ICMAB INSTITUT DE CIÈNCIA DE MATERIALS DE BARCELONA · EXCELENCIA SEVERO OCHOA · CSIC CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS · Inorganic Materials & Catalysis Laboratory

9 EUROPEAN CONFERENCE ON BORON CHEMISTRY

Campus de la UAB, Barcelona, Spain
July 3-7, 2022

Detailed Conference Program

Rosario Núñez, *chairwoman*
José Giner, *chairman*

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Sunday (3rd July)

Auditorium, Faculty of Philosophy and Arts/Facultat de Filosofia I lletres, UAB

16:30-19:30	**Documentation**
19:30-21:30	**Welcome cocktail**

Boron containing materials, polymers, ceramics, borides, boron nitride, boron oxides
Organoboron compounds and their metal complexes
Boron compounds in medicine
Other aspects of boron chemistry, including characterization and modelling
Cluster boron chemistry
Asymmetric synthesis via organoboron compounds, enantioselective reductions, chiral boron compounds

Monday (4th July)

Auditorium

08:00	**Registration**
08:40	**Open Ceremony**
Session 1	*Chair: Philippe Miele*
09:00	**KN1 Todd Marder** *3-Coordinate Organoboron Compounds Light The Way: Synthesis, Optical Properties and Cell Imaging*
09:45	**INV1 Emmanuel Lacôte** *Photopolymerization with Boron Radicals*

Room	**Auditorium**	**501 (parallel room)**
	Chair: Philippe Miele	*Chair: Todd Marder*
10:20	**O1A Holger Helten** *Macromolecular Organoborane Chemistry: Developing Sustainable Approaches*	**O1B Juan Z Davalos** *Experiment vs. theory in paramagnetic [FeIII(1,2-$C_2B_9H_{11})_2]^-Cs^+$: Mössbauer spectroscopy and electronic structure computations*
10:40	**O2A Sabine Müller** *Assembly of Functional Nucleic Acid Enzymes and Aptamers from Short Borono-Modified Oligonucleotides*	**O2B Taiki Morita** *Asymmetric Synthesis of Oxazaborolidines via Palladium-Catalyzed N-H/B-H Double Functionalization of 1,2-Azaborines*
11:00	**Coffee Break**	
Session 2	*Chair: William Harman*	*Chair: Todd Marder*
11:30	**O3A Pavel Matejicek** *Anionic boron clusters in supramolecular and polymer chemistry*	**O3B Andrea Olmos** *Mild synthesis of polypyrazolylborates: completing the family*
11:50	**O4A Lei Gan** *A Highly Water-Stable meta-Carborane-Based Copper Metal-Organic Framework for Efficient High-Temperature Butanol Separation*	**O4B Christian Kleeberg** *Transition metal boryl complexes: New answers to old questions?*
12:10	**SC1A Ainee Ibrahim** *Solid-state green hydrogen export utilising the regeneration of BH_4^- from $B(OH)_4^-$ and $B(OCH_3)_4^-$*	**SC1B Ludwig Zapf** *Tricyanoboraneimidazoline-2-ylidenate Anions – Ditopic N-Heterocyclic Carbene Ligands*
12:25	**SC2A Louis Le Moigne** *Catalyst free transfer hydrogenation from amine-borane dimers and oligomers to different substrates*	**SC2B Masato Tsuda** *Synthesis of Isoxazoloazaborines via Gold(I)-Catalyzed Propargyl Aza-Claisen Rearrangement/Borylative Cyclization Cascade*
12:40	**SC3A Romane Bellec** *New energetics polynitrogen-boron compounds for space propulsion*	**SC3B Michele Tomasini** *Arylic C-H Bond Activation and Borylation*
12:55	**SC4A Jonas Bachmann** *Difurodiborepins: New Heteroaromatic Building Blocks for Extended π-Conjugated Materials*	**SC4B Marion Boyet** *Photodecaging of boronic and borinic acids under uv-light irradiation*
13:10	**Lunch**	

	Auditorium	
Session 3	*Chair: Francesc Teixidor*	
14:30	**INV2 Alan Welch** *Bridges, Vertices and How to Distinguish Them*	
Room	**Auditorium**	**501 (parallel room)**
	Chair: Francesc Teixidor	*Chair: Eliseo Ruiz*
15:05	**O5A Jonas Warneke** *Reactivity of $[B_{12}X_{11}]^-$ fragment anions (X=halogen, CN) in the gas phase and in surface layers.*	
15:25	**O6A Ramón Macías** *Ten-vertex Rhodathiaborane Reactivity: Cluster Modular Tuning and Catalysis*	**O6B Jordi Poater** *Aromaticity in Boron Clusters Survives Radical Structural Changes*
15:45	**O7A Zsolt Kelemen** *The „chemical tug-of-war" in boron clusters, beyond the elongation of the C-C bonds of o-carboranes – a combined theoretical and experimental study*	**O7B Ricardo José Maza Quiroga** *Mapping the Electronic Structure and the Reactivity Trends for Stabilized α-Boryl Carbanions*
16:05	**SC5A Sohini Sinha** *Diverse and unique photophysics of new o-carborane cluster based luminescent materials*	**SC5B Daniel Vogler** *Highly selective dipolar cycloaddition reactions of a diazido-diborane*
16:20	**SC6A Zhen Li** *Rational design and synthesis of carborane-based Luminescence lanthanide metal organic frameworks and their application for anticounterfeiting*	**SC6B Julia Ruhl** *Bidentate Lewis Acid Catalyzed IEDDA/PIRO Reaction as Synthetic Tool for Medium-Sized Carbocycles*
16:35	**SC7A Liridona Useini** *Carboranyl analogues of the non-steroidal anti-inflammatory drug mefenamic acid*	**SC7B Arnaud Osi** *9-Boratriptycenes: A Lewis Superacids Story*
16:50	**SC8A Neville Murphy** *Metallacarboranes as triple-negative breast cancer therapeutics and diagnostics*	**SC8B Damien Mahaut** *Metal-free hydrogenation of unactivated olefins by weakly basic 9-phosphatriptycene derivatives and tris(pentafluorophenyl)borane*
17:05	**Coffee Break** **Poster Session A (P1A-P26A)**	
19:00	**Free Time to Discover Barcelona**	

Tuesday (5th July)

	Auditorium	
Session 4	*Chair: Bohumir Grüner*	
09:00	**KN2 Clara Viñas** *Towards the application of purely inorganic anionic icosahedral boron clusters in nanomedicine*	
09:45	**INV3 Elena Fernandez** *Site-selective C-B functionalization of 1,1-diborylalkenes*	
Room	**Auditorium**	**501 (parallel room)**
	Chair: Bohumir Grüner	*Chair: Zsolt Kelemen*
10:20	**O8A Hiroyuki Nakamura** *Comprehensive Exploration of Chemical Space Using Trisubstituted Carboranes*	**O8B Krzysztof Durka** *Heavy-atom free spiro organoboron complexes as triplet excited states photosensitizers for singlet oxygen activation*
10:40	**O9A Fernanda Marques** *Metallacarboranes (Co, Fe) as multifunctional molecules for multimodal cancer treatment*	**O9B Tomasz Kliś** *Organoboron compounds in photocatalysis*
11:00	**Coffee Break**	
Session 5	*Chair: Zbigniew Leśnikowski*	*Chair: Elena Fernandez*
11:30	**O10A Simonetta Geninatti Crich** *Histidine containing PLGA nanoparticles as novel theranostic agents for Boron Neutron Capture Therapy (BNCT)*	**O10B William Harman** *Boron-Doped Acenes as Ligands and Reaction Centers*
11:50	**O11A Stefano Parisotto** *Exploring the Activity of ortho-Carboranes as Therapeutic Agents against Alzheimer's Disease*	**O11B Merle Arrowsmith** *Facile access to iminoboranes via the Staudinger-type reaction of boron(I) compounds with organic azides*

12:10	**SC9A Miquel Nuez-Martínez** *Fingerprint of the Small Anionic Molecule Cobaltabis(dicarbollide) Uptake in Glioma Stem Cells using Synchrotron-Based Fourier-Transform Infrared Micro-Spectroscopy (SR- FTIRM)*	**SC9B Jana Sendra Viscarro** *Catalytic Stereoselective Borylative Transannular reaction*
12:25	**SC10A Jakub Cebula** *In vitro evaluation of biological activity of cobalta bis(dicarbollide) derivatives on eukaryotic cell lines and bacteria*	**SC10B Oriol Salvadó Ruiz** *Olefination reaction between aldehydes and diborylsilylmethide lithium salts*
12:40	**SC11A Amanda Muñoz-Juan** *In vivo insights of carboranes using C. elegans*	**SC11B Kieran Nicholson** *Transborylation as a General Turnover Strategy for Main-group Catalysis.*
12:55	**Lunch** *(Int. Committee Meeting)*	

	Auditorium	
Session 6	*Chair: Evamarie Hey-Hawkins*	
14:30	**INV4 Zbigniew Leśnikowski** *Composites of DNA and boron clusters and their assembly into functional nanoparticles*	
	Auditorium	**501 (parallel room)**
	Chair: Evamarie Hey-Hawkins	*Chair: Hiroyuki Nakamura*
15:05	**O12A Agnieszka Adamczyk-Woźniak** *Studies of the molecular mechanism of action of Tavaborole and its analogues as anti C. albicans agents*	**O12B Antonio Sousa-Pedrares** *Modulation of the coordinating ability of an iminophosphorane group using a carborane moiety.*
15:25	**O13A Krzysztof Fink** *Metallacarborane-ultrashort cationic peptide conjugates with antimicrobial activity*	**O13B Andrea Barba-bon** *Boron clusters as broadband membrane carriers*
15:45	**SC12A Sebastiano M. S. Micocci** *Novel Boronated Monocarbonyl Analogues of Curcumin (BMAC): A new approach to fighting Alzheimer disease (AD)*	**SC12B Diego Holanda Pereira de Souza** *Hydrated Metal Boranes for Solid-State Batteries*
16:00	**SC13A Alberto Lanfranco** *Synthesis of Bifunctional Agents for the Treatment of Mesothelioma by Coupling BNCT with Inhibition of CAIX*	**SC13B Amanda Berger** *Divalent closo-monocarbadodecaborane salts as solid-state electrolytes.*
16:15	**SC14A Nils Schopper** *Alkyl-, alkenyl- and alkynylcyanoborates: Syntheses and properties of low-viscosity ionic liquids*	**SC14B Thomas Hales** *Heavy metal substituted closo-dodecaborane salts for future battery applications*
16:30	**SC15A Martin Orságh** *Novel LMW gelator based on phenylboronic acid and its stimuli-responsivity*	**SC15B Ioanna Chazapi** *Specific interactions of nano-ions with proteins*
16:45	**SC16A Andrei Bita** *Diester chlorogenoborate complex: synthesis method and uses thereof*	
17:00	**Coffee Break** **Poster Session B (P1B-P27B)**	
19:00	***Free Time to Discover Barcelona***	

Wednesday (6 July)

	Auditorium	
Session 7	*Chair: Alan Welch*	
09:00	**KN3 Francesc Teixidor** *Metallacarboranes as Seen Through my Eyes*	
09:45	**INV5 Evamarie Hey-Hawkins** *Carboranes and Metallacarboranes as Building Blocks for the Design of Novel Anti-Tumour Agents*	
Room	**Auditorium**	**501 (parallel room)**
	Chair: Alan Welch	*Chair: Jordi Poater*
10:20	**O14A Isabel Romero Garcia** *Ruthenium-Cobaltabis(dicarbollide) as Efficient Photoredox Catalyst through Proton Coupled Electron Transfer processes (PCET)*	**O14B Jedrzej Walkowiak** *Green catalysis in organoboron and related compounds synthesis*
10:40	**O15A Maria José Mostazo-López** *Synthesis and electrochemical performance of fluorine-functionalized cobaltabisdicarbollide*	**O15B Terry Humphries** *Regeneration of sodium borohydride by reactive ball milling with Mg_2Si*
11:00	**Coffee Break**	

Session 8	*Chair: Deflet Gabel*	*Chair: Jordi Poater*
11:30	**O16A Aleš Růžička** *Opening Cationic Heteroboranes Era*	**O16B**
11:50	**O17A Fabrizio Murgia** *Metastable NaCB11H12 polymorph prepared by mechanical milling as new superionic conductor for post-Li solid-state batteries*	**O17B Eliseo Ruiz** *Theoretical Approach to Carborane-based Systems: From Magnetism to Photochemistry*
12:10	**O18A Isabel Guerrero Troyano** *Metallabis(dicarbollide) a green and efficient photoredox catalyst for epoxidation reactions*	**O18B Laura Caggiu** *Novel closo-hydridoborates of K, Mg and Ca as potential solid electrolytes for post-lithium solid-state batteries*
12:30	**SC17A Jewel A M Xavier** *Tapping the potential of Metallacarboranes as Standard Internal Reference*	**SC17B Philipp Grewelinger** *Facile access to non-classical 1,2-diboriranes*
12:45	**SC18A Tarek Marei** *Host-guest interaction of substituted dodecaborate anions with hydrophobic hosts*	**SC18B Dominic Willcox** *Borane-Catalysed C(sp3)–F Bond Arylation and Esterification Enabled by Transborylation*
13:00	**Lunch**	

Auditorium

Session 9	*Chair: Clara Viñas*
14:30	**INV6 Bohumír Grüner** *Boron Cluster Inhibitors of Cancer Associated CA-IX Enzyme- an Overview*
15:05	**O19A Agnieszka Olejniczak** *Compounds containing boron clusters with antibacterial and anticancer activity.*
15:25	**O20A Marcos Couto** *Carbaboranyl-based tyrosine Kinases inhibitors as bimodal therapeutic agents against Glioblastoma, the worst Prognosis Brain Cancer*
15:45	**O21A Christoph Selg** *Borinostats: Solid-Phase Synthesis of Carborane-Capped Histone Deacetylase Inhibitors with a Tailormade Selectivity Profile*
16:05	**Excursion + Dinner**

Thursday (7th July)

Auditorium

Session 10	*Chair: Emmanuel Lacôte*
09:15	**KN4 Philippe Miele** *Boron nitride based nanostructured materials for energy, health and environmental applications.*
10:00	**INV7 Detlef Gabel** *The functionalization of dodecaborate - an ongoing challenge*
10:35	**O22A Mahmoud Al-Joumhawy** *Insight into synthesis and properties of functionalized dodecaborates*
10:55	**Coffee Break**
Session 11	*Chair: Pavel Matejicek*
11:30	**O23A Michael Beckett** *Hydroxidooxidohexaborate chemistry: 1-D coordination polymers with Zn(II) and Cu(II) amine complexes.*
11:50	**O24A Bérangère Toury** *Excellent Boron Nitride Nanosheets from a new source of large hBN single crystals*
12:10	**O25A Eric Rivard** *Polyacetylenes with Redox Active Boryl Groups and the Quest to Prepare BN at Low Temperature*
12:30	***Prizes + Closing Ceremony***
13:00	***Lunch + Departure***

Poster Session A (Monday 4th July 17:05-19:00)

Syrine Affes	*Graphene, Polyaromatic Hydrocarbons and Cosane*	**P1A**
Virinder Bhagat	*Reactivity studies of a Donor Stabilized Borylnitrene*	**P2A**
Charlotte Bodin	*Borates based interface for calcium metal batteries*	**P3A**
Fabian Burzlaff	*Synthesis and reactions of fluorinated closo-dodecaborates*	**P4A**
Deniz Cam	*N-Functionalization of the closo-Dodecaborate Anion [B12H12]2- via Arylation of [B12H11NH3]-*	**P5A**
Vicente Compañ	*Metallacarborane salts as doping agents in polybenzimidazole-based membranes with enhanced proton conductivity for high temperature proton exchange membranes*	**P6A**
AnnaMaria Deagostino	*Synthesis of a new Theranostic Agent Containing Boron and Biotin for BNCT/MRI Applications*	**P7A**
Paula Dominguez Molano	*Transborylation between diboron reagents and alkenylboranes*	**P8A**
Ferdinand Ehlers	*Synthesis and spectroscopic properties of the cyanated closo-Dodecaborates [B12(CN)11X]2- anions (X = F, Cl, Br, I, NH2)*	**P9A**
Sarah Fellinger	*A New Synthesis to C-substituted 1-Carba-closo-dodecaborates*	**P10A**
Roman Franz	*Phosphanyl-Boranes embedded into a [3]ferrocenophane scaffold*	**P11A**
Gerard Bru	*Mechanistic insights into the transborylation between diboron reagents and alkenylboranes: A DFT study*	**P12A**
Sara González Morán	*1,2-Dicarbofunctionalization of 1,1-arylborylalkenes*	**P13A**
Divanshu Gupta	*Computational Studies of Reactivity and Nature of B≡N bond Containing Cyclic Rings*	**P14A**
Tobias Heitkemper	*Reactivity of novel 2,5-silyl substituted Boroles*	**P15A**
Belhssen Hleli	*Associative behavior of dodecaborate conjugates with alkyl tails*	**P16A**
Drahomir Hnyk	*Reactions of icosahedral, bicapped-square antprismatic and octahedral heteroboranes with n-heterocyclic carbenes: computational studies of origination of the corresponding heteroborane cations*	**P17A**
Josef Holub	*The Establishment of the Class of Non-Covalent Organic Framework Materials by Phenyl-Substituted Thiaboranes – linked 2D and 3D Aromatics*	**P18A**
Evelyn Hümpfner	*Aromatic conjugation between the 2D and 3D systems*	**P19A**
Pawel Huninik	*Transition-metal catalyzed Markovnikov and anti-Markovnikov selective hydroboration of mono- and disubstituted alkenes*	**P20A**
Litwin Jacob	*Ionic materials based on [closo-B10H10]2- anion for modern technological applications*	**P21A**
Rafal Jakubowski	*Photophysical and thermal properties of self-organizing derivatives of 10- and 12-vertex p-carboranes*	**P22A**
Mari Janse van Rensburg	*Synthesis and Electrochemical Investigation of Boron Verdazyl Radicals*	**P23A**
Damian Kaniowski	*Highly boron-loaded antisense oligonucleotides conjugated with target-directed ligands for dual anticancer therapy: anti-EGFR and BNCT*	**P24A**
Denis Kargin	*Examples of chalcogen transfer and reactivity of boron based compounds*	**P25A**
Roman Keder	*Polyborazylene: A precursor for the formation and deposition of boron nitride layers*	**P26A**

Poster Session B (Tuesday 5th July 17:00-19:00)

Willi Keller	*Synthesis and Structural Verification of the First Small Polyhedral Telluraborane closo-TeB5Cl5: How Far can Molecular Octahedral Distortion go?*	**P1B**
Barbara Krupa	*Catalytic hydroboration of carbonyl compounds in traditional and green reaction media*	**P2B**
Min Hyung Lee	*TADF Emitters Based on Boron-Carbonyl Hybrid Acceptors: Achieving Fast Spin-Flip and High-Efficiency OLEDs*	**P3B**
Xiaobao li	*Towards the Generation of Hierarchical Porosity in Carborane-Based Metal-Organic Frameworks*	**P4B**
Falk Lissner	*SYNTHESIS AND STRUCTURE OF A LONG PREDICTED SMALL POLYHEDRAL THIABORANE: closo-SB5Cl5*	**P5B**
Matthias Maier	*Poly(iminoborane)s: An Elusive Class of Main Group Polymers?*	**P6B**
Jelena Matovic	*Glycoconjugates for boron neutron capture therapy*	**P7B**
Soňa Mesíková	*Nanomaterials based on electrostatic interaction of triblock copolymers with closo-dodecaborate*	**P8B**
Max Milewski	*Carboranylphosphines meet dendrimers - New scaffolds for ligand design*	**P9B**
Moheera Noor	*Halogenation of substituted dodecaborate clusters*	**P10B**
Lucia Pazderova	*Derivatives of conformationally restrained cobalt bis(dicarbollide) ion as a new chiral platform and a tool for electrolabeling of biomolecules*	**P11B**
Mireia Pujol Marti	*Copper Catalyzed Stereoselective cross coupling of gem-diborylalkenes*	**P12B**
Carmen Ramirez de Arellano	*Free scorpionate ligands ready for metal complexation*	**P13B**
Gabriela Ramos	*Binding of substituted dodecaborate clusters to cyclodextrins*	**P14B**
Daria Różycka	*Isoniazid containing boron clusters – synthesis and activity*	**P15B**
Sebastian Rykowski	*3- and 4-Substituted naphthalimide DNA intercalators bearing carborane cluster – synthesis, physicochemical and biological properties*	**P16B**
Julijan Sarcevic	*Neutral half-sandwiches of silicon, germanium and tin*	**P17B**
Marvin Sindlinger	*Structural characterization and reactivity of a kinetically stabilized benzoborirene*	**P18B**
Krzysztof Śmiałkowski	*Oligofunctionalization of cobalt-bis(1,2-dicarbollide)ate (COSAN) as a building block for nanoconstructions*	**P19B**
Tomasz Sokolnicki	*Ru-catalyzed Coupling of Vinylsilanes with Vinyl Boronates in PEGs and scCO2 – A Green Approach Towards 1-Boryl-1-silylethenes.*	**P20B**
Philipp Stockmann	*Reversion of drug resistance – a carboranic approach*	**P21B**
Lukas Swoboda	*Furan Based Diboraporphyrins – Broadband UV-vis to NIR Absorbers*	**P22B**
Jakub Szyling	*TM-catalyzed diboration and hydroboration of 1,3-diynes – efficient access to boryl-functionalized enynes*	**P23B**
Ece Zeynep Tüzün	*Boron Clusters in Design of Fluorescent Probes and Kinase Inhibitors*	**P24B**
Lea Ueberham	*Synthesis of carborane-based ligands for theranostic approaches*	**P25B**
Ziyan Warneke	*Gas phase reactivity of functionalized halogenated closo-dodecaborate anions*	**P26B**
Ryotaro Yamanashi	*A base-stabilized neutral B=O species supported by a bis(oxazolinyl)methanide ligand*	**P27B**

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