

Dalton 2023
18-20 April 2023, Coventry, UK

OVERVIEW PROGRAMME

Tuesday 18 April 2023

Registration					
Chairs' welcome (OC1.05 Lecture Theatre)					
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					
PLENARY (PL1) - Session Chair: David Liprott (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	OC1.04 (1st floor)	OC1.06 (1st 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, University 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] hydrogenases 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)	Intermolecular primary C-H oxidation catalyzed by bioinspired manganese catalyst Siu-Chung Chan, Universitat de Girona, Spain (OB3)	Coordination chemistry of WSeC4 and WSeC4 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 Liprott, 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 Stańca, 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)	A fluorospar alternative? - journey towards a terminal calcium monofluoride Mathias Ellwanger, University of Oxford, UK (OB9)	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)	Catalyst speciation and deactivation in the Ru-mediated meyer-schuster rearrangement of ethynyl-β-iodol for vitamin A production Asad Saib, University of Bath, UK (OB10)	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)		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 phosphametalloene 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 Chemistry, 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-Diboraphthalene to 6,13-Diborapentacene Merle Arrowsmith, Universität Würzburg, Germany (DD12)		
17:30-18:00	Committee meeting IBDG	Committee meeting IRMG	Committee meeting CODG	Committee meeting MGDG	
17:30	Dinner - Rootes Restaurant				
19:00	Poster session with drinks reception (Oculus Building)				
22:00	Close				

Wednesday 19 April 2023

09:00	PLENARY (PL2) - Session Chair: Kyle Vincent (OC1.05 Lecture Theatre) Monitoring of electrocatalytic reactions Jana Rothova, 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 Yttride ligands: synthesis, structure and reactivity of rhodium complexes with a PCy2N pincer ligand Sébastien Lapointe, Ruhr-Universität 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 dysprosium 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(III) 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 (Ag, Cu, Au) 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 Alumanyl 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-Alumanyl Liam Griffin, University of Oxford, UK (OD17)	Making science greener: Community perspectives & solutions Clare Dyer-Smith, Royal Society of Chemistry, UK (OE17)
12:15	Lunch - Rootes Restaurant				
13:45	SUSTAINABILITY - Session Chair: Uli Hintermaier (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 Sastry	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 R4R'4 [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 Sirlata Polepalli, University of Warwick, UK (OA21)	SNAr Reactions of [(η ⁶ 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 Methylation 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 Erlu Lu, Newcastle University, UK (OD22)	Towards New and Improved Pressure Sensitive Paint Formulations for Aerodynamic Measurements Elliott Nunn, University 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 CO ₂ 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 Heterometallic 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 Wroclaw, 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	Erlu Lu	Sebastian Pike
09:45	Bacterial metalloproteases as medicinal targets – coordination chemistry of possible metal-based inhibition Paulina Potok, University of Wroclaw, Poland (OA25)	Shining a new light on photoredox catalysis Daniel Scott, University of Bath, UK (OB25)	¹⁸ F-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(II) 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 Andry Borys, Universität Bern, Switzerland (OB27)	Recent Adventures in Lanthanide and Actinide Silicon Chemistry David Mills, University of Manchester, UK (OC27)	Reactivity of Tretrel 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)	Vinyllic 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 Metallyenes Lewis Wales, University of Oxford, UK (OD28)	Formation, Characterisation and Disassembly of Metallousupramolecular 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				