dinuclear metal complexes with M2O2 core</i> <b>Akiko Hori</b> Shibaura Institute of Technology, Japan	<b>O8:</b> <i>Exploiting hydrogen bonds to enhance aluminum catalyst performances in lactide ring-opening polymerization</i> <b>Charles Romain</b> Imperial College London, UK
18.45-19.00	<b>O3:</b> <i>3-aminopyrazine-2-carboxylate based coordination compounds: from crystal engineering to catalysis</i> <b>Anirban Karmakar</b> Universidade de Lisboa, Portugal	<b>O6:</b> <i>Mechanistic details of ethanol to butadiene conversion over metal oxides: a DFT Study</i> <b>Yoong-Kee Choe</b> National Institute of Advanced Industrial Science and Technology, Japan	<b>O9:</b> <i>Crystal engineering with chalcogen bonds: X-ray crystallography and multinuclear magnetic resonance spectroscopic investigations</i> <b>Vijith Kumar</b> University of Ottawa, Canada
19.00-21.00	<b>WELCOME RECEPTION</b>		



<b>Tuesday, September 3, 2019</b>			
09.00-09.45	<b>Room A</b> Chair: <b>Hans-Jörg Schneider</b>		
09.45-10.30	<b>PL5: IUPAC Lecture</b> <i>Halogen, chalcogen, pnictogen, and tetrel bonds: structural aspects</i> <b>Giuseppe Resnati</b> Politecnico di Milano, Italy		
10.30-11.00	<b>COFFEE BREAK</b>		
11.00-11.45	<b>Room A</b> Chair: <b>Matti Haukka</b>		
11.45-12.15	<b>Room A</b> Chair: <b>Matti Haukka</b>	<b>Room B</b> Chair: <b>Elena S. Shubina</b>	<b>Room C</b> Chair: <b>Catharine Esterhuysen</b>
11.45-12.15	<b>KL7:</b> <i><math>\sigma</math>-Hole bonds of tetrahedral centres</i> <b>Slawomir J. Grabowski</b> <sup>1,2</sup> <sup>1</sup> University of the Basque Country and Donostia International Physics Center (DIPC), Spain <sup>2</sup> Basque Foundation for Science, Spain	<b>IL19:</b> <i>Solid-state NMR and NQR studies of noncovalent interactions</i> <b>David L. Bryce</b> University of Ottawa, Canada	<b>IL22:</b> <i>Porphyrin-based metal-organic frameworks as multifunctional materials</i> <b>Filipe A. Almeida Paz</b> University of Aveiro, Portugal
12.15-12.45	<b>KL8:</b> <i>Probing weak interactions in molecular crystals via electron density analysis</i> <b>Deepak Chopra</b> Indian Institute of Science Education and Research Bhopal, India	<b>IL20:</b> <i>NMR spectral diagnostics of strong hydrogen bonds: case of phosphinic acids</i> <b>Peter M. Tolstoy</b> St. Petersburg State University, Russia	<b>IL23:</b> <i>Harnessing outer-sphere interactions in homogeneous catalysis</i> <b>Manuel Iglesias</b> Universidad de Zaragoza, Spain
12.15-12.45	<b>IL 21:</b> <i>Halogenated isophthalamides and dipicolineamides: the role of the halogen substituent on the anion binding and transport properties</i> <b>Claudia Caltagirone</b> Università degli Studi di Cagliari, Italy	<b>IL 24:</b> <i>Redox-responsive supramolecular behaviors of TTF-annulated subphthalocyanine</i> <b>Soji Shimizu</b> Kyushu University, Japan	



12.45-14.15		LUNCH		
14.15-15.00	<b>Room A</b> Chair: <b>Kazuaki Ishihara</b>			
	<b>PL8:</b> <i>Experimental and theoretical interplay in the study of organometallic, underligated Cr(II) complexes</i> <b>Pierre Braunstein, Vincent Robert</b> Universite de Strasbourg, France			
15.00-15.45	<b>PL9:</b> <i>Cyclodextrin-based supramolecular materials</i> <b>Akira Harada</b> Osaka University, Japan			
15.45-16.15	<b>Room A</b> Chair: <b>Kazuaki Ishihara</b>	<b>Room B</b> Chair: <b>Kevin E. Riley</b>	<b>Room C</b> Chair: <b>Jean-Pierre Djukic</b>	
	<b>KL9:</b> <i>Multimolecular tectons in crystal engineering</i> <b>Roger Bishop</b> University of New South Wales, Australia	<b>IL25:</b> <i>Noncovalent chemistry with carbon</i> <b>Tiddo J. Mooibroek</b> University of Amsterdam, The Netherlands	<b>IL28:</b> <i>Dithiadiazolyl radicals in functional materials: understanding 'pancake' bonding</i> <b>Delia A. Haynes</b> Stellenbosch University, South Africa	
		<b>IL26:</b> <i>Carbohydrogen bond: a new noncovalent interaction</i> <b>Himansu S. Biswal</b> <sup>1,2</sup> <sup>1</sup> National Institute of Science Education and Research (NISER), India <sup>2</sup> Homi Bhabha National Institute, India	<b>IL29:</b> <i>Pnictogen bonding in solution: from catalysis to reversed bilayer formation</i> <b>Anthony F. Cozzolino</b> Texas Tech University, USA	
16.15-16.45	<b>KL10:</b> <i>Anion-anion and cation-cation complexes</i> <b>Ibon Alkorta</b> Instituto de Química Médica (CSIC), Spain	<b>IL27:</b> <i>Carbonyl-carbonyl interactions in transition metal complexes</i> <b>Jorge Echeverría</b> Universitat de Barcelona, Spain	<b>IL30:</b> <i>Common quantitative trends for the halogen, chalcogen, and pnictogen bonds</i> <b>Ekaterina Bartashevich</b> Ural State University, Russia	



16.45-17.15	<p><b>KL11:</b> <i>Modelling of noncovalent interactions in excited states</i> <b>Dana Nachtigalova</b> Intstitute of Organic Chemistry and Biochemistry of the CAS, Czech Republic</p>	<p><b>O10:</b> <i>Halogen bond and electrochemistry: a strong cooperation for anion detection in solution and at the interface</i> <b>Claire Fave</b> Université Paris Diderot, France</p> <p><b>O11:</b> <i>D4 goes periodic: improving the applicability of the dispersion correction for condensed-phase systems</i> <b>Jan-Michael Mewes</b> Bonn University, Germany</p>	<p><b>F1:</b> <b>Elisabete C.B.A. Alegria</b></p> <p><b>F2:</b> <b>Olga Kulikova</b></p> <p><b>F3:</b> <b>Asja A. Kroeger</b></p> <p><b>F4:</b> <b>Tannistha Roy Barman</b></p> <p><b>F5:</b> <b>Bruno G. M. Rocha</b></p> <p><b>F6:</b> <b>Mohamed M.A. Soliman</b></p> <p><b>F7:</b> <b>Ekaterina S. Gulyaeva</b></p>
<b>Detail information on Flash Presentations</b>			
16.45-16.50	<p><b>F1:</b> <i>Mechanochemical activation of noncovalent interactions</i> <b>Elisabete C.B.A. Alegria</b><sup>1,2</sup> <sup>1</sup>Universidade de Lisboa, Portugal <sup>2</sup>Instituto Politécnico de Lisboa, Portugal</p>		
16.50-16.55	<p><b>F2:</b> <i>Noncovalently linked water-soluble metalloporphyrin-quantum dot conjugates with potential application in photodynamic therapy</i> <b>Olga Kulikova</b> G.A. Krestov Institute of Solution Chemistry, Russia</p>		
16.55-17.00	<p><b>F3:</b> <i>Catalysis by pure graphene - from supporting actor to protagonist through <math>\pi</math>-<math>\pi</math> interactions</i> <b>Asja A. Kroeger</b> The University of Western Australia, Australia</p>		
17.00-17.05	<p><b>F4:</b> <i>Cu(II) complexes: structures, noncovalent interactions and microwave assisted oxidation of alkanes</i> <b>Tannistha Roy Barman</b> Universidade de Lisboa, Portugal</p>		
17.05-17.10	<p><b>F5:</b> <i>Nickel(II) tetrazole-saccharinate complex as homogeneous catalyst on the reduction of aldehydes: scope and reaction mechanism</i> <b>Bruno G. M. Rocha</b> Universidade de Lisboa, Portugal</p>		
17.10-17.15	<p><b>F6:</b> <i>ZnO nanoparticles: an efficient catalyst for transesterification reaction of <math>\alpha</math>-keto carboxylic esters</i> <b>Mohamed M.A. Soliman</b> Universidade de Lisboa, Portugal</p>		





17.15-17.20	<b>F7:</b> <i>Amine-boranes dehydrogenation catalyzed by bimetallic W/Pd complex</i> <b>Ekaterina S. Gulyaeva</b> <sup>1,2</sup> <sup>1</sup> M.V. Lomonosov Moscow State University, Russia <sup>2</sup> A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Russia
17.20-19.00	<b>POSTER SESSION</b>
20.00-23.00	<b>SPEAKERS' DINNER</b>



<b>Wednesday (<math>\pi</math>-day), September 4, 2019</b>			
09.00-09.45	<b>Room A</b> Chair: <b>Djamaladdin G. Musaev</b>		
09.45-10.30	<b>PL10: Tutorial Lecture</b> <i>Cation-<math>\pi</math> interactions in organic synthesis</i> <b>Shinji Yamada</b> Ochanomizu University, Japan		
10.30-11.00	<b>COFFEE BREAK</b>		
11.00-11.45	<b>Room A</b> Chair: <b>Andrew S. Weller</b>		
11.45-12.15	<b>PL12: Tutorial Lecture</b> <i><math>\pi</math>-<math>\pi</math> interactions in organic, coordination, and organometallic compounds</i> <b>Snežana D. Zarić</b> <sup>1,2</sup> <sup>1</sup> University of Belgrade, Serbia <sup>2</sup> Texas A&M University at Qatar, Qatar		
12.15-12.45	<b>Room A</b> Chair: <b>Andrew S. Weller</b>	<b>Room B</b> Chair: <b>Anton Vidal-Ferran</b>	<b>Room C</b> Chair: <b>Antonio Romerosa</b>
11.45-12.15	<b>KL12:</b> <i>Putting small molecules into open-cage fullerenes</i> <b>Yasujiro Murata</b> Kyoto University, Japan	<b>IL 31:</b> <i>Noncovalent interactions in Ir-catalyzed enantioselective C(sp<sup>3</sup>)-H borylation</i> <b>Masaya Sawamura</b> Hokkaido University, Japan	<b>IL 34:</b> <i>Crystalline phase transition and related events of organometallic rotaxanes</i> <b>Kohtaro Osakada</b> Tokyo Institute of Technology, Japan
12.15-12.45	<b>KL13:</b> <i>Enantio- and site-selective <math>\alpha</math>-fluorination of N-Acyl-3,5-dimethylpyrazoles catalyzed by chiral <math>\pi</math>-Cu(II) complexes</i> <b>Kazuaki Ishihara</b> Nagoya University, Japan	<b>IL 32:</b> <i>"C-H<math>\cdots</math><math>\pi</math> interaction" regulates rtereoselectivity in olefin polymerization</i> <b>Yi Luo</b> Dalian University of Technology, China	<b>IL 35:</b> <i>Noncovalent interactions in carboranes</i> <b>Vladimir I. Bregadze</b> A.N.Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Russia
12.45-14.15	<b>LUNCH</b>		
<b>EXCURSION</b> (Tour Sintra, starting at 14.30)			



<b>Thursday, September 5, 2019</b>			
09.00-09.45	<b>Room A</b> Chair: <b>Lee Brammer</b>		
09.45-10.30	<b>PL13:</b> <i>Noncovalent interactions: selectivity and reactivity of transition-metal catalyzed C–H functionalization</i> <b>Djamaladdin G. Musaev</b> Emory University, USA		
10.30-11.00	<b>COFFEE BREAK</b>		
11.00-11.45	<b>Room A</b> Chair: <b>Ibon Alkorta</b>		
11.45-12.15	<b>PL15:</b> <i>The nature of dative or Lewis acid-base interactions between lanthanides and transition-metals</i> <b>Michael B. Hall</b> Texas A&M University, USA		
12.15-12.45	<b>Room A</b> Chair: <b>Ibon Alkorta</b>	<b>Room B</b> Chair: <b>Elangannan Arunan</b>	<b>Room C</b> Chair: <b>Ignacio Vargas-Baca</b>
11.45-12.15	<b>KL14:</b> <i>Dihydrogen bonding as a driving force in hydride chemistry</i> <b>Elena S. Shubina</b> A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Russia	<b>IL 37:</b> <i>Noncovalent interactions as viewed through the source function descriptor</i> <b>Carlo Gatti</b> Istituto di Scienze e Tecnologie Molecolari ISTM-CNR, Italy	<b>IL 40:</b> <i>Macrocyclic assemblies via Watson-Crick Pairing</i> <b>David Gonzalez-Rodriguez</b> Universidad Autónoma de Madrid, Spain
12.15-12.45	<b>KL15:</b> <i>Covalent and noncovalent polymers: syntheses and applications</i> <b>Kana M. Sureshan</b> School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram, India	<b>IL 38:</b> <i>Comprehensive benchmark data sets for testing and development of approximate computational methods</i> <b>Jan Řezáč</b> Academy of Sciences of the Czech Republic, Czech Republic	<b>IL 41:</b> <i>Molecular-targeted photodynamic therapy with bioconjugates</i> <b>João P. C. Tomé</b> Universidade de Lisboa, Lisboa, Portugal
12.15-12.45	<b>KL15:</b> <i>Covalent and noncovalent polymers: syntheses and applications</i> <b>Kana M. Sureshan</b> School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram, India	<b>IL 39:</b> <i>Tackling halogen bonds with computational methods: from anion binding affinity to solvation free energies</i> <b>Paulo J. Costa</b> Faculdade de Ciências da Universidade de Lisboa, Portugal	<b>IL 42:</b> <i>Design function in Porous organic cages</i> <b>Ming Liu</b> University of Liverpool, UK



12.45-14.15	<b>LUNCH</b>		
14.15-15.00	<b>Room A</b> <i>Chair: Yasujiro Murata</i>		
15.00-15.45	<b>P16:</b> <i>Nonporous adaptive crystals (NACs) for separation and adsorption</i> <b>Feihe Huang</b> Zhejiang University, China		
15.45-16.15	<b>P17:</b> <i>Extended molecular assemblies – linking molecular moieties by noncovalent contacts</i> <b>Matti Haukka</b> University of Jyväskylä, Finland		
	<b>Room A</b> <i>Chair: Yasujiro Murata</i>	<b>Room B</b> <i>Chair: Kana M. Suresha</i>	<b>Room C</b> <i>Chair: Ekaterina Bartashevich</i>
16.15-16.45	<b>KL16:</b> <i>Neutron scattering: a valuable procedure to study the interaction of water molecules with catalytic intermediates</i> <b>Antonio Romerosa</b> Universidad de Almería, Almería, Spain	<b>IL43:</b> <i>Cinchona-based primary amine catalyzed a proximal fluorination of dienamines: importance of C-H hydrogen bonding for stereoselectivity</i> <b>Satoru Arimitsu</b> University of the Ryukyus, Japan  <b>IL44:</b> <i>Role of noncovalent interactions in asymmetric induction: cycloadditions between aldehydes and enolisable anhydrides</i> <b>Cristina Trujillo</b> TBSI - Trinity College Dublin, Ireland  <b>IL45:</b> <i>Anion-<math>\pi</math> catalysis on carbon nanotubes</i> <b>Javier López-Andarias</b> University of Geneva, Switzerland	<b>IL46:</b> <i>Tuning mechanical responses of crystalline coordination polymers via altering the influence of a variety of noncovalent interactions</i> <b>Marijana Đaković</b> University of Zagreb, Croatia  <b>IL47:</b> <i>Crystal engineering and supramolecular chemistry as tools to rejuvenate old drugs</i> <b>Vânia André</b> Universidade de Lisboa, Portugal  <b>IL48:</b> <i>Influence of halogen vs hydrogen bonding on the properties of inclusion compounds</i> <b>Susan A. Bourne</b> University of Cape Town, South Africa
16.45-17.15	<b>COFFEE BREAK</b>		



	Room A <i>Chair: Dominik Cinčić</i>	Room B <i>Chair: Israel Fernández</i>	Room C <i>Chair: Antonio Caballero</i>
17.15-17.45	<p><b>KL18:</b> <i>The role of noncovalent interactions in the properties of porous compounds</i> <b>Catharine Esterhuysen</b> Stellenbosch University, South Africa</p>	<p><b>IL49:</b> <i>Understanding and improving the stability of noncovalently immobilized lanthanide and actinide complexes at interfaces</i> <b>James Blakemore</b> University of Kansas, USA</p> <p><b>IL50:</b> <i>Synthesis and catalytic applications of iron(II) polyhydride and aminoborane pincer complexes</i> <b>Karl Kirchner</b> Vienna University of Technology, Austria</p> <p><b>IL51:</b> <i>Macrocyclic copper(I) and silver(I) pyrazolates: principles of supramolecular assemblies with Lewis bases</i> <b>Oleg A. Filippov</b> A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Russia</p>	<p><b>IL52:</b> <i>Origin of attraction in aromatic charge-transfer complexes: importance of dispersion interactions</i> <b>Seiji Tsuzuki</b> National Institute of Advanced Industrial Science and Technology, Japan</p> <p><b>IL53:</b> <i>Stacking of planar organic radicals: strong noncovalent or weak covalent interactions?</i> <b>Krešimir Molčanov</b> Ruđer Bošković Institute, Croatia</p> <p><b>IL54:</b> <i>Local energy decomposition analysis of noncovalent interactions</i> <b>Giovanni Bistoni</b> Max-Planck-Institut für Kohlenforschung, Germany</p>
17.45-18.15			
18.15-18.30	<p><b>O12:</b> <i>Halomethane-halide and halomethane-metal halogen bonding in adducts of Pd(II) and Pt(II) dialkylcyanamide complexes with iodoform, bromoform, and tetrabromomethane</i> <b>Daniil M. Ivanov</b> Saint Petersburg State University, Russian Federation</p>	<p><b>O15:</b> <i>The X40×10 halogen bonding benchmark revisited: surprising importance of (n-1)d subvalence correlation</i> <b>Nitai Sylvetsky</b> Weizmann Institute of Science, Israel</p>	<p><b>O18:</b> <i>Theoretical study on conducting properties of heteroatom mono-substituted coronenes and their interplanar π-π interactions</i> <b>Francis A. S. Chipem</b> Manipur University, India</p>



18.30-18.45	<b>O13:</b> <i>Functional materials discovery using energy–structure–function maps</i> <b>Marc A. Little</b> University of Liverpool, UK	<b>O16:</b> <i>Multicomponent crystals of nitrofurazone–when more is less</i> <b>Nikoletta B. Báthori</b> Cape Peninsula University of Technology, South Africa	<b>O19:</b> <i>Molecular dynamics simulations of halogen bond-mediated biomolecular recognition events</i> <b>Rafael Nunes</b> Faculdade de Ciências da Universidade de Lisboa, Portugal
18.45-19.00	<b>O14:</b> <i>Crystal engineering of large, supramolecular assemblies of C-methylcalix[4]-resorcinarene</i> <b>Clive L. Oliver</b> University of Cape Town, South Africa	<b>O17:</b> <i>NMR crystallographic investigations of a series of organic cocrystals exhibiting tetrel bonds</i> <b>Scott A. Southern</b> University of Ottawa, Canada	<b>O20:</b> <i>Endoplasmic reticulum-targeting fluorescent probes to image mobile Zn<sup>2+</sup></i> <b>Le Fang</b> Queen Mary University of London, UK
20.00-23.00	<b>CONFERENCE DINNER</b>		



Friday, September 6, 2019			
09.15-09.45	<b>Room A</b> <i>Chair: G. Narahari Sastry</i>		
	<b>PL18:</b> <i>Unorthodox interactions at work</i> <b>Stefan Matile</b> University of Geneva, Switzerland		
09.45-10.30	<b>PL19:</b> <i>Noncovalent interactions in truncated menaquinone derivatives; effects on reactivity and biological functions</i> <b>Debbie C. Crans</b> Colorado State University, USA		
10.30-11.00	<b>COFFEE BREAK</b>		
11.00-11.30	<b>Room A</b> <i>Chair: Karl Kirchner</i>	<b>Room B</b> <i>Chair: Jan Řezáč</i>	<b>Room C</b> <i>Chair: Roberto Quesada</i>
	<b>KL20: IUPAC Lecture</b> <i>The alkalene bond</i> <b>Elangannan Arunan</b> Indian Institute of Science, India	<b>IL55:</b> <i>Design of novel luminescent complexes based on cyclic hybrid phosphines for chemo- and biosensing via molecular recognition</i> <b>A.A. Karasik</b> A.E. Arbusov Institute of Organic and Physical Chemistry - Subdivision of FIC KazanSC of RAS, Russia	<b>IL58:</b> <i>NCIPLOT4 and NCIweb: towards the quantification of noncovalent interactions in complex systems</i> <b>Francesca Peccati</b> <sup>1,2</sup> <sup>1</sup> Laboratoire de Chimie Théorique, Sorbonne Université/CNRS, France <sup>2</sup> Institut des Sciences du Calcul et des Données, Sorbonne Université, France
11.30-12.00	<b>KL21:</b> <i>Self assembled supramolecular polymers in solution by halogen bonding interactions</i> <b>Antonio Caballero</b> Universidad de Murcia, Spain	<b>IL56:</b> <i>Metallophilic interactions for phosphorescent complexes and supramolecular assemblies</i> <b>Wei Lu</b> Southern University of Science and Technology, China	<b>IL59:</b> <i>Platinum, gold, and silver standards of intermolecular interaction energy calculations</i> <b>Konrad Patkowski</b> Auburn University, USA
		<b>IL57:</b> <i>Where to stop by accounting for effects of noncovalent interactions in condensed matter?</i> <b>Ilya G. Shenderovich</b> University of Regensburg, Germany	<b>IL60:</b> <i><math>\sigma</math>- and <math>\pi</math>-hole bonds: emergent noncovalent interactions in liquid-chromatography enantiodiscrimination</i> <b>Paola Peluso</b> Istituto di Chimica Biomolecolare ICB CNR, Italy



12.00-12.30	<p><b>KL22:</b> <i>Noncovalent interactions involving noble gas hydrides</i> <b>Jan Lundell</b> University of Jyvaskyla, Finland</p>	<p><b>O22:</b> <i>Noncovalent rhodium-rhodium interactions</i> <b>Jeanet Conradie</b> University of the Free State, South Africa</p> <p><b>O23:</b> <i>Crystal structure predictions and analysis</i> <b>Sten O. Nilsson Lill</b> Pharmaceutical Sciences R&amp;D, AstraZeneca Gothenburg, Sweden</p>	<p><b>O25:</b> <i>Noncovalent catalysis as powerful biomimetic approaches in strain-release glycosylations</i> <b>Charles C. J. Loh</b><sup>1,2</sup> <sup>1</sup>Max-Planck Institute of Molecular Physiology, Germany <sup>2</sup>Technische Universität Dortmund, Germany</p> <p><b>O26:</b> <i>Noncovalent interactions in bis(dicarbollide) complexes of transition metals and their role in rotamer stabilization</i> <b>Igor B. Sivaev</b> A.N.Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Russia</p>
12.30-12.45	<p><b>O21:</b> <i>Noncovalent interactions in compartmental Schiff base heterometallic M-Sn(II/IV) Systems</i> <b>Susanta Hazra</b> Universidade de Lisboa, Portugal</p>	<p><b>O24:</b> <i>Introducing halogen bonding to platinum luminophores</i> <b>Igor O. Koshevoy</b> University of Eastern Finland, Finland</p>	<p><b>O27:</b> <i>Conformation analysis and tautomeric forms of supramolecular synthons</i> <b>Ivan Fedyanin</b> A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Russia</p>
12.45-14.15	<b>LUNCH</b>		
	<p><b>Room A</b> Chair: <b>Sander J. Wezenberg</b></p>	<p><b>Room B</b> Chair: <b>Paulo J. Costa</b></p>	<p><b>Room C</b> Chair: <b>Vânia André</b></p>
14.15-14.45	<p><b>KL23:</b> <i>Noncovalent interactions in metal complex catalysis</i> <b>Kamran T. Mahmudov</b><sup>1,2</sup> <sup>1</sup>Universidade de Lisboa, Portugal <sup>2</sup>Baku State University, Azerbaijan</p>	<p><b>O32:</b> <i>Delocalization in halogen and hydrogen bonded molecules and solids</i> <b>Alberto Otero de la Roza</b> University of Oviedo, Spain</p> <p><b>O33:</b> <i>Stacking interactions of aromatic ligands in transition metal complexes</i> <b>Dušan P. Malenov</b> University of Belgrade, Serbia</p>	<p><b>O38:</b> <i>C-S...X-C halogen bond: reality or artefact?</i> <b>Maciej Kubicki</b> Adam Mickiewicz University in Poznan, Poland</p> <p><b>O39:</b> <i>Noncovalent interactions in the new nonclassical compounds based on boron tetrahedrons</i> <b>Vitaliy V. Koval</b> Southern Federal University, Russia</p>





14.45-15.00	<p><b>O28:</b> <i>XPS demonstration of noncovalent interactions</i> <b>Ana M. C. Ferraria</b> Universidade de Lisboa, Portugal</p>	<p><b>O34:</b> <i>New porphyrin "hosts" for ion-dependent binding of organic "guests" of different nature</i> <b>N.Zh. Mamardashvili</b> G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences, Russia</p>	<p><b>O40:</b> <i>Hierarchy of intermolecular bonding in organometallic co-crystals: search and validation of supramolecular synthons</i> <b>Yury Torubaeu</b> N.S. Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Russia</p>
15.00-15.15	<p><b>O29:</b> <i>Study on Photoluminescent Properties of Supramolecular Compounds Constructed by Substituted Terpyridine Ligands and Inorganic and Organic Acids</i> <b>Zhen Ma</b> Guangxi University, China</p>	<p><b>O35:</b> <i>Interaction of Carbon Nanotubes with Nanoparticles, Dyes or DNA Fragments as a Fundamental Factor for the Design of Drugs Carriers. Insights from Molecular Dynamics Studies</i> <b>Tomasz Pańczyk</b> Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy for Sciences, Poland</p>	<p><b>O41:</b> <i>Supramolecular hydrogen-bonding chains and networks from copper(II) halogenobenzoates with N-methylnicotinamide</i> <b>Jan Moncol</b> Slovak University of Technology, Slovakia</p>
15.15-15.30	<p><b>O30:</b> <i>Noncovalent interactions in adducts of platinum(II) halide 1,5-cyclooctadiene complexes with I<sub>2</sub>, CHI<sub>3</sub>, and 1,4-diodotetrafluorobenzene</i> <b>Margarita Bulatova</b> University of Jyväskylä, Finland</p>	<p><b>O36:</b> <i>Computational study of noncovalent interactions in cyclotetranavanadate complexes</i> <b>María Eugenia Castro</b> Benemérita Universidad Autónoma de Puebla, Mexico</p>	<p><b>O42:</b> <i>NH...N hydrogen bonds energy and geometry evaluation from <sup>1</sup>H NMR</i> <b>Elena Tupikina</b> St. Petersburg State University, Russia</p>
15.30-16.45	<p><b>O31:</b> <i>Noncovalent interactions in stoichiometric and catalytic reactions of iridium pincer complexes</i> <b>Elena Osipova</b> A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Russia</p>	<p><b>O37:</b> <i>Noncovalent interaction in cyclic heterocomplexes of phosphinic and phosphoric acids studied by 1H NMR spectroscopy</i> <b>Valeriya Mulloyarova</b> St. Petersburg State University, Russia</p>	<p><b>O43:</b> <i>Polyproline II type helices are stabilized by carbonyl-carbonyl noncovalent Interactions</i> <b>Biswajit Sahariah</b> Shiv Nadar University, India</p>
15.45-16.00	<b>Poster Awards</b>		
16.00-16.15	<b>CLOSING</b>		



## Posters

Tuesday, September 3, 2019	
Poster Session (17.15-19.00)	
P1	<b>Synthesis of mono and bimetallic precious metal nanoparticles using noncovalent interactions</b> <a href="#">Agnieszka Jędrych</a> , <a href="#">Michał Wójcik</a> , <a href="#">Agnieszka Krogul-Sobczak</a> University of Warsaw, Poland
P2	<b>Theoretical studies of noncovalent interactions in chemical systems promising for catalysis, materials science, and medicine</b> <a href="#">Alexander S. Novikov</a> Saint Petersburg State University, Russia
P3	<b>Valorisation of waste coffee grounds into activated carbon for support of metal salts</b> <a href="#">Egle Rosson</a> , <sup>1</sup> <a href="#">Paolo Sgarbossa</a> , <sup>1</sup> <a href="#">Roberta Bertani</a> , <sup>1</sup> <a href="#">Ana Dias</a> , <sup>2,3</sup> <a href="#">Elisabete C.B. Alegria</a> , <sup>2,3</sup> <a href="#">Ana Paula da Costa Ribeiro</a> <sup>3</sup> <sup>1</sup> Dipartimento Ingegneria Industriale, UNIPD, Italy <sup>2</sup> ADEQ-ISEL-Instituto Politécnico de Lisboa, Portugal <sup>3</sup> Universidade de Lisboa, Portugal
P4	<b>Noncovalent interactions involving fluorinated iodobenzenes: halogen bond supported (anion/lp)•••<math>\pi</math>-hole interactions</b> <a href="#">Anastasiya A. Eliseeva</a> , <sup>1</sup> <a href="#">Daniil M. Ivanov</a> , <sup>1</sup> <a href="#">Vadim Yu. Kukushkin</a> <sup>1,2</sup> <sup>1</sup> Saint Petersburg State University, Russia <sup>2</sup> Institute of Macromolecular Compounds, Russian Academy of Sciences, Russia
P5	<b>Anion-<math>\pi</math> catalysis with peptides</b> <a href="#">Anh Tuan Pham</a> , <a href="#">Naomi Sakai</a> , <a href="#">Stefan Matile</a> University of Geneva, Switzerland
P6	<b>Study of catalytic intermediate states in water by X-ray pair distribution function.</b> <a href="#">Antonio Romerosa</a> , <a href="#">Franco Scalambra</a> , <a href="#">Belén López-Sánchez</a> Universidad de Almería, Spain
P7	<b>Transformation of an amide functionalised mononuclear Zn(II) complex to a Cu(II) complex through transmetalation</b> <a href="#">Anup Paul</a> , <a href="#">A.J.L. Pombeiro</a> Universidade de Lisboa, Portugal
P8	<b>Experimental and theoretical investigation of inter/intramolecular interactions in selfassembly of supramolecular isomers controlled by hydrogen and chalcogen bonding capability of component</b> <a href="#">Ghodrat Mahmoudi</a> , <sup>1</sup> <a href="#">Atash V. Gurbanov</a> <sup>2,3</sup> <sup>1</sup> University of Maragheh, Iran <sup>2</sup> Baku State University, Azerbaijan <sup>3</sup> Universidade de Lisboa, Portugal
P9	<b>On the importance of Pb•••X (X = N, S) tetrel bonding interactions of extended lead(II) MOF's</b> <a href="#">Ghodrat Mahmoudi</a> , <sup>1</sup> <a href="#">Atash V. Gurbanov</a> <sup>2,3</sup> <sup>1</sup> University of Maragheh, Iran <sup>2</sup> Baku State University, Azerbaijan <sup>3</sup> Universidade de Lisboa, Portugal
P10	<b>Salts of mefenamic acid with selected amines</b> <a href="#">Avesha Jacobs</a> , <a href="#">Jacky S. Bouanga Boudiombo</a> Cape Peninsula University of Technology, South Africa
P11	<b>Carbonyl-carbonyl noncovalent interactions</b> <a href="#">Biswajit Sahariah</a> , <a href="#">Bani Kanta Sarma</a> Shiv Nadar University, India
P12	<b>Crystal structure and hirshfeld surface of a new copper(II) complex with hydrazone derived of B6 vitamin</b> <a href="#">Claudia C. Gatto</a> , <a href="#">Clarisse A. Paiva</a> , <a href="#">Pedro H. de O. Santiago</a> University of Brasília, Brazil



## Posters

P13	<b>Fundamentals of the hydrogen bond enhanced halogen bond</b> <a href="#">Daniel A. Decato</a> , <a href="#">Asia Marie S. Riel</a> , <a href="#">James May</a> , and <a href="#">Orion B. Berryman</a> University of Montana, USA
P14	<b>Triple hydrogen bond-directed assembly of transition metal-containing tectons</b> <a href="#">David A McMorran</a> , <a href="#">Aidan P McKay</a> University of Otago, New Zealand
P15	<b>Revealing the spin state of isolated iron(II) phthalocyanine followed by its tuning via non-covalent interaction</b> <a href="#">Rabindranath Lo</a> , <sup>1,2</sup> <a href="#">Debashree Manna</a> , <sup>1,2</sup> <a href="#">Dana Nachtigallová</a> , <sup>1,2</sup> <a href="#">Radek Zbořil</a> , <sup>1</sup> <a href="#">Pavel Hobza</a> , <sup>1,2</sup> <a href="#">Pavel Jelínek</a> <sup>1,3</sup> <sup>1</sup> Palacký University, Czech Republic <sup>2</sup> Institute of Organic Chemistry and Biochemistry (IOCB), Academy of Sciences of the Czech Republic, Czech Republic <sup>3</sup> Institute of Physics of the Czech Academy of Sciences, Czech Republic
P16	<b>Folding of cyclic peptides stabilized by noncovalent interactions</b> <a href="#">Diogo Vila-Viçosa</a> , <a href="#">Rafael Nunes</a> , <a href="#">Paulo J. Costa</a> Faculdade de Ciências da Universidade de Lisboa, Portugal
P17	<b>Copper(II) complexes with bulky N-substituted diethanolamines: high-field electron paramagnetic resonance, magnetic, and catalytic studies</b> <a href="#">Dmytro S. Nesterov</a> , <sup>1</sup> <a href="#">Oksana V. Nesterova</a> , <sup>1</sup> <a href="#">Julia Jezierska</a> , <sup>2</sup> <a href="#">Andrew Ozarowski</a> , <sup>3</sup> <a href="#">Armando J. L. Pombeiro</a> <sup>1</sup> <sup>1</sup> Universidade de Lisboa, Portugal <sup>2</sup> University of Wrocław, Poland <sup>3</sup> Florida State University, USA
P18	<b>The effect of cucurbit[7]uril on the cytotoxicity of carboplatin</b> <a href="#">Ekaterina Pashkina</a> , <sup>1,2</sup> <a href="#">Alina Aktanova</a> , <sup>2</sup> <a href="#">Irina Mirzaeva</a> , <sup>3</sup> <a href="#">Ekaterina Kovalenko</a> , <sup>3</sup> <a href="#">Nadezhda Knauer</a> , <sup>1</sup> <a href="#">Natalya Pronkina</a> , <sup>1</sup> <a href="#">Aleksandr Kozlov</a> <sup>1,2</sup> <sup>1</sup> Research Institute of Fundamental and Clinical Immunology, Russia <sup>2</sup> Novosibirsk State Medical University, Russia <sup>3</sup> Nikolaev Institute of Inorganic Chemistry, Siberian Branch of the Russian Academy of Sciences, Russia
P19	<b>Hydrogen bonds anticooperativity in (FH)<sub>n</sub>Cl<sup>-</sup> clusters</b> <a href="#">Elena Tupikina</a> , <sup>1,2</sup> <a href="#">Gleb Denisov</a> , <sup>1</sup> <a href="#">Peter Tolstoy</a> <sup>2</sup> <sup>1</sup> Faculty of Physics, St. Petersburg State University, Russia <sup>2</sup> Institute of Chemistry, St. Petersburg State University, Russia
P20	<b>PDB and the hidden secrets – do we know everything about anion–π interactions in macromolecules?</b> <a href="#">Emilia Kuźniak</a> , <sup>1</sup> <a href="#">Michał Glanowski</a> , <sup>2</sup> <a href="#">Rafał Kurczab</a> , <sup>3</sup> <a href="#">Andrzej J. Bojarski</a> , <sup>3</sup> <a href="#">Robert Podgajny</a> <sup>1</sup> <sup>1</sup> Jagiellonian University, Poland <sup>2</sup> Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Poland <sup>3</sup> Institute of Pharmacology, Polish Academy of Sciences, Poland
P21	<b>Dihalobenzene shape sorting by nonporous adaptive crystals of perbromoethylated pillararenes</b> <a href="#">Errui Li</a> , <a href="#">Yujuan Zhou</a> , <a href="#">Run Zhao</a> , <a href="#">Kecheng Jie</a> , <a href="#">Feihe Huang</a> Zhejiang University, China
P22	<b>Novel series of nano-sized mono- and homobi-nuclear metal complexes of sulfathiazoleazodye ligand: Synthesis, characterization, DNA-binding affinity, and anticancer activity</b> <a href="#">Fawaz A. Saad</a> , <a href="#">Abdalla M. Khedr</a> , <a href="#">Hoda El-Ghamry</a> , <a href="#">Mohammed A. Kassem</a> , <a href="#">Nizar El-Guesmi</a> Umm Al-Qura University, Saudi Arabia
P23	<b>Novel Cu(II)-NSAID complexes with isonicotinamide – structure and bioactivity</b> <a href="#">Flóra Jozefiková</a> , <sup>1,2</sup> <a href="#">George Psomas</a> , <sup>2</sup> <a href="#">Ján Moncol</a> <sup>1</sup> <sup>1</sup> Slovak University of Technology in Bratislava, Slovakia <sup>2</sup> Aristotle University of Thessaloniki, Greece

## Posters

P24	<p><b>Theoretical study of the interactions of copper complexes with organic ligands as possible photosensitizers</b></p> <p><a href="#">Francisco J. Melendez</a>,<sup>1</sup> <a href="#">Lisset Noriega</a>,<sup>1</sup> <a href="#">María Eugenia Castro</a>,<sup>2</sup> <a href="#">Norma A. Caballero</a>,<sup>3</sup> <a href="#">Jose Manuel Perez-Aguilar</a>,<sup>1</sup> <a href="#">Brenda L. Sánchez-Gaytán</a>,<sup>2</sup> <a href="#">Enrique González-Vergara</a>,<sup>2</sup></p> <p><sup>1</sup>Facultad de Ciencias Químicas, Benemérita Universidad Autónoma de Puebla, Mexico <sup>2</sup>Centro de Química, ICUAP, Benemérita Universidad Autónoma de Puebla, Mexico <sup>3</sup>Facultad de Ciencias Biológicas, Benemérita Universidad Autónoma de Puebla, Mexico</p>
P25	<p><b>The Sn(IV)-tetra(4-sulfonatophenyl)porphyrin complexes with fluorescein: synthesis, structure, properties</b></p> <p><a href="#">G. Mamardashvili</a>, <a href="#">D. Lazovskiy</a>, <a href="#">O. Dmitrieva</a>, <a href="#">O.I. Koifman</a></p> <p>G.A. Krestov Institute of Solution Chemistry, Russian Academy of Sciences, Russia</p>
P26	<p><b>Effect of meso-nitrophenyl substitution on the Co(II)porphyrins <math>\beta</math>-pyrrole fragments bromination</b></p> <p><a href="#">A. Rusanov</a>, <a href="#">N. Chizhova</a>, <a href="#">G. Mamardashvili</a>, <a href="#">N. Mamardashvili</a></p> <p>G.A. Krestov Institute of Solution Chemistry, Russian Academy of Sciences, Russia</p>
P27	<p><b>Theoretical mechanistic studies on B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>/amine-catalyzed C(sp)-H silylation of terminal alkynes with hydrosilanes</b></p> <p><a href="#">Gen Luo</a>,<sup>1</sup> <a href="#">Yi Luo</a>,<sup>1</sup> <a href="#">Yuanhong Ma</a>,<sup>2</sup> <a href="#">Zhaomin Hou</a><sup>1,2</sup></p> <p><sup>1</sup>Dalian University of Technology, China <sup>2</sup>Organometallic Chemistry Laboratory, RIKEN Cluster for Pioneering Research, Japan</p>
P28	<p><b>Cyanosilylation of aldehydes catalyzed by Ag(I)- and Cu(II)-arylhydrazone coordination compounds</b></p> <p><a href="#">Gonçalo A.O. Tiago</a>,<sup>1</sup> <a href="#">M. Fátima C. Guedes da Silva</a>,<sup>1</sup> <a href="#">Ana P.C. Ribeiro</a>,<sup>1</sup> <a href="#">Luís C. Branco</a>,<sup>2</sup> <a href="#">Armando J.L. Pombeiro</a><sup>1</sup></p> <p><sup>1</sup>Universidade de Lisboa, Portugal <sup>2</sup>Universidade Nova de Lisboa, Portugal</p>
P29	<p><b>Chiral OligoEG's as Evolved Cation-Binding Catalysts</b></p> <p><a href="#">In-Soo Hwang</a>, <a href="#">Choong Eui Song</a></p> <p>Sungkyunkwan University, Korea</p>
P30	<p><b>Zinc metal-organic frameworks hybrid materials and their application in catalysis</b></p> <p><a href="#">Inês A.S. Matias</a>,<sup>1</sup> <a href="#">Mohamed M.A. Soliman</a>,<sup>1</sup> <a href="#">Joana M.N. Brás</a>,<sup>2</sup> <a href="#">Maximilian N. Kopylovich</a>,<sup>1</sup> <a href="#">Elisabete C.B.A. Alegria</a>,<sup>1,2</sup> <a href="#">Ana P.C. Ribeiro</a>,<sup>1</sup> <a href="#">Armando J.L. Pombeiro</a><sup>1</sup></p> <p><sup>1</sup>Universidade de Lisboa, Portugal <sup>2</sup>Instituto Politécnico de Lisboa, Portugal</p>
P31	<p><b>Induced circular dichroism in zinc porphyrin complexes</b></p> <p><a href="#">Irina Osadchuk</a>,<sup>1,2</sup> <a href="#">Riina Aav</a>,<sup>1</sup> <a href="#">Eric Clot</a><sup>2</sup></p> <p><sup>1</sup>Tallinn University of Technology, Estonia <sup>2</sup>University of Montpellier, France</p>
P32	<p><b>Catalytic activity of carbon supported Cu(I) complexes for the synthesis of 1,2,3-triazoles</b></p> <p><a href="#">Ivy L. Librando</a>,<sup>1</sup> <a href="#">Abdallah G. Mahmoud</a>,<sup>1</sup> <a href="#">Sónia A.C. Carabineiro</a>,<sup>1</sup> <a href="#">Carlos F.G.C. Geraldes</a>,<sup>2</sup> <a href="#">M. Fátima C. Guedes da Silva</a>,<sup>1</sup> <a href="#">Armando J.L. Pombeiro</a><sup>1</sup></p> <p><sup>1</sup>Universidade de Lisboa, Portugal <sup>2</sup>Universidade de Coimbra, Portugal</p>
P33	<p><b>A hydrogen bonding definition based on spatial distribution functions and its extension to quantitative structural analysis of general intermolecular bonds in solutions and other fluids</b></p> <p><a href="#">Jan Dočkal</a>, <a href="#">Filip Moučka</a></p> <p>J. E. Purkinje University, Czech Republic</p>
P34	<p><b>Cell-penetrating streptavidin: a new tool for cellular uptake</b></p> <p><a href="#">Javier López-Andarias</a>, <a href="#">Yangyang Chen</a>, <a href="#">Eline Bartolami</a>, <a href="#">Naomi Sakai</a>, <a href="#">Stefan Matile</a></p> <p>University of Geneva, Switzerland</p>



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P35	<b>Structures and hydrogen bond networks of molecular clusters</b> <a href="#">Alhadji Malloum</a> , <sup>1,2</sup> <a href="#">Jean Jules Fifen</a> , <sup>2</sup> <a href="#">Jeanet Conradie</a> <sup>1</sup> <sup>1</sup> University of the Free State, South Africa <sup>2</sup> The University of Ngaoundere, Cameroon
P36	<b>Anion-<math>\pi</math> catalysis on functional fullerene oligomers</b> <a href="#">Jiajia Wang</a> , <a href="#">Xiang Zhang</a> , <a href="#">Javier López-Andarias</a> , <a href="#">Xiaoyu Hao</a> , <a href="#">Anh-Tuan Pham</a> , <a href="#">Naomi Sakai</a> , <a href="#">Stefan Matile</a> University of Geneva, Switzerland
P37	<b>Successful combination of copper(II)-triazapentadienate complexes and carbon nanotubes in alcohol oxidation</b> <a href="#">Jiawei Wang</a> , <sup>1</sup> <a href="#">Ana P. Ribeiro</a> , <sup>1</sup> <a href="#">Marta S. Saraiva</a> , <sup>2,3</sup> <a href="#">Maximilian N. Kopylovich</a> , <sup>1</sup> <a href="#">Luísa M.D.R.S. Martins</a> <sup>1</sup> <sup>1</sup> Universidade de Lisboa, Portugal <sup>2</sup> Centro de Química e Bioquímica, DQB, Faculdade de Ciências, Universidade de Lisboa, Portugal; <sup>3</sup> BioISI -Biosystems & Integrative Sciences Institute, Departamento de Química e Bioquímica, Faculdade de Ciências, Universidade de Lisboa, Portugal
P38	<b>Hydrophobically directed organocatalytic synthesis of chiral GABA Analogues with all-carbon quaternary stereogenic center at <math>\beta</math>-Position</b> <a href="#">Jin Hyun Park</a> , <a href="#">Jae Hun Sim</a> , <a href="#">Pintu Maity</a> , <a href="#">Young Jun Chang</a> , <a href="#">Choong Eui Song</a> Sungkyunkwan University, Korea
P39	<b>Dye sensitized solar cells based on porphyrins</b> <a href="#">Gabriel F. Gika</a> , <sup>1,2</sup> <a href="#">Francisco M. Ferraz</a> , <sup>1,2</sup> <a href="#">Joana M. D. Calmeiro</a> , <sup>1,3</sup> <a href="#">Leandro M. O. Lourenço</a> , <sup>3</sup> <a href="#">Cláudia C. L. Pereira</a> , <sup>2</sup> <a href="#">João P. C. Tomé</a> <sup>1</sup> <sup>1</sup> Universidade de Lisboa, Portugal <sup>2</sup> Universidade NOVA de Lisboa, Portugal <sup>3</sup> University of Aveiro, Portugal
P40	<b>A GROMOS force field for furanose-based carbohydrates</b> <a href="#">Karina Nester</a> , <a href="#">Karolina Gawęda</a> , <a href="#">Wojciech Płaziński</a> <sup>1</sup> Polish Academy of Sciences, Poland
P41	<b>Conformation of the furanose ring. THE QM/MM molecular dynamics simulations.</b> <a href="#">Karolina Gawęda</a> , <a href="#">Wojciech Plazinski</a> Polish Academy of Sciences, Poland
P42	<b>Testing of semiempirical quantum mechanical methods on model systems relevant in drug design</b> <a href="#">K. Kříž</a> , <sup>1,2</sup> <a href="#">J. Řezáč</a> <sup>1</sup> <sup>1</sup> Academy of Sciences of the Czech Republic, Czech Republic <sup>2</sup> Charles University of Prague, Czech Republic
P43	<b>Synthesis of stable, industrially scalable, efficient metathesis Hoveyda-Grubbs catalysts with a S<math>\rightarrow</math>Ru coordinate bond in a six-membered ring</b> <a href="#">K. A. Alekseeva</a> , <a href="#">F. I. Zubkov</a> , <a href="#">K. B. Polyanskii</a> , <a href="#">P. V. Raspertov</a> , <a href="#">P. A. Kumandin</a> Peoples' Friendship University of Russia (RUDN University), Russia
P44	<b>Understanding the Molecular Structure of 3-[(5-methyl-1,3,4-thiadiazol-2-yl)sulfanyl]-1,2- benzothiazole 1,1-dioxide. The Importance of S<math>\cdots</math>N Interaction in a Thiadiazolyl-Saccharinate Derivative</b> <a href="#">L. M. T. Frija</a> , <sup>1</sup> <a href="#">L. I. L. Cabral</a> , <sup>2,3</sup> <a href="#">E. M. Brás</a> , <sup>4</sup> <a href="#">M. S. C. Henriques</a> , <sup>5</sup> <a href="#">C. Marques</a> , <sup>3</sup> <a href="#">L. Barreira</a> , <sup>2,3</sup> <a href="#">J. A. Paixão</a> , <sup>5</sup> <a href="#">R. Fausto</a> , <sup>4</sup> and <a href="#">M. L. S. Cristiano</a> <sup>2,3</sup> <sup>1</sup> University of Lisbon, Portugal <sup>2</sup> Department of Chemistry and Pharmacy, F.C.T., University of Algarve, Portugal <sup>3</sup> Center of Marine Sciences, CCMar, University of Algarve, Portugal <sup>4</sup> CQC, Department of Chemistry, University of Coimbra, Portugal <sup>5</sup> CFisUC, Department of Physics, University of Coimbra, Portugal
P45	<b>Topological analysis of intermolecular interactions involving chlorine; an experimental charge density study</b> <a href="#">Maciej Kubicki</a> , <a href="#">Agata Owczarzak</a> Adam Mickiewicz University, Poland

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P46	<p><b>Photochromic benzo[<i>b</i>]phosphole alkynylgold(I) complexes with mechanochromic property to serve as multi-stimuli-responsive materials</b>  <a href="#">Nathan Man-Wai Wu</a>, <a href="#">Maggie Ng</a>, <a href="#">Vivian Wing-Wah Yam</a>            The University of Hong Kong, China</p>
P47	<p><b>Intramolecular H bonds (IHB) of acylphloroglucinol derivatives: AIM theory and molecular docking studies</b>  <a href="#">María Eugenia Castro</a>,<sup>1</sup> <a href="#">Luis Fernando Paredes</a>,<sup>1,2</sup> <a href="#">Norma A. Caballero</a>,<sup>3</sup> <a href="#">Sergio Luis García</a>,<sup>2,4</sup> <a href="#">Jose Manuel Perez-Aguilar</a>,<sup>2</sup> <a href="#">Liliana Mammino</a>,<sup>5</sup> <a href="#">Francisco J. Melendez</a>,<sup>2</sup>  <sup>1</sup>Centro de Química, ICUAP, Benemérita Universidad Autónoma de Puebla, Mexico  <sup>2</sup>Facultad de Ciencias Químicas, Benemérita Universidad Autónoma de Puebla, Mexico  <sup>3</sup>Facultad de Ciencias Biológicas, Benemérita Universidad Autónoma de Puebla, Puebla, Mexico  <sup>4</sup>Universidad Abierta y a Distancia de México, Mexico  <sup>5</sup>University of Venda, South Africa</p>
P48	<p><b>Synthesis and study of crown-containing bisstyryl dye complexes with various metal cations by using FRET process</b>  <a href="#">M.A. Ustimova</a>,<sup>1</sup> <a href="#">O.A. Fedorova</a>,<sup>1,2</sup> <a href="#">Yu.V. Fedorov</a> <sup>1</sup>  <sup>1</sup>A.N. Nesmeyanov Institute of Organoelement Compounds, RAS, Russia  <sup>2</sup>D. Mendeleev University of Chemical Technology of Russia, Russia</p>
P49	<p><b>Engineering mechanical flexibility in crystalline coordination polymers and their two-component systems</b>  <a href="#">Mateja PISAČIĆ</a>, <a href="#">Ozana Mišura</a>, <a href="#">Marijana Đaković</a>            University of Zagreb, Croatia</p>
P50	<p><b>Carbon materials as supports for a dioxidovanadium(V) complex: application in catalytic cyclohexane oxidation</b>  <a href="#">Marta A. Andrade</a>, <a href="#">Manas Sutradhar</a>, <a href="#">Sónia A.C. Carabineiro</a>, <a href="#">Luísa M.D.R.S. Martins</a>, <a href="#">Armando J.L. Pombeiro</a>            Universidade de Lisboa, Portugal</p>
P51	<p><b>Hydrogen bonds hierarchy in theobromine cocrystals with hydroxybenzoic acids</b>  <a href="#">Mateusz Gołdyn</a>, <a href="#">Weronika Nowak</a>, <a href="#">Elżbieta Bartoszak-Adamska</a>            Adam Mickiewicz University, Poland</p>
P52	<p><b>Relationships between halogen bond strength and electron density properties</b>  <a href="#">Maxim L. Kuznetsov</a>            Universidade de Lisboa, Portugal</p>
P53	<p><b>Synthesis of copper-organic frameworks for the capture and electrocatalysis of carbon dioxide</b>  <a href="#">Mei-Jywan Syu</a>, <a href="#">Yan-Lin Wang</a>            National Cheng Kung University, Taiwan</p>
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Wednesday, 4 September	09.00 – 12.45
Thursday, 5 September	09.00 – 19.00
Friday, 6 September	09.00 – 16.00



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# XXII INTERNATIONAL SYMPOSIUM ON HOMOGENEOUS CATALYSIS



## XXII International Symposium on Homogeneous Catalysis (XXII ISHC)

6-11 September 2020, Lisbon

### Topics

Metal complex catalysis  
Organocatalysis  
Biocatalysis and bioinspired catalysis  
Electrocatalysis  
Photocatalysis  
Cooperative and tandem catalysis  
Heterogenized homogeneous catalysis  
Multiphasic homogeneous catalysis  
Asymmetric catalysis  
Nanocatalysis  
Applied catalysis  
Catalysis in non conventional media  
Noncovalent interactions in catalysis  
Mechanistic investigations  
Computational approaches  
Emerging directions  
Others

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### Important Dates

Early Bird Registration: October 1, 2019 – April 30, 2020

Normal Registration: May 1 - July 20, 2020

Late Registration: from July 21, 2020

Abstract Submission: October 1, 2019 - May 10, 2020



**Chairperson - Armando J. L. Pombeiro**  
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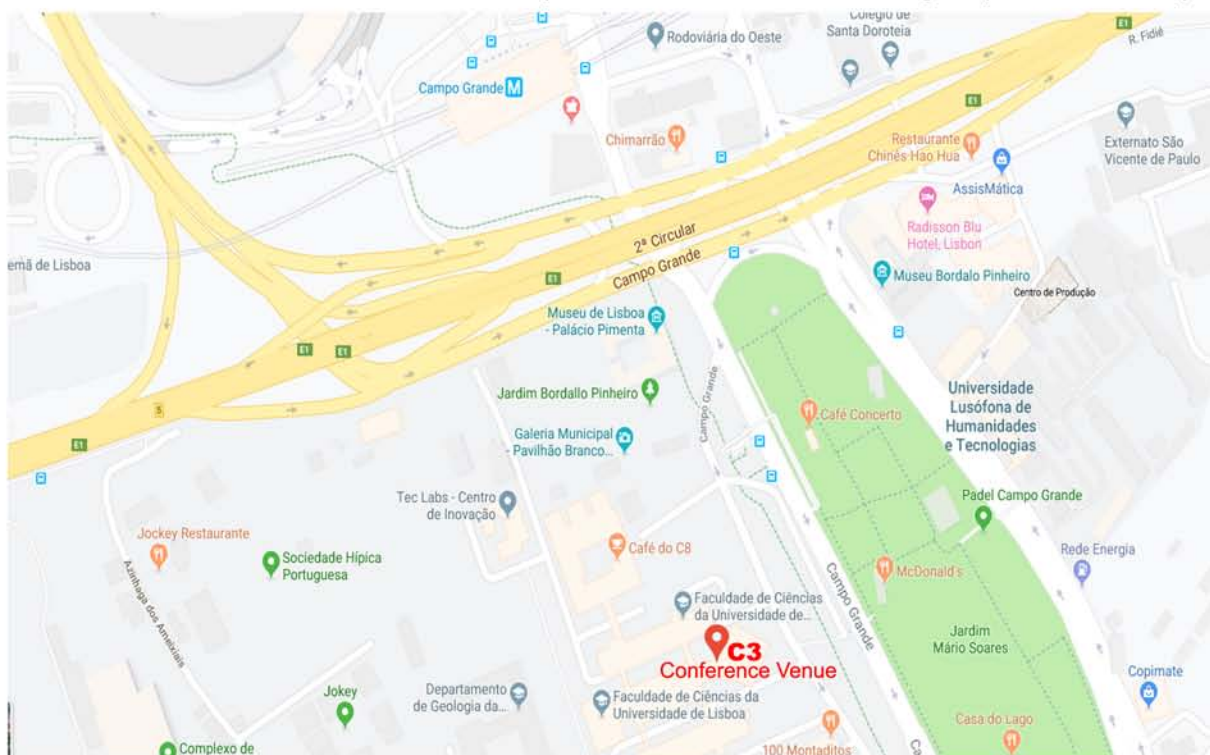
Venue : Faculdade de Ciências da Universidade de Lisboa, Campo Grande 016, 1749-016 Lisboa, Portugal

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## Conference Venue

Venue address:

Faculdade de Ciências da Universidade de Lisboa, Campo Grande 016, 1749-016 Lisboa, Portugal. <https://ciencias.ulisboa.pt/en>



## Campus Map



**C3** Registration & Conference Hall  
**C6** Welcome Reception

# Program at a Glance

Monday - September 2		Tuesday - September 3		Wednesday (Fri-day) - September 4		Thursday - September 5	
<b>Registration</b>							
<b>Opening ceremony</b>		P5 - Resnati (IUPAC Lecture)		P10 - Yamada (Tutorial Lecture)		P13 - Museev	
P1 - Hobza		P6 - Kitagawa		P11 - Frontera (Tutorial Lecture)		P14 - Narahari Sastry	
<b>Coffee break</b>		<b>Coffee break</b>		<b>Coffee break</b>		<b>Coffee break</b>	
P2 - Schneider		P7 - Weller		P12 - Zarić (Tutorial Lecture)		P15 - Hall	
K1 - Akeröy	IL1 - Mosquera	IL19 - Bryce	IL22 - Paz	IL31 - Sawamura	IL34 - Osakada	IL37 - Gatti	IL40 - González-Rodríguez
K2 - Grepioni	IL2 - Cincić	IL20 - Tolstoy	IL23 - Iglesias	IL32 - Luo	IL35 - Bregadze	IL38 - Režić	IL41 - Tomé
	IL3 - Zeng	IL21 - Caltagirone	IL24 - Shimizu	IL33 - Podgajny	IL36 - Maeda	IL39 - Costa	IL42 - Liu
<b>LUNCH</b>		<b>LUNCH</b>		<b>LUNCH</b>		<b>LUNCH</b>	
P3 - Braga		P8 - Braunstein & Robert		<b>EXCURSION</b> (Tour Sintra, starting at 14.30)		P16 - Huang	
P4 - Carpentier		P9 - Harada				P17 - Haukka	
K3 - Nau	IL7 - Werenberg	IL25 - Moobroek	IL28 - Haynes	F1 - Algeria	IL43 - Arimitsu	IL46 - Đaković	
K4 - Jin	IL8 - Nabeshima	IL26 - Biswal	IL29 - Cozzolino	F2 - Kuilkova	IL44 - Trujillo	IL47 - André	
	IL9 - Quesada	IL27 - Echeverría	IL30 - Bartashevich	F3 - Kroeger	IL45 - López-Andarias	IL48 - Bourne	
<b>Coffee break</b>		IL10 - Riley	O10 - Fave	F4 - Roy Barman	<b>Coffee break</b>		
K5 - Brammer	IL13 - Breugst	IL11 - Novikov	O11 - Mewes	F5 - Rocha	K18 - Esterhuysen	IL49 - Blakemore	IL52 - Tsuzuki
K6 - Djukić	IL14 - Fernández	IL12 - Vogtziš		F6 - Sollman	K19 - Vidal-Ferran	IL50 - Kirchner	IL53 - Moičanov
O1 - Sutradhar	IL15 - Kanger	K11 - Nachtgallova	<b>POSTER SESSION</b> (Posters will remain hanged at the proper place during whole conference)		O12 - Nanov	IL51 - Filipov	IL54 - Bistoni
O2 - Rosokha	O4 - Stilianovic				O13 - Little	O15 - Svetsky	O18 - Chigem
O3 - Karmakar	O5 - Hort			O14 - Oliver	O16 - Bálhori	O20 - Fang	
<b>WELCOME RECEPTION</b> (19:00-21:00)		<b>SPEAKERS DINNER</b> (20:00-23:00)		<b>SPEAKERS DINNER</b> (20:00-23:00)		<b>CONFERENCE DINNER</b> (20:00-23:00)	

Friday - September 6	
08:00-09:00	12:45 - 14:15
09:00 - 09:15	14:15 - 14:30
09:15 - 09:30	14:30 - 14:45
09:30 - 09:45	14:45 - 15:00
09:45 - 10:00	15:00 - 15:15
10:00 - 10:15	15:15 - 15:30
10:15 - 10:30	15:30 - 15:45
10:30 - 10:45	15:45 - 16:00
10:45 - 11:00	16:00 - 16:15
11:00 - 11:15	
11:15 - 11:30	
11:30 - 11:45	
11:45 - 12:00	
12:00 - 12:15	
12:15 - 12:30	
12:30 - 12:45	

LUNCH	
O32 - Otero de la Rosa	O38 - Kubicki
O33 - Malenov	O39 - Koval
O34 - Mamaradshvili	O40 - Torubayev
O35 - Pańczyk	O41 - Moncol
O36 - Bulatova	O42 - Tupolina
O37 - Orjipova	O43 - Shariyah

Poster Awards CLOSING	
IL58 - Peccati	
IL59 - Patkowski	
IL60 - Peluso	
O25 - Loh	
O26 - Skarev	
O27 - Fedyanin	

Poster Prizes	
Chemical Science	
Dalton Transactions	
RSC Advances	
Inorganics	
Pharmaceuticals	



## Metro Map

