
## Sunday - 17 July

**Belle Electrique**
***12 Esplanade Andry Farcy, 38000 Grenoble***
***Tram station "Berriat -Le Magasin"***

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| 15h00-17h30 | **Registration** |
| 17h30 - 18h30 | **Welcome party** |
| 18h30 - 19h00 | **Opening Ceremony**<br>***Chairs: Carole DUBOC - Stéphane MENAGE*** |
| 19h00 - 19h30 | ***Chair Eva Freisinger***<br>**EUROBIC Medal 2020 - Aidan MCDONALD**<br>**Mimicking class Ib dimanganese ribonucleotide reductase** |
| 19h30 - 20h00 | **EUROBIC Medal 2020 - Kallol RAY**<br>**Small molecule activation at transition metal centers: structure-function correlations** |

# Monday - 18 July

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| **8h30 - 9h20** | **PL1 - Elisabeth NOLAN**<br>**Exploring siderophore scaffolds for antibacterial strategies**<br>***Room A - Chair Roland SIGEL*** | | |
| | **Session 1 - Room B** | **Session 2 - Room C** | **Session 3 - Room D** |
| | ***Chair* Isabel CORREIA** | ***Chair* Nick LE BRUN** | ***Chair Vincent ARTERO*** |
| **9:30 - 10:00** | **KN1 ROMPEL Annette**<br>*Interweaving disciplines to advance chemistry: applying polyoxometalates in biology* | **KN3 CIURLI Stefano**<br>*Advances in the biochemistry of urease and related systems* | **KN5 NAM Wonwoo**<br>*Biomimetic Metal-Oxygen Intermediates in Dioxygen Activation Chemistry* |
| 10:00 - 10:20 | **OC1 HADJIKAKOU Sotiris**<br>*Drug activation for the discovery and development of new targeted chemotherapeutic formulations* | **OC5 WONG Kam Bo**<br>*Structural insights into nickel trafficking along the urease maturation pathway* | **OC9 JACKSON Timothy**<br>*Geometric and Electronic Influences on the Reactivity of Mn(III)-hydroxo and Mn(III)-alkylperoxo Complexes* |
| 10:20 - 10h40 | **OC2 MARMION Celine**<br>*Multi-Targeted Metallodrugs Rationally Designed to Overcome Drug Resistance* | **OC6 FURTMUELLER Paul**<br>*Structural and mechanistic insights in dimeric chlorite dismutase - Impact of pH and the dynamics of the catalytic arginine* | **OC10 DEY Abhishek**<br>*Nitric Oxide Reactivity with Iron Porphyrins* |
| **10h40-11h10** | **Coffee Break** | | |
| | **Session 1 - Room B** | **Session 2 - Room C** | **Session 3 - Room D** |
| | ***Chair Juan FONTECILLA-CAMPS*** | ***Chair Catherine BELLE*** | ***Chair Ewen BODIO*** |
| 11h10 - 11h40 | **KN2 EINSLE Oliver**<br>*Towards a Unified Concept of Nitrogenase Catalysis* | **KN4 TUCZEK Felix**<br>*Model systems of copper-containing monooxygenases with pyridazine backbone* | **KN6 DAUMANN Lena**<br>*Inspired by Nature: Separation of Lanthanides and Actinides* |
| 11h40 - 12h00 | **OC3 BERTEAU Olivier**<br>*Crystallographic snapshots of Mmp10, a B12-dependent radical SAM methyltransferase involved in methane biosynthesis* | **OC7 STOKOWA Kamila**<br>*Cu(II) and Fe(II) binding, DNA cleavage and radicals production by outer-membrane protein fragments from F. nucleatum* | **OC11 ELISEEVA Svetlana**<br>*Tuning functional properties of lanthanide(III)-based metallacrowns* |
| 12h00 - 12h20 | **OC4 ASH Philip**<br>*Unifying Mechanism in NiFe Hydrogenase Using Advanced Spectroscopic Techniques* | **OC8 NEUMANN Wilma**<br>*Dithiolopyrrolones are Prochelators that Mediate the Redox Cycling of Copper* | **OC12 HAMON Nadège**<br>*Design of specific regio-functionnalized pyclen-based Ln(III) complexes for two-photon excitation and application to imaging or theranostic* |
| **12h20 - 14h00** | **LUNCH** | | |
| **14h00 - 15h00** | **Discussion around Gender in Science**<br>*Room A - Chair Carole DUBOC & Pascale DELANGLE* | | |
| | **Session 1 - Room B** | **Session 2 - Room C** | **Session 3 - Room D** |
| | ***Chair Abhishek DEY*** | ***Chair* Luca BERTINI** | ***Chair Bas DE BRUIN*** |
| 15h00 - 15h30 | **KN7 AUKAULOO Ally**<br>*Coupling photoredox with bioinspired molecular catalysts for $O_2$ and $CO_2$ activation* | **KN9 PETOUD Stéphane**<br>*Metals for Biological and Medical Diagnostics: Dual-mode Nearinfrared Optical and Photoacoustic Imaging Agent based on Low Energy Absorbing Ytterbium Complex* | **KN11 GALLO Emma**<br>*Synthesis of Biologically Relevant Heterocycles Mediated by Porphyrin-based Catalysts* |
| 15h30 - 15h50 | **OC13 ARTERO Vincent**<br>*Proton relays in molecular electrocatalysis: specifications for efficiency and insights into their relevance for reversible behavior* | **OC15 IVANOVIC-BURMASOVIC Ivar**<br>*Is Zn redox "innocent"? Redox modulation and signaling by Zn vs Fe and Mn* | **OC17 SRNEC Martin**<br>*On the role of asynchronicity and frustration in C-H bond activation by metal-oxo complexes* |
| 15h50 - 16h10 | **OC14 LOURO Ricardo**<br>*Exploring the molecular mechanisms of electron uptake by (photo)electro-autotrophic organisms* | **OC16 GAMBINO Dinorah**<br>*Multi-functional organometallic compounds as prospective antitrypanosomal agents: new approaches* | **OC18 AVENIER Frédéric**<br>*Bioinspired Iron Chemistry: i) Heterolytic O-O Bond Breaking Reaction and ii) Unprotected Nitrene Transfer Reactions* |
| 16h10 - 16h40 | **KN8 MINTEER Shelley**<br>*Enzymatic and Microbial Bioelectrocatalysis for Electrosynthesis* | **KN10 VILAR Ramon**<br>*Targeting and imaging DNA with metal complexes* | **KN12 MORGAN Grace**<br>*Dioxygen Activation by Electronic Modulation of Redox and Spin State Choice in Mn and Co Chelate Complexes* |
| **16h40 - 17h10** | **Coffee Break** | | |
| **17h10 - 18h00** | **PL2 - Jana ROITHOVA**<br>**Bioinspired catalysis investigated by mass spectrometry**<br>***Room A - Chair Pascale MALDIVI*** | | |
| 18h00 - 19h30 | Poster Session<br>*Hall SUD* | | |

# Tuesday - 19 July

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| **8h30 - 9h20** | **PL3 - Nick LE BRUN**<br>**Adventures with iron-sulfur cluster-containing regulators: elucidation of sensing mechanisms**<br>***Room A - Chair Sandrine OLLAGNIER*** | | |
| | **Session 1 - Room B** | **Session 2 - Room C** | **Session 3 - Room D** |
| | ***Chair Sven STRIPP*** | ***Chair Christelle HUREAU*** | ***Chair Shelley MINTEER*** |
| **9:30 - 10:00** | **KN13 AGAPIE Theodor**<br>*Cluster Models of the Nitrogenase Active Site* | **KN15 BLINDAUER Claudia**<br>*How marine cyanobacteria deal with zinc in an ocean desert* | **KN17 HELLWIG Petra**<br>*Electrocatalytic and Spectroscopic Studies on Cytochrome bd Oxidase, a Highly Diverse Bacterial Defense Factor* |
| 10:00 - 10:20 | **OC19 ANXOLABEHERE Elodie**<br>*Electrochemical O2 activation by Fe and Mn porphyrins. Towards electrocatalytic aerobic oxidations of organic substrates* | **OC23 JANCSO Attila**<br>*On the metal site stabilizing role of the C-terminal CCHHRAG fragment of the metalloregulatory protein CueR* | **OC27 FOLGOSA Filipe**<br>*The conserved amino acid motif -GSSYN- is essential for the E. coli flavorubredoxin NO reductase its activity* |
| 10:20 - 10h40 | **OC20 MILET Anne**<br>*Theoretical Mechanistical Study of CO2 Reduction to CH4 by a Bio-Inspired NiFe Hydrogenase Model on graphite.* | **OC24 KIELB Patrycja**<br>*Do Tyr/Trp redox pathways protect O2-reducing S. Coelicolor laccase from oxidative damage?* | **OC28 ZHANG Huijie**<br>*Development of Multiheme Cytochromes-Carbon Dots Biohybrids for Solar Chemicals and Fuels Generation* |
| **10h40-11h10** | **Coffee Break** | | |
| | **Session 1 - Room B** | **Session 2 - Room C** | **Session 3 - Room D** |
| | ***Chair Oliver EINSLE*** | ***Chair Jens MÜLLER*** | ***Chair Liviu MIRICA*** |
| 11h10 - 11h40 | **KN14 HÖGBOM Martin**<br>*Toward geometric structures of oxidized cofactors and high-valent metal-oxygen intermediates in di-metal proteins by femtosecond XFEL crystallography* | **KN16 HANNON Mike**<br>*Supramolecular recognition of DNA and RNA junction structures for anti-viral and anti-cancer therapy* | **KN18 HERRES-PAWLIS Sonja**<br>WILEY<br>*Manipulating the Electron Transfer in Entatic State Model - The Influence of Substituents on Novel Copper Guanidine Quinoline Complexes* |
| 11h40 - 12h00 | **OC21 WORRALL Jonathan**<br>*Serial femtosecond X-ray crystallography reveals the role of water molecules in the chemistry of compound I reduction in dye-decolorizing peroxidases* | **OC25 SIGEL Roland**<br>*Programmed cell death and SARS-CoV-2; two RNA G-quadruplexes in the focus of metal ions, their complexes, and small molecules* | **OC29 KULAK Nora**<br>*Prodigiosin derivatives and their Cu(II)-dependent antimicrobial and photoinduced anticancer activity* |
| 12h00 - 12h20 | **OC22 RABE Patrick**<br>*X-ray free electron laser studies reveal dioxygen binding to isopenicillin N synthase induces correlated motions during catalysis* | **OC26 PRATIK Shah**<br>*Noncanonical Head-to-Head Hairpin DNA Dimerization at Interfacial Binding Sites by Orange Emissive Silver Nanocluster* | **OC30 RONCONI Luca**<br>*Tale of a successful failure: gold(III)-glycoconjugates as antiviral agents against SARS-CoV-2* |
| **12h20 - 14h00** | **LUNCH** | | |
| **14h00 - 15h00** | **Discussion around Integrity in Science**<br>*Room A - Chairs Sandrine OLLAGNIER & Stéphane MENAGE* | | |
| | **Session 1 - Room B** | **Session 2 - Room C** | **Session 3 - Room D** |
| | ***Chair Pascale DELANGLE*** | ***Chair Vincent FOURMOND*** | ***Chair Jean-Pierre MAHY*** |
| 15h00 - 15h30 | **KN19 HUREAU Christelle**<br>*Natural polyanions to tune the metal-modulated self-assembly of Aβ amyloid-forming peptides* | **KN21 NICOLET Yvain**<br>*FeFe-hydrogenase active site assembly: the case of HydE* | **KN23 PECORARO Vincent**<br>*de Novo Designed Protein Catalysis* |
| 15h30 - 15h50 | **OC31 MIRICA Liviu**<br>*Novel Theranostic Agents for Alzheimer's Disease* | **OC33 CASERTA Giorgio**<br>*Stepwise assembly of the [NiFe]-hydrogenase active site* | **OC35 CHAKRABORTY Saumen**<br>*De Novo Designed Artificial Cu Proteins (ArCuPs) as O-H/O-O/C-H Activation Catalysts* |
| 15h50 - 16h10 | **OC32 BERTINI Luca**<br>*Membrane damages induced by Cu(II)-Aβ•OH radical species. OH propagation toward polar head groups and lipid tails of membrane phospholipid* | **OC34 STRIPP Sven**<br>*Proton-coupled Electron Transfer in the Catalytic Mechanism of [FeFe]-Hydrogenase* | **OC36 LEONE Linda**<br>*Unveiling selectivity in indole oxidation catalyzed by artificial heme-enzymes* |
| 16h10 - 16h40 | **KN20 GOSH DEY Somdatta**<br>*Heme and Copper bound Amyloid β Peptides: Reactive Intermediates relevant to Oxidative Degradation of Neurotransmitters* | **KN22 LEIMKÜHLER Silke**<br>*Modulation of the Molybdenum Coordination Sphere of E. coli Trimethylamine N-oxide reductase and role of the nucleotides in the bis-MGD molybdenum cofactor* | **KN24 WARD Thomas**<br>*Artificial Metalloenzyme for in vivo Catalysis: Challenges and Opportunities* |
| **16h40 - 17h10** | **Coffee Break** | | |
| **17h10 - 18h00** | **PL4 - Clotilde POLICAR**<br>**Metal complexes in biological environments: a new frontier in inorganic chemistry**<br>***Room A - Chair Vincent PECORARO*** | | FrenchBIC |
| 18h00 - 19h30 | Poster Session<br>*Hall SUD* | | |

# Wednesday - 20 July

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| **8h30 - 9h20** | **PL5 - Franc MEYER**<br>**Unusual Spin States and Spin-Dependent Reaction Trajectories in Biorelevant Dicopper/O2 and Diiron/NO Chemistry**<br>***Room A - Chair Carole DUBOC*** | | |
| | **Session 1 - Room B** | **Session 2 - Room C** | **Session 3 - Room D** |
| | ***Chair Fabrice THOMAS*** | ***Chair Claudia BLINDAUER*** | ***Chair Mike HANNON*** |
| **9:30 - 10:00** | **KN25 COMPANY Anna**<br>*Exploring the oxidation chemistry of iron(V)-oxo-carboxylato species* | **KN27 FREISINGER Eva**<br>*Metallothioneins – looking beyond the fully metalated state* | **KN29 MEZLER-NOLTE Nils**<br>*New Chemistry of Organometallic Rhenium Complexes for Drug Development* |
| 10:00 - 10:20 | **OC37 ARRIGONI Federica**<br>*Exploring novel features of [FeFe]-hydrogenase models through non-biomimetic modifications and reactivity: a DFT viewpoint* | **OC41 BYRNE Joseph**<br>*Carbohydrate-functionalised metal complexes: targeting bacterial carbohydrate-binding proteins for therapeutic and sensing applications* | **OC45 COVERDALE James**<br>*Advances in Os(II)-catalysed intracellular asymmetric reduction: new targets, stability improvement and anticancer potency enhancement* |
| 10:20 - 10h40 | **OC38 MARTINI Maria Alessandra**<br>*Inhibition by CN- provides insight into the catalytic mechanism of [FeFe] hydrogenases* | **OC42 CORREIA Isabel**<br>*Liposomal formulation of a new Zn(II) complex exhibiting high therapeutic potential in a murine colon cancer model* | **OC46 MASSAI Lara**<br>*Internalization of Anticancer Gold(I) Complexes in Human H Ferritin to Improve Drug Selectivity* |
| **10h40-11h10** | | | |
| | **Session 1 - Room B** | **Session 2 - Room C** | **Session 3 - Room D** |
| | ***Chair Emma GALLO*** | ***Chair Ragnar BJORNSSON*** | ***Chair* Roland SIGEL** |
| 11h10 - 11h40 | **KN26 DE BRUIN Bas**<br>*Bio-Inspired Synthesis of Ring Compounds using Metalloradical Catalysis* | **KN28 PEREIRA Ines**<br>*High activity metalloenzymes for sustainable production of fuels* | **OC47 MÜLLER Jens**<br>*Light-Induced Formation of Metal-Mediated Base Pairs* |
| 11h40 - 12h00 | **OC39 ZLATAR Matija**<br>*Coordination preferences of Shiff base ligands with transition metals: DFT study* | **OC43 BIRRELL James**<br>*Structural insights on the mechanism of the electron-bifurcating [FeFe] hydrogenase from Thermotoga maritima* | **OC48 SANTOS Joana**<br>*Mitochondria-targeted Radiocomplexes for Auger Electron Therapy of Cancer* |
| 12h00 - 12h20 | **OC40 SILAGHI-DUMITRESCU Radu**<br>*Old dogs, old tricks, new glasses: hydrogen peroxide, cobalamin and others* | **OC44 FOURMOND Vincent**<br>*Exploring the reactivity of CO dehydrogenases* | **OC49 VAZQUEZ LOPEZ Miguel**<br>*Selective Cleavage of DNA Replication Foci in Cell Nuclei by Peptide Helicates* |
| | **FREE AFTERNOON - ACTIVITIES AROUND GRENOBLE** | | |
| 19h30 | **GALA DINER**<br>**Stade des Alpes**<br>Boulevard Jean Pain 38000 Grenoble<br>Tram station "Grenoble Hôtel de Ville" | | |

# Thursday - 21 July

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| **8h30 - 9h20** | **PL6 - Gerard ROELFES**<br>**Artificial Metalloenzymes going Live**<br>***Room A - Chair Thomas WARD*** | | |
| | **Session 1 - Room B** | **Session 2 - Room C** | **Session 3 - Room D** |
| | ***Chair Luca RONCONI*** | ***Chair Dinorah GAMBINO*** | ***Chair Philip ASH*** |
| **9:30 - 10:00** | **KN30 PIKRAMENOU Zoe** | **KN32 SUMAN Sigridur** | **KN35 LEPOUL Nicolas** |
| | *Luminescent Nanoparticles in detection and triggered drug release* | *Molybdenum Complexes as Catalytic Cyanide Antagonists: Bicompatibility, Intracellular Distribution and Mechanism.* | *Electrochemical and spectroelectrochemical approaches for the characterization of transient copper-oxygen models of oxygenases* |
| 10:00 - 10:20 | **OC50 BODIO Ewen** | **OC55 PIZZARO Ana** | **OC59 GUIGLIARELLI Bruno** |
| | *Aza-BODIPY and metal, a winning association for multimodal imaging and theranostics* | *Potent Tethered Osmium(II) Half-Sandwich Anticancer Agents Bearing Phenylpyridine* | *Deciphering the Metal Ion Environment in Formate Dehydrogenases: Insights from EPR, Isotopic Enrichment and DFT Calculations in a Tungsten and Selenium Dependent Enzyme* |
| 10:20 - 10h40 | **OC51 MOLLOY Jennifer** | **OC56 ENYEDY Eva** | **OC60 GHATTAS Wadih** |
| | *Design and synthesis of a multitopic pro radical probe for the detection of oxidative stress* | *Water-soluble 8-hydroxyquinoline-amino acid hybrids and their interaction with various metal ions: relationship between solution chemistry and cytotoxicity* | *Artificial metalloenzymes for in vitro and in vivo catalysis* |
| **10h40-11h10** | **Coffee Break** | | |
| | **Session 1 - Room B** | **Session 2 - Room C** | **Session 3 - Room D** |
| | ***Chair Olivier BERTEAU*** | ***Chair Attila JANCSO*** | ***Chair Frédéric AVENIER*** |
| 11h10 - 11h40 | **KN31 CIOFI BAFFONI Simone** | **KN33 GUMIENNA-KONTECKA Elzbieta** | **KN36 SHOJI Osami** |
| | *The intriguing puzzle of iron-sulfur protein biogenesis* | *Inspired by siderophores: from structural probes of ferric ions assimilation to Ga-68/Zr-89 nuclear imaging* | *Hydroxylation of Nonnative Substrates by Wild-type Cytochrome P450BM3 with Decoy Molecules* |
| 11h40 - 12h00 | **OC52 MOUGEL Victor** | **OC57 MICHAUD-SORET Isabelle** | **OC61 HAGEDOORN Peter-Leon** |
| | *Iron-sulfur clusters: synthetic challenges and applications to catalysis* | *Is the iron homeostasis under the control of an iron-sulfur cluster in Fur?* | *Unique Biradical Intermediate in the Mechanism of the Heme Enzyme Chlorite Dismutase discovered using microsecond timescale freeze hyperquench* |
| 12h00 - 12h20 | **OC53 CUTSAIL George** | **OC58 RODRIGUEZ MACIA Patricia** | **OC62 GYURCSIK Béla** |
| | *Stabilization of Intermediate Spin-States in Mixed-valent Diiron Dichalcogenide Complexes* | *How accessory iron-sulfur clusters influence catalytic bias, O2 tolerance and overpotential in [FeFe] hydrogenases* | *Interplay of multiple metal ion binding sites regulates the catalytic activity of metalloenzymes* |
| 12h20 - 12h50 | **OC54 DECAMPS Laure** | **KN34 SCHALK Isabelle** | **KN37 TRON Thierry** |
| | *Nitrogenase P-cluster biosynthesis: unraveling the role of NifW with spectroscopy* | *Cancelled* | *Hybrid catalysis and Multi-Copper oxidases* |
| **12h50 - 14h30** | **LUNCH** | | |
| **14h30 - 15h20** | ***Room A - Chair Stéphane MENAGE***<br>**PL7 Marc FONTECAVE**<br>*From $CO_2$ to fuels: bioinspired metal catalysts* | | |
| **15h20 - 15h50** | ***Room A - Chair Eva FREISINGER***<br>**EUROBIC Medal 2022 - Maxie ROESSLER**<br>*Controlling and exploiting intrisic unpaired electrons in metalloproteins* | | |
| **15h50 - 16h20** | **Closing Ceremony - Eurobic Awards**<br>**Chairs : Carole DUBOC - Stéphane MENAGE** | | |
| **16h20 - 17h00** | **Coffee Break** | | |

# Coordination preferences of Shiff base ligands with transition metals: DFT study

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The chemistry of the first-row transition metals is highly diverse, with a multitude of different reactivity and property patterns. This richness results from a wide range of ligands and coordination flexibility around the central metal ion. Still, it results from the partial occupation of the metal d-orbitals, which leads to different oxidation and spin states.[1] For the past years, our research has focused on investigating transition metal complexes with hydrazone-based ligands and studying their catalytic[2], magnetic[3], and biological activities.[4] We have studied a series of tridentate NNO/NNS and pentadentate NNNOO/NNNSS ligands obtained by condensation reactions of 2-acetylpyridine, 2-quinolinecarboxaldehyde, 2-acetylthiazole, or 2,6-diacetylpyridine and Girard's reagents (N-substituted glycine hydrazides) or thiosemicarbazide, and their mono- and binuclear complexes with various transition metal ions ($Fe^{2+}$, $Fe^{3+}$, $Co^{2+}$, $Co^{3+}$, $Ni^{2+}$, $Cu^{2+}$).

To rationalize coordination preferences of the ligands to form mono- or binuclear complexes and coordinate differently, together with the electronic structure of transition metal ions, we performed Density Functional Theory (DFT) calculations accompanied by the Energy Decomposition Analysis and Ligand Field Theory. The results explain the different ways of ligand binding and how the electronic structure of the central metal ion and the spin state affect the coordination pattern. Our results pave the way for the rational design of transition-metal complexes.

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[1] M. Zlatar, M Gruden in *Practical Approaches to Biological Inorganic Chemistry, 2nd Edition*, **2020**, 17-67
[2] M. Milenković, A. T. Papastavrou, D. Radanović, A. Pevec, Z. Jagličić, M. Zlatar, M. Gruden, G. C. Vougioukalakis, I. Turel, K. Anđelković, B. Čobeljić, *Polyhedron*, **2019**, *165*, 22-30.
[3] D. Darmanović, I. N. Shcherbakov, C. Duboc, V. Spasojević, D. Hanžel, K. Anđelković, D. Radanović, I. Turel, M. Milenković, M. Gruden, B. Čobeljić, M. Zlatar, *The Journal of Physical Chemistry C*, **2019**, *123*, 31142-31155.
[4] N. Stevanović, M. Zlatar, I. Novaković, A. Pevec, D. Radanović, I. Matić, M. Đorđić Crnogorac, T. Stanojković, M. Vujčić, M. Gruden, D. Sladić, K. Anđelković, I. Turel, B. Čobeljić *Dalton Transactions*, **2022**, *51*, 185-196.