Dalton 2023
18-20 April 2023, Coventry, UK

OVERVIEW PROGRAMME

Tuesday 18 April 2023

	Registration				
11:30	**Chairs' welcome (OC1.05 Lecture Theatre)**				
11:30	**AWARD LECTURE (AL1) -** Session Chair: Sam de Visser (OC1.05 Lecture Theatre) **Texas-inspired metallodrug discovery efforts** Jonathan Sessler, The University of Texas at Austin, USA				
12:15	**PLENARY (PL1) -** Session Chair: David Liptrot (OC1.05 Lecture Theatre) **The new chemistry of old PN cages** Saurabh Chitnis, Dalhousie University, Canada				
13:00	**Lunch - Rootes Restaurant**				
Theme	**Inorganic Biochemistry**	**Inorganic Reaction Mechanisms**	**Coordination and Organometallic Chemistry**	**Main Group Chemistry**	**Sustainability**
Room	**Faculty of Arts Bldg, 0.08 (Ground floor)**	**Faculty of Arts Bldg, 0.03 (Ground floor)**	**OC1.05 (1st floor)**	**OCO.04 (Ground floor)**	**OCO.02 (Ground Floor)**
Session chair	Luisa Ciano	Ian Fairlamb	Richard Layfield	Cath Weetman	Matthias Stein
14:00	**Exquisite fine-tuning of the active-site electronic structure in [FeFe] hydrogenases** James Birrell, Univeristy of Essex, UK (OA1)	**Oxidative dehalogenation of halophenols by high-valent nonheme Iron(IV)-Oxo intermediates** CV Sastri, Indian Institute of Technology Guwahati, India (OB1)		**Probing the Active Encounter Complex in Frustrated Lewis Pair Chemistry** Andrew Jupp, University of Birmingham, UK (OD1)	
14:15	**Concerted or sequential: Time-resolved methods to probe proton coupled electron transfer in [NiFe] hydogenases** Dmitry Sedush, University of Leicester, UK (OA2)	**Using parametrised descriptor-outcome modelling and in-situ FTIR to gain mechanistic insight to the Pauson-Khand reaction** Theo Tanner, University of York, UK (OB2)	**Coaxing Cobalt With 'PNP' Ligands** Adam Carrick, Durham University, UK (OC2)	**A Zintl Cluster for Transition Metal-Free Catalysis: C=O Bond Reductions** Bono van Ijzendoorn, University of Manchester, UK (OD2)	**Controlled biocatalytic synthesis of metal nanoparticle-enzyme hybrids: demonstration for catalytic hydrogen-driven NADH or flavin recycling** Lucy Browne, University of Oxford, UK (OE1)
14:30	**An electrochemical flow cell allows in situ X-ray spectroscopy of sensitive metalloproteins** Rufus Frew, University of Leicester, UK (OA3)	**Intemolecular primary C-H oxidation catalyzed by bioinspired manganese catalyst** Siu-Chung Chan, Universitat de Girona, Spain (OB3)	**Coordination chemistry of WSCl4 and WSeCl4 with the development of precursors for WE2 thin film deposition** Victoria Greenacre, University of Southampton, UK (OC3)	**Activation Modes of Boron Lewis Acid Catalysts with Nitrogen-Containing Substrates** Yara van Ingen, Cardiff University, UK (OD3)	**Asymmetric transfer hydrogenation of ketones using ruthenium(II) complexes** Martin Wills, University of Warwick, UK (OE2)
14:45	**Using in situ spectroscopic methods to study the electron relay and active site interplay in [FeFe] hydrogenases** Zehui Duan, University of Oxford, UK (OA4)	**Investigating the mechanism and origins of selectivity in palladium-catalysed carbene insertion cross-coupling reactions** Paul Dingwall, Queen's University Belfast, UK (OB4)	**Copper(I) boryl anions supported by ring-expanded N-heterocyclic carbenes: breaking the cycle** David Liptrot, University of Bath, UK (OC4)	**Designing Highly Electronically Tuneable FLPs** Aisling Ropers, University of Oxford, UK (OD4)	**Borates versus aluminates: electrolyte salts for sodium-ion batteries** Darren Ould, University of Cambridge, UK (OE3)
15:00	**Unravelling the reaction mechanism of ortho-hydroxylation of phenolic substrates by coupled-binuclear copper enzyme tyrosinase (Ty)** Agnieszka Stańczak, Czech Academy of Sciences, Czech Republic (OA5)	**Investigating the role of magic size clusters in the growth of InP quantum dots** Theodore Gazis, Keele University, UK (OB5)	**Design of High-relaxivity MRI nanoprobes for multimodal imaging** Thomas Price, King's College London, UK (OC5)	**Planar Bismuth Triamides: A Tunable Platform for Main Group Lewis Acidity and Polymerization Catalysis** Tyler Hannah, Dalhousie University, Canada (OD5)	**Homogeneous (De)hydrogenative Catalysis for A Circular Economy** Amit Kumar, University of St Andrews, UK (OE4)
15:15	**Heme Oxygenase-1 (HO-1) activity in human-derived macrophages with an aminocoumarin-porphyrin FRET 'break-apart' probe** Saul Cooper, Imperial College London, UK (OA6)	**Mechanisms of the reactivity of N-heterocyclic carbene supported copper(I) tetranides** Rex Charman, University of Bath, UK (OB6)	**A New Vision for the Electronic and Molecular Structures of Inorganic Molecules** Robert Deeth, University of Warwick, UK (OC6)	**Weakly coordinating chiral anions** Richard Collins, Imperial College London, UK (OD6)	**Mechanistic insights of metal oxide mediated photocatalytic and photoelectrochemical C-C coupling using visible light** Richard Douthwaite, University of York, UK (OE5)
15:30	**Refreshments**				
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Session chair	Justin Bradley	Aidan McDonald	Adrian Chapman	Andrew Jupp	Georgia Orton
16:00	**'Turn On' lanthanide fluorescent probes for imaging in hypoxic environments** Charlie Sims, Oxford University, UK (OA7)	**Understanding reactions of nickel(0) relevant to cross-coupling catalysis** David Nelson, University of Strathclyde, UK (OB7)	**Electrochemically Switched 2nd Order Non-Linear Optical Responses in Arylimido-Polyoxometalate Derivatives** Bethany Hood, University of East Anglia, UK (OC7)	**Exploring the Chemistry of the Cyaphide Ion** Eric Yang, University of Oxford, UK (OD7)	**N-heterocyclic Phosphines as Pre-catalysts for the Selective Degradation of Poly(lactic acid)** Laura English, University of Bath, UK (OE8)
16:15	**Quantum dots for targeted multimodal MRI/NIR fluorescence imaging of glioblastoma** Kanik Chelani, King's College London, UK (OA8)		**Enhancing the Air Stability of Dimolybdenum Paddlewheel Complexes: Redox Tuning through Fluorine Substituents** Luke Wilkinson, University of York, UK (OC8)	**Phosphabora-[3]Dendralenes: The Next Polycyclic Precursors** Vesela Zarkina, University of Edinburgh, UK (OD8)	**Automating Inorganic Chemistry** Nicola Bell, University of Glasgow, UK (OE9)
16:30	**Versatile diphosphine platforms for molecular radiopharmaceuticals based on technetium 99m and rhenium 188** Michelle Ma, King's College London, UK (OA9)	**Shining a new light on photoredox catalysis** Daniel Scott, University of Bath, UK (OB25)	**Germole-ligated Organometallic Lanthanide Single-Molecule Magnets** Siddhartha De, University of Sussex, UK (OC9)	**Main group gallyl and gallylene complexes: gallane dehydrogenation, "redox" isomerisation, and small molecule activation** Louis Morris, University of Oxford, UK (OD9)	**Tris(β-ketoiminate) AlIII Compounds as Aluminium Oxide Precursors** Erica Faria, University College London, UK (OE11)
16:45	**Diphosphine bioconjugates via Pt(0)-catalysed hydrophosphination – a versatile chelator platform for Tc-99m and Re-188 radiolabelling of biomolecules** Rachel Nuttall, King's College London, UK (OA10)	**Catalyst speciation and deactivation in the Ru-mediated meyer-schuster rearrangement of ethynyl-β-ionol for vitamin A production** Asad Saib, University of Bath, UK (OB10)	**How to make substituted pentalenide ligands less exotic** Niko Jenek, University of Bath, UK (OC10)	**Reaction of Zn–H bonds with Transition Metal(I) fragments** Marina Perez Jimenez, Imperial College London, UK (OD10)	**Bn2DT3A complexes with Ga-68 and Cu-64 for application in PET – radiolabelling and biological evaluation** Veronika Rosecker, King's College London, UK (OE12)

17:00	**Functional and structural diversity in thiosemicarbazone complexes and related fluorescent and radiolabelled molecules** Sofia Pascu, University of Bath, UK (OA11)	**Computational Studies on the Mechanistic Diversity of Rhodium- and Iridium-Catalysed Amine-Borane Dehydropolymerisation** Lia Sotorrios, Heriot-Watt University, UK (OB11)	**Synthesis of 3d transition metal(II) bis-phospholyl complexes and reduction to phosphametallocene anions** Corentin Magnoux, University of Manchester, UK (OC11)	**Identity of Group 1 Metal in Stabilisation of Reduced Mg-Diamide** Han-Ying Liu, University of Bath, UK (OD11)	**How to Publish with Impact.** Sally Howells, Executive Editor, Royal Society of Chemsitry, UK (OE21)
17:15		**A combined Heterogeneously/Homogeneously Catalysed Approach to the Direct Hydrogenation of Captured Carbon Dioxide** Matthew Quesne, Cardiff University, UK (OB12)	**Properties and Applications of Gold Complexes with Multifunctional L-Shaped N-Heterocyclic Carbenes** Paul Davies, University of Birmingham, UK (OC12)	**Structure and Electronics of Symmetrically Diboron-Doped Acenes – From 1,4-Diboranaphtalene to 6,13-Diborapentacene** Merle Arrowsmith, Universität Würzburg, Germany (OD12)	
17:30-18:00	**Committee meeting IBDG**	**Committee meeting IRMG**	**Committee meeting CODG**	**Committee meeting MGDG**	
17:30	**Dinner - Rootes Resturant**				
19:00	**Poster session with drinks reception (Oculus Building)**				
22:00	**Close**				

Wednesday 19 April 2023

09:00	**PLENARY (PL2) -** Session Chair: Kylie Vincent (OC1.05 Lecture Theatre) **Monitoring of electrocatalytic reactions** Jana Roithova, Radboud University Nijmegen, Netherlands				
09:45	**AWARD LECTURE (AL2) -** Session Chair: John Fielden (OC1.05 Lecture Theatre) **Oxidative addition and multiple bonds in aluminium chemistry** Michael Cowley, University of Edinburgh, UK				
10:30	**Refreshments**				
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Session chair	Philip Ash	James Walton	Nicola Bell	Michael Cowley	Darren Willcox
11:00	**Semi-synthetic and artificial metalloenzymes for energy conversion: from catalytic insight to catalyst design** Patricia Rodriguez-Macia, University of Oxford, UK (OA13)	**Exploiting Cobalt(II) Amide Complexes in Deprotonative Metalation of Fluoroaromatic Molecules** Alessandra Logallo, University of Bern, Switzerland (OB13)	**Probing the donor strength of Yldiide ligands: synthesis, structure and reactivity of rhodium complexes with a PCylideN pincer ligand** Sébastien Lapointe, Ruhr-Universitat Bochum, Germany (OC13)	**C–H bond activation and higher-order cycloaddition reactions between polyolefins and a dinuclear main-group ambiphile** Robert Kretschmer, Chemnitz University of Technology, Germany (OD13)	**Influence of equatorial ligand fields on magnetic relaxation pathways of dysprosocenium cations** Sophie Corner, University of Manchester, UK (OE13)
11:15		**High-valent metal-halides for hydrocarbon oxidation and halogenation** Aidan McDonald, Trinity College Dublin, Ireland (OB14)	**Imido-Functionalised Polyoxometalates for Photonics** Claire Jones, University of East Anglia, UK (OC14)	**A Quantum Chemical Study of Base-Coordinated Dialumenes** Keelan Byrne, Maynooth University, Ireland (OD14)	**Synthesis and Reactivity of Lanthanide(II) Hydrides** Georgia Richardson, Victoria University of Wellington, New Zealand (OE14)
11:30	**Cooperative Chemobio-Catalysts for Hydrogenation Reactions** Tim Sudmeier, University of Oxford, UK (OA15)	**Computational Design of a Heterogeneous Catalyst for Efficient Dehydrogenation of Alcohols: A Pincer-based Metal-Organic Framework** Bengt Tegner, University of Liverpool, UK (OB15)	**Self-Assembly of Benzimidazole Derived NHC Ligands and Coinage ions (AgI, CuI, AuI) to Organometallic Cages and Their Unusual Transmetalation Chemistry** Rajeev Nishad, King's College London, UK (OC16)	**Synthesis and Reactivity of the Indyl Anion** Tylah Sweet, Victoria University of Wellington, New Zealand (OD15)	**Adventures in alkaline earth and rare earth chemistry: ligand design, catalysis and low-oxidation state chemistry** Fabrizio Ortu, University of Leicester, UK (OE15)
11:45	**Electronic structure and bonding in heterometallic clusters** Daniel Wilson, King's College London, UK (OA16)	**From cradle to grave – a combined kinetic, mechanistic and structural study of palladacycles in Suzuki-Miyaura reactions** David Husbands, University of York, UK (OB16)	**Sequential Molecular Surface Modification of Cuprous Oxide Nanoparticles by Organometallic Reactivity** Bradley Cowie, University of Oxford, UK (OC17)	**An Acyclic Aluminyl Anion** Ross Jackson, University of Bath, UK (OD16)	**Computational Mechanistic Studies on Iron-Catalysed Dehydrogenation of Amines Involving Cyclopentadienone Iron Complexes.** Joannes Peters, Stockholm University, Sweden (OE16)
12:00	**Exploring the Design of Copper Artificial Metalloenzymes** Eva Klemencic, University of Edinburgh, UK (OA17)	**Hydrogen peroxide reduction to dioxygen on a nonheme iron centre. A computational study** Henrik Wong, University of Manchester, UK (OB17)		**Synthesis and Reactivity of a Homoleptic Magnesium Bis-Aluminyl** Liam Griffin, University of Oxford, UK (OD17)	**Making science greener: Community perspectives & solutions** Clare Dyer-Smith, Royal Society of Chemisty, UK (OE17)
12:15	**Lunch - Rootes Restaurant**				
13:45	**SUSTAINABILITY -** Session Chair: Uli Hintermair (OC1.05 Lecture Theatre) **Activation of Small Molecules: Can Boron act as a Transition Metal?** Holger Braunschweig, Universität Würzburg, Germany				
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Session chair	Anna Peacock	CV Sastri	Maxie Roessler	Robert Kretschmer	John Slattery
14:30	**How universal is the role of tyrosine in oxygen activation by ferritin?** Justin Bradley, University of East Anglia, UK (OA18)	**Synthesis, Size Effects and Photoredox Reactivity of Metal-oxo Clusters** Sebastian Pike, University of Warwick, UK (OB18)	**sigma-Aromatic Metal-Metal Bonding in Molecular Actinide Chemistry** Steve Liddle, University of Manchester, UK (OC18)	**Development of Main Group NHC complexes for stabilisation of Low-Oxidation State Group 2 and 13 elements** Catherine Weetman, University of Strathclyde, UK (OD18)	**Flame retardant Phosphonate-functionalised Poly(propylene)s** Alex Evans, University of Oxford, UK (OE18)
14:45	**Iron Oxidation and Detoxification in Human Mitochondrial Ferritin** Zinnia Bugg, University of East Anglia, UK (OA19)		**In-Crystallo Lattice Adaptivity Triggered by Solid/Gas Reactions of Group 7 Cationic Pincer Complexes** Joe Goodall, University of York, UK (OC19)	**Structural and dimensional control of porphyrin capsules using group 15 tris(3-pyridyl) linkers** Álvaro García-Romero, Universidad de Valladolid, Spain (OD19)	**Probing the Speciation and Electronic Structure of Organozinc Reagents using X-ray Spectroscopy** Lewis Parker, University of Reading, UK (OE19)

15:00	**Stabilisation of the RirA [4Fe-4S] cluster results in loss of iron-sensing function** Elizabeth Gray, University of East Anglia, UK (OA20)	**Mechanistic investigations of CO homologation in iron terphenyl complexes** Nathan Coles, University of Nottingham, UK (OB20)	**Synthesis, magnetic properties, and reactivity of lanthanide complexes featuring bulky silylamide ligands** Jack Emerson-King, University of Manchester, UK (OC20)	**Comparing carbon disulfide activation reactions of Terphenyl-stabilized potassium phosphides and potassium phosphinophosphides** Lilian Sophie Szych, University of Oxford, UK (OD20)	**Small molecule activation with titanium 'POCOP' pincer complexes** Leah Webster, Imperial College London, UK (OE20)
15:15	**Consequences of fatty acid-mediated changes in blood plasma zinc speciation** Sirilata Polepalli, University of Warwick, UK (OA21)	**SNAr Reactions of [(η6 arene)RuCp]+ Complexes and Catalysis Via Arene Exchange** James Walton, Durham University, UK (OB21)	**Non-Covalent Interactions in Organic and Organometallic Crystals** Matthias Stein, Max Planck Institute for Dynamics of Complex Technical Systems, Germany (OC21)	**Li vs Na: Divergent Reaction Patterns between Organo–Lithium and –Sodium Complexes, and Ligand-catalysed Ketone/Aldehyde Methylenation** Nathan Davison, Newcastle University, UK (OD21)	
15:30	**Refreshments**				
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Session chair	Patricia Rodriguez-Macia	David Nelson	Anbu Sellamuthu	Meera Mehta	Amit Kumar
16:00	**Coiled coils as ligands for inclusion in the inorganic chemist's toolbox** Anna Peacock, University of Birmingham, UK (OA22)	**Investigating the effects of Pd speciation on cross-coupling reactions** Neil Scott, University of York, UK (OB22)	**Valence Electron Configurational Isomerism in the f-block** Conrad Goodwin, University of Manchester, UK (OC22)	**Room-Temperature Stable Electride (RoSE): Synthesis, Structure, Reactivity** Erli Lu, Newcastle University, UK (OD22)	**Towards New and Improved Pressure Sensitive Paint Formulations for Aerodynamic Measurements** Elliott Nunn, Univeristy of Manchester, UK (OE22)
16:15	**Generating Evolvable, Artificial Metalloenzymes Containing Organometallic Cofactors via Ligand Exchange** Oskar James Klein, University of Cambridge, UK (OA23)	**Oxazolidinones vs. Piperazines: The temperature dependant conundrum for the cycloaddition of aziridines and CO2** Ryan Lewis, Sheffield Hallam University, UK (OB23)	**Coordination and activation of germanes by ruthenium diphosphine complexes** Aswin Chandran, Laboratoire de chimie de coordination - LCC-CNRS, France (OC23)	**Tailoring sodium organometallic reagents for arene functionalisation** Andreu Tortajada Navarro, University of Bern, Switzerland (OD23)	**Group 10 Heteromettallic Hydride Complexes: Hexagonal Planar Geometries and Hydrogen Activation** Andreas Phanopoulos, Imperial College London, UK (OE24)
16:30	**Histidine-Rich C-terminus of mycobacterial GroEL1 and its Copper Complex – the Impact of Point Mutations** Anna Rola, University of Wrocław, Poland (OA24)	**Stability and C–H bond activation reactions of palladium(I) and platinum(I) metalloradicals** Adrian Chaplin, University of Warwick, UK (OB24)	**Unsubstituted trispyrazolylborate lanthanide complexes: reduction to Ln(II), and synthetic routes to radical-bridged heterobimetallics** Tajrian Chowdhury, University of Glasgow, UK (OC24)	**A Blueprint for the Synthesis of Low-Valent Alkaline Earth Metal Complexes** Alex Bowles, University of Leicester.UK (OD24)	
16:45	**AWARD LECTURE (AL3) -** Session Chair: Nick Le Brun (OC1.05 Lecture Theatre) **Oxygen-Sensing Enzymes in Plants and Animals** Emily Flashman, University of Oxford, UK				
17:30	**PLENARY (PL3) -** Session Chair: Joseph Wright (OC1.05 Lecture Theatre) **Making supramolecular assemblies that could be used in quantum information processing** Richard Winpenny, University of Manchester, UK				
18:15	Close				
19:00	**Conference dinner - Panorama Suite (Rootes Building)**				

Thursday 20 April 2023

09:00	**PLENARY (PL4) -** Session Chair: Claudia Blindauer (OC1.05 Lecture Theatre) **Mechanistic insights into bio- and electro-catalytic reactions from EPR spectroscopy** Maxie Roessler, Imperial College London, UK				
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Session chair	Isolda Romero-Canelon	Amanda Jarvis	Gill Reid	Erli Lu	Sebastian Pike
09:45	**Bacterial metallopeptidases as medicinal targets – coordination chemistry of possible metal-based inhibition** Paulina Potok, University of Wroclaw, Poland (OA25)	**A fluorspar alternative? - journey towards a terminal calcium monofluoride** Mathias Ellwanger, University of Oxford, UK (OB9)	**18F-labelling via halide exchange reactions on main group and transition metal based-chelates for PET applications** Danielle Runacres, University of Southampton, UK (OC25)	**Inducing nucleophilic reactivity at beryllium with an aluminyl ligand** Josef Boronski, University of Oxford, UK (OD25)	**Synthesis of new gold(I) complexes containing an ortho-trifluoromethylphenyl phosphine. Hydroamination catalysis.** Itxaso Bustos, University of the Basque Country, Spain (OE25)
10:00	**The structural activity and anion impact of quinolinyl Ag(I) complexes: molecular docking, in vitro biological studies and their interactions with biomolecules** Adesola Abimbola Adeleke, Olabisi Onabanjo University Ago-Iwoye, Nigeria (OA26)	**The Importance of Water in Homogeneous Ruthenium Catalysed Aerobic Olefin Epoxidation** Mark Muldoon, Queen's University of Belfast, UK (OB26)	**Cobalt Schiff-Base Complexes as Catalysts for Multi-electron Reductions** John Fielden, Lancaster University, UK (OC26)	**Beryllium-centred C-H Activation of Benzene** Kyle Pearce, University of Bath, UK (OD26)	**Synthetic Iron Chemistry with Z-type Ligands** Laura Grose, University of Manchester, UK (OE26)
10:15	**Exploring the antimicrobial activity of cobalt(II) picolinamide complexes** Rianne Lord, University of East Anglia (OA27)	**Unveiling Structure-Property Correlations in Alkali-Metal Nickelates** Andryj Borys, Universität Bern, Switzerland (OB27)	**Recent Adventures in Lanthanide and Actinide Silicon Chemistry** David Mills, University of Manchester, UK (OC27)	**Reactivity of Tetrel Functionalised Heptapnictogen Clusters Towards Heteroallenes** William Jobbins, University of Manchester, UK (OD27)	**Ta/Ir Heterobimetallics Supported on Mesoporous Silica Surface for C–H Bond Activation** Rosalyn Falconer, University of British Columbia, Canada (OE27)
10:30	**Biological evaluation of homoleptic bimetallic silver(I) N-heterocyclic carbene complexes** Oliver King, University of East Anglia (OA28)	**Vinylic C–H activation of styrenes by an iron–aluminium complex** Nikolaus Gorgas, Imperial College London, UK (OB28)	**Exploring the chemistry of super-reduced uranium organometallics** Luciano Barluzzi, University of Sussex, UK (OC28)	**Exploring the Insertion Chemistry of Silyl Substituted Metalylenes** Lewis Wales, University of Oxford, UK (OD28)	**Formation, Characterisation and Disassembly of Metallosupramolecular Complexes in vacuo** Niklas Geue, Manchester Institute of Biotechnology, UK (OE28)
10:45	**Refreshments**				
11:10	**AWARD LECTURE (AL4) -** Session Chair: TBC (OC1.05 Lecture Theatre) **Sequential carbon monoxide homologation with transition metal carbonyls and an aluminium (I) reductant** Richard Kong, Cornell University, USA				
11:55	**Closing remarks from Conference Organisers**				