



Indaba 8

Serendipity vs Prediction

16 - 21 August 2015

Skukuza, Kruger National Park, South Africa

PROGRAMME

SUNDAY 16 August 2015		
Time	Event	
14:00- 17:00	Registration	Nombolo Mdhuli Conference Centre, Skukuza
17:00	Welcoming function	Game drive & bush braai (all delegates to convene at parking area in front of conference centre)
MONDAY 17 August 2015		
Time	Event/ Speaker	Title
07:30	Breakfast	Cattle Baron Restaurant
08:45-13:00	Morning Session Chair: TBA	
08:45	Opening	Andreas Roodt / IUCr/ ICSU
09:15	Alberto, Roger	Prediction in High Dilution 99mTc Chemistry - or Serendipity?
09:45	Schubert, Wulf-Dieter	Resolving Bacterial Infections in Atomic Detail
10:15	Tea/Coffee	Nombolo Mdhuli Conference Centre
11:00	Comba, Peter	Design, Optimization and Applications of an Efficient Platform for Targeted PET I89maging
11:30	Billing, David	From Quantum Well to Solar Cell: The Hybrid Perovskite Story
12:00	Fahrni, Christoph	Fluorescence Sensing of Biological Trace Metals
12:30	Kingsford-Adaboh, Robert	Refunctionalization of natural products for structural, antioxidant and in vitro antimicrobial SAR studies: Case study of alpinumisoflavones
13:00	Lunch	Nombolo Mdhuli Conference Centre
14:30	Sightseeing	Delegates using conference transport will leave from the conference centre: delegates with their own transport make their own arrangements:
18:30-21:30	Evening Session Chair: TBA	
18:30	Ott, Holger	Bruker presentation
18:45	Poster flash presentations	2 minutes (2-3 Slides) per presenter All presentations have to be loaded before 13:00
20:15	Poster Session	Snacks and drinks

TUESDAY 18 August 2015

Time	Event/ Speaker	Title
06:00	Sightseeing	Delegates using conference transport will leave from the conference centre: delegates with their own transport make their own arrangements
07:30	Breakfast	Cattle Baron Restaurant
08:45-13:00	Morning Session Chair: TBA	
08:45	Stalke, Dietmar	Lewis diagrams match charge density distribution – serendipity or predication?
09:15	Levendis, Demetrius	Crystallization is serendipity in action
09:45	Roodt, Andreas	Predicting a chemical process
10:15	Tea/Coffee	Nombolo Mdhuli Conference Centre
11:00	DeBeer, Serena	X-ray spectroscopic studies of biological dinitrogen reduction in molybdenum and vanadium nitrogenases
11:30	Koch, Klaus	What's in the ^{195}Pt and ^{103}Rh NMR Chemical Shift of deceptively 'simple' complexes of such precious metals? Unique intrinsic isotope effects in ^{195}Pt and ^{103}Rh NMR as "spectroscopic-fingerprints"
12:00	Nenwa, Justin	Nanochannelled silver-deficient oxalatochromate(III) salts with H_2O -guest molecules carrying protons
12:30	Munro, Orde	Gold(III) Macrocycles: Nucleotide-Specific Unconventional Catalytic Inhibitors of Human Topoisomerase I
13:00	Lunch	Nombolo Mdhuli Conference Centre
14:00	Sightseeing	Delegates using conference transport will leave from the conference centre: delegates with their own transport make their own arrangements
18:30	Dinner	Cattle Baron Restaurant
19:30 -21:45	Jan Boeyens Session Chair: Demi Levendis	
19:30	Boeyens, Jan	Wishful Thinking or Serendipity?
20:00	Fernandes, Manuel	Prediction and Serendipity: Cooperativity, Feedback Mechanisms, and Structure Annealing in Solid-State Reactions
21:00	Haynes, Delia	Framework materials based on organic components: from happy accident towards design

WEDNESDAY 19 August 2015

Time	Event/ Speaker	Title
06:00	Sightseeing	Delegates using conference transport will leave from the conference centre: delegates with their own transport make their own arrangements
07:30	Breakfast	Cattle Baron Restaurant
08:45-13:00	Morning Session Chair: TBA	
08:45	Bernhardt, Paul	An electrochemical perspective on Cu-catalysed atom transfer radical polymerisation
09:15	Thiel, Walter	Prediction vs: serendipity in computational chemistry
09:45	Sewell, Trevor (+15min Instruct)	The Mechanism of Amidases and Nitrilases
10:15	Tea/Coffee	Nombolo Mdhuli Conference Centre
11:00	Jensen, Vidar	In Silico Design of Homogeneous Catalysts
11:30	Shanmugam, Maheswaran	Switching the Sign of Magnetic Anisotropy in Tetrahedral Co(II) complexes
12:00	Yamashita, Masahiro	Frontier of Quantum Molecular Spintronics Based on Single-Molecule Magnets: Toward Green IT Innovation
12:30	Wendt, Ola	Unexpected molecular structure: careful observation paves the way for new reactivity in the organometallic chemistry of pincer complexes
13:00	Lunch	Nombolo Mdhuli Conference Centre
14:00	Sightseeing	Delegates using conference transport will leave from the conference centre: delegates with their own transport make their own arrangements
19:00	Dinner	Cattle Baron Restaurant

THURSDAY 20 August 2015

Time	Event/ Speaker	Title
06:00	Sightseeing	Delegates using conference transport will leave from the conference centre: delegates with their own transport make their own arrangements
07:30	Breakfast	Cattle Baron Restaurant
08:45-13:00	Morning Session Chair: TBA	
08:45	Neese, Frank	Understanding Single Molecule Magnets through a Combination of Experiment and Quantum Chemistry
09:15	Pace, Ron	Computational Chemical Studies of the Structure and Mechanism of the Water Oxidising Complex in Photosystem II
09:45	Dillen, Jan	The topology of the Ehrenfest force density revisited: A different perspective based on Slater-type orbitals
10:15	Tea/Coffee	Nombolo Mdhuli Conference Centre
11:00	Karsten Meyer	TBA
11:30	Esterhuysen, Catharine	Gold as hydrogen-bond acceptor
12:00	Krossing, Ingo	From Weakly Coordinating Anions to the Protoelectric Potential Map
12:30	Lemmerer, Andreas	Optical Heating and Crystallization Device – Fun with a CO ₂ Laser
13:00	Lunch	Nombolo Mdhuli Conference Centre
14:00-16:00	Afternoon Session Chair: TBA	
14:00	SAASTA	TBA
15:00	Hackert, Marvin	Surprising versatility within the 4-OT family of proteins
15:30	P Comba/ A Roodt	Concluding remarks
16:00	Sightseeing	Delegates using conference transport will leave from the conference centre: delegates with their own transport make their own arrangements
19:00	Farewell function	Boma next to restaurant

FRIDAY 21 August 2015

Time	Event	Title
07:30	Breakfast	Cattle Baron Restaurant
09:00	Departure	Delegates using conference transport will leave from the conference centre: delegates with their own transport make their own arrangements

POSTER PRESENTATIONS

Note: All Presenters have to do a 2 minute (2-3 Slides) 'flash' presentation on Monday evening preceding the formal Poster Session

Presenting Author	Title
Akerman, Matthew	Novel Metallodrugs: Targeted Chemotherapeutic Agents
Akpan, Ekemini	Synthesis and structural investigation of formamidine Zn(II) and Cu(I) complexes
Alexander, Orbett	Structure and Spectroscopic Correlation of M(Ox) ₃ complexes (M = Al, Ga, In, Eu: Ox = 8-hydroxyquinolate and derivatives thereof)
Antwi, Boniface	Investigation of the efficient conversion of photon energy to electricity by newly synthesized, well-ordered, low band gap semiconducting polymers:
Belay, Alebel	Synthesis and characterization of Nb(V) complexes with O,O' bidentate ligands:
Bezuidenhout, Charl	Pleochroism as a probe to monitor the solvent exchange process in a 1-D metal-organic framework with 1-D solvent accessible channels:
Bhikraj, Sandipa	Gold(III) Pseudomacrocyclic Bis(Pyrrrolide-Imine) Schiff Base Complexes: Potential Chemotherapeutic Agents
Chatturgoon, Teshica	An X-ray crystallographic and DFT study of bis(pyrrrolide-imine) nickel(II) Schiff base chelates
De Kock, Sunel	Gold anticancer prodrugs and their interactions with selenium and sulfur containing polypeptides
Dippenaar, Alwyn	Hydrate formation in pharmaceutically relevant salts
Duma, Nontokoza	Novel Isoquinolyl Amides: Structural and Spectroscopic Studies
Elmakki, Mohammed	Synthesis and characterisation of rhodium cupferrate and substituted cupferrate complexes:
Frei, Angelo	Multi-functional Re/ ^{99m} Tc-Cyclopentadienyl and Carbonyl Complexes for Theranostic Applications
Groenewald, Ferdi	Gold acting as Lewis base in the formation of hydrogen and halogen bonds
Hean, Duane	Structural Insights into the Rampant Polymorphism of an Isoniazid Derivative
Hill, Tania	The beginning of a multi-component crystal chemistry quest
Hunter, Leigh	Derivatised Phenanthroline Transition Metal Chelates: Targeted Chemotherapeutic Agents

Kerscher, Marion	Electrochemical properties of iron bispidine catalysts
Khorasani, Sanaz	Dynamic Reaction Pathways in the Single-Crystal-to-Single-Crystal Solid-State Diels-Alder Reaction of N,N'-bis(cyclobutylimino)-1,4-dithiin with 9-Vinylanthracene
Koen, Renier	Comparing tantalum and niobium: The β -diketone approach
Kpomah, Bridget	Synthesis, Characterization and Activity of Copper(II) Complex of 1, 10-Phanthroline with Isopropylideneamino)thiourea
Le Roex, Tanya	Formation and properties of some hydrogen-bonded frameworks based on organic components
Makgae, Ofentse	Morphogenic and polymorphic transition between calcite and hollow vaterite spheres in binary polar aprotic-protic solvent mixtures: The effect of the solvent ratio
Mnguni, Malitsatsi	The Search for Polymorphic Co-Crystals from Polymorphic Co-Formers:
Moodley, Desigan	Gold(III) DNA Intercalators: Targeted Chemotherapeutic Agents
O'Connor, James	Investigation of the potential porosity of various 1,2,3,5-dithiadiazolyl radicals:
Pretorius, Carla	Assembly of one-dimensional metal chains via metallophilic interactions using Rh(I) metal centres
Sayed, Amina	Solvent manipulation of N-methylacetamide inclusion compounds with a xanthenol host:
Schutte-Smith, Marietjie	A mechanistic study of rhenium (I) complexes: aqua vs methanol substitution:
Tanyi, Rogers	New pyrazole and its chelating aptitude towards some transition metal salts
Van Heerden, Dewald	Elucidating the mechanism responsible for anisotropic thermal expansion in a Metal-Organic Framework
Van Laeren, Laura	Investigation of Dithiadiazolyl Radical – Metalloporphyrin Complexes
Venter, Gerhard	Predicting the Strength and Character of Hydrogen Bonding in Imidazolium-based Ionic Liquids:
Viljoen, Johannes	Is Hafnium Zirconium's chemical twin?
Zacharias, Savannah	Characterization and dye sorption studies of iron(III) supramolecular gels