

PART 1

Conference details

Abstract for oral presentations

Registrants list

Conference of the Inorganic Chemistry Division

Royal Australian Chemical Institute

Inorganic and Organometallic Specialist Group

New Zealand Institute of Chemistry

4-8 February 2007
Wrest Point Convention Centre
Hobart Tasmania



IC
07



PROGRAM AND CONFERENCE PAPERS



WELCOME

Welcome to IC07, the 2007 Conference of the Inorganic Division of the Royal Australian Chemical Institute and the Inorganic and Organometallic Specialist Group of the New Zealand Institute of Chemistry.

An outstanding group of researchers have contributed plenary and other oral presentations to the meeting across a range of current themes in inorganic chemistry, together with a comprehensive array of poster presentations.

The conference is an opportunity to recognise outstanding contributions by Australian and New Zealand researchers, and to capture the research in progress by postgraduate students. In this regard, the Burrows and the D.R. Stranks Award sessions are highlights of the conference program.

We extend a particular welcome to international visitors, whose contributions will enrich the program, and we hope that you take the opportunity to network and build constructive cooperations with Australian and New Zealand inorganic chemists.

Enjoy your time in Tasmania.

Allan Canty and Michael Gardiner

ORGANISING COMMITTEE

Professor Allan Canty
University of Tasmania (Co-Chair)

Dr Michael Gardiner
University of Tasmania (Co-Chair, Treasurer and Secretary)

CONFERENCE ORGANISERS

Leishman Associates
113 Harrington Street, Hobart TAS 7000
Ph: (03) 6234 7844 Fax: (03) 6234 5958
Email: paula@leishman-associates.com.au
Website: www.leishman-associates.com.au

CONFERENCE INFORMATION

Registration Desk

The Registration Desk is located near the main entrance to the Convention Centre. Staff are there to assist you with any questions you may have regarding registration, attendance, accommodation or social functions.

REGISTRATION TIMES

Sunday February 4:	4.00pm – 8.30pm
Monday February 5:	8.00am – 5.00pm
Tuesday February 6:	8.00am – 5.00pm
Wednesday February 7:	8.00am – 2.00pm
Thursday February 8:	8.00am – 2.30pm

Accommodation

If you have any queries relating to your accommodation booking, please see the staff at the registration desk, or alternatively the staff at your hotel.

Your deposit has been transferred to the hotel you have selected – please confirm this on check in with your hotel. If you have arrived 24 hours later than your indicated arrival day you may find that you have forfeited your deposit.

Additional Tickets: Conference Social Program

The Welcome Reception ticket is included with full conference registration. If you have purchased additional tickets to the dinner or welcome function, these may be collected from the Registration Desk on arrival.

The Conference Dinner is an additional cost for all delegates. Please see the Registration Desk if you would like to purchase a ticket to the dinner and haven't already done so.

Conference Name Badges

All delegates will be provided with an identifying name badge, which also lets organisers know which events that you have elected to attend. **Please ensure that you wear your name tag at all times as it is required for access to conference events.**

Disclaimer

The ICO7 Conference reserves the right to amend or alter any advertised details relating to dates, program and speakers if necessary, without notice, as a result of circumstances beyond their control. All attempts have been made to keep any changes to an absolute minimum.

Entry to Conference Sessions

It is suggested that delegates arrive at preferred sessions promptly to ensure a seat.

Mobile Phones and Pagers

As a courtesy to other delegates, please ensure that all mobile phones and pagers are turned off or in silent mode during all sessions.

Photographs, videos, recording of sessions

Delegates are not permitted to use any type of camera or recording device at any of the sessions unless written permission has been obtained from the relevant speaker.

Special Diets

Wrest Point and the Henry Jones have been advised of any special diet preferences you have indicated on your registration form. Please identify yourself to catering staff at each venue - they will be happy to assist you to obtain your appropriate meal.

PRESENTERS' INFORMATION

Preparation Room

The speakers' preparation room is located near the registration desk. A technician will be available in this room throughout the conference. Computer and audio visual equipment will be available for speakers wishing to review their presentations.

- All speakers should present themselves to the technician at least four hours before their scheduled presentation time to hand over and test their presentation.

Time Guidelines

- Allocated time includes questions – please allow at least 5 minutes for questions within your allotted time, as indicated in the program.
- The chair of each session is tasked with keeping the session running to time. Please be considerate of other speakers by arriving promptly and adhering to the chairs' instructions.

Poster Presentations

Poster Presentations have been divided into 2 sessions, scheduled on Monday or Tuesday from 5pm to 7pm in the Boardwalk Gallery, which is located down the escalators at the far end of the Convention Foyer.

- Presenters must be in attendance with that their posters for the entire session.
- All poster presenters are asked to ensure their poster is ready for viewing on their scheduled day.
 - Posters must be mounted on the poster boards by 10:30am on the day of your session and removed by 9:00am on the following day.
- Please check the location number for your poster in the handbook program.
 - There are two numbers, the first is the location of your poster board, the second is the abstract number. Both are numerically listed.
 - Find your abstract number and confirm its location on the poster boards.
 - Velcro is available at the registration desk.
 - Presenters are responsible for placing their own posters in the correct location.

Chair Guidelines

All chairpersons are asked to familiarise themselves with the room and equipment prior to the commencement of their session. Chairpersons are asked to keep all presenters strictly to time.

SOCIAL FUNCTIONS

Welcome Reception

Time: 6.30 – 8.30

Place: Wrest Point Convention Centre Foyer

The Welcome Function is included with full registration; additional tickets can be purchased for \$65 from staff at the Registration Desk.

Conference Dinner

Time: 7.00pm for 7.30

Place: Henry Jones Art Hotel, IXL Jam Factory, Hunter Street, Hobart

The hotel is located on the Hobart Waterfront, a few minutes walk from Salamanca Place. Taxis from Wrest Point will take 10 – 15 minutes.

The Conference Dinner is an additional cost for all delegates. If you did not book a ticket when you registered, but would like to purchase a ticket at a cost of \$100.00 - please see staff at the Registration Desk by 5.00pm on Monday 5 February.

Lunch Suggestions

Lunch is not provided as part of the Conference, so delegates will have a 1.5 hour lunch break (except Thursday). There are a number of venues for lunch located within Wrest Point, including Pier One, Riverview Snacks, Anchors Bistro and the Coffee Shop. Sandy Bay precinct, 15 minutes walk from Wrest Point, offers a wide range of cafes, takeaways, restaurants and shops.

Wednesday Tours

We can accept bookings for the following tours until Tuesday 6 February at 12noon. Please see the staff at the Registration Desk for more details.

Those with Tour Bookings, please be sure to arrive at the departure location, 10 minutes before the departure time as tours MUST leave on schedule. Please Note: Appropriate clothing is required for some tours.

Tour	Departure Time	Meeting Place	Special Clothing
Sea Kayaking	12noon	Hotel Foyer	Comfortable sports clothing
Cascades and the Mountain	1.00pm	Hotel Foyer	Comfortable shoes
Mountain Descent	1.15pm	Hotel Foyer	Comfortable sports clothing and shoes
Discover Hobart	12.45pm	Hotel Foyer	Comfortable shoes
Chocolate and Wine	12.45pm	Hotel Foyer	Closed toe shoes, no jewelry (wedding ring accepted), no loose clothing.
Peppermint Bay Cruise	11.15am	Hotel Foyer	Casual, bring a warm jacket or sweater.

GENERAL INFORMATION

Banking - Banking hours in the city of Hobart are Monday to Friday 9.30am – 4.00pm. Banks are closed on weekends. There is an ATM situated in the hotel lobby and at the entrance to the Convention Centre.

Bus services in Hobart - The Metro Busy Bee bus service runs frequently from the City (GPO on Elizabeth Street in the city centre) to the Wrest Point Hotel front entrance. In addition, there is a Sandy Bay – Casino –Taroona service. The Casino Bus stop on Sandy Bay Road (stop 15) is only a few minutes from the Casino & Convention Centre entrance.

Metro Bus Information: 13 22 01

Emergency Medical Care – The emergency phone number in Australia is 000. 24 hour emergency care is available at the Royal Hobart Hospital (RHH) via the Argyle Street entrance and the Hobart Private Hospital (HPH). The hotel reception desk is staffed 24 hours and they can assist you to locate an after hours medical facility in a non-emergency situation. All hospitals are located within a 5 – 10 minute drive from Wrest Point.

Internet Access - Wrest Point does not offer wireless internet access – however delegates may access their emails via the Business Centre located on the Mezzanine Level of the Hotel (access via Reception). Cards enabling access may be purchased at the hotel reception - \$5 for 30 minutes and \$10 for 60 minutes.

Messages - Messages can be left on the message board located near the registration desk. Please check this board regularly as no responsibility can be taken to deliver messages.

Non-smoking - Wrest Point Hotel and Convention Centre are non smoking venues - no rooms are designated smoking rooms however guests are allowed to smoke in the covered smoking area accessible via the Sports Bar, or outside the venue.

Parking Information - Free parking for delegates is available at Wrest Point.

Public Telephones - These are available just outside the entrance to the Convention Centre foyer, standard pay phone charges apply.

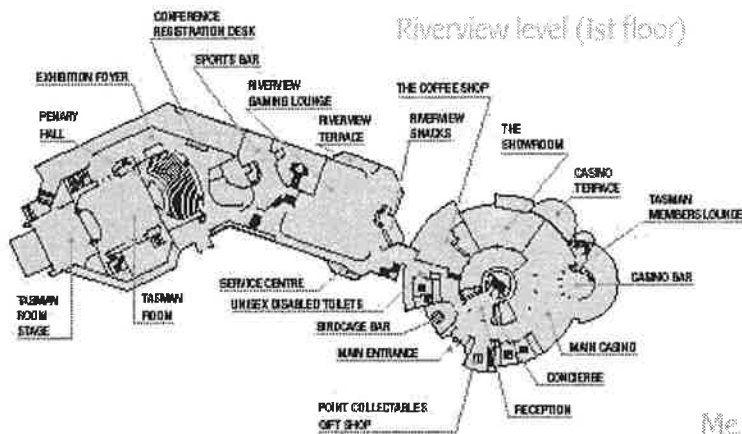
Shopping - Sandy Bay (approximately 10 minutes walk on Sandy Bay Rd, towards the city) is the closest shopping centre to the hotel for supermarkets, restaurants and anything else you may require.

Special Interest Groups - Want to connect with other registrants during the Conference to meet to discuss a common interest? You may wish to register a "Special Interest Group" on the whiteboard provided for this purpose located near the Registration Desk. Please include your name, the topic, time you wish to get together and where you plan to meet.

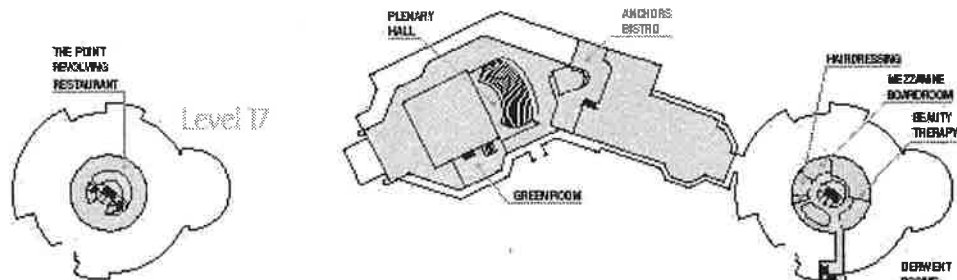
Taxis - Taxi's from Wrest Point to Hobart CBD or Salamanca cost approximately \$10 – \$15.

City Cabs	131 008
Taxi Combined	132227
Associated Taxis	6273 2244

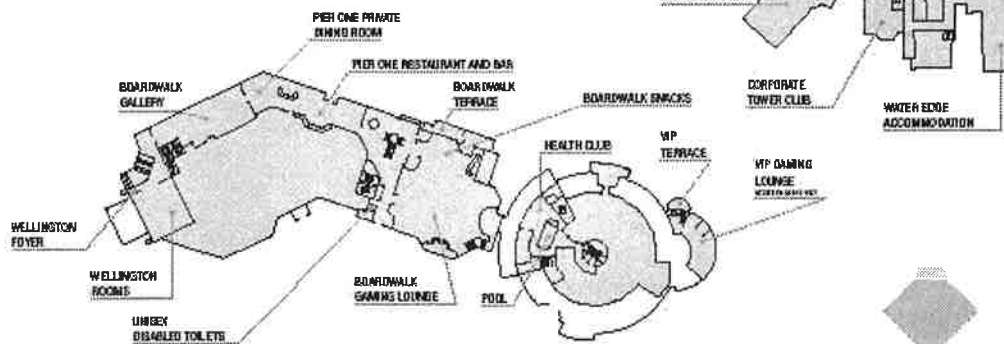
Wrest Point Directory



Mezzanine level (2nd floor)



Boardwalk level (ground floor)



Wrest Point

SUNDAY

4 February, 2007

16.00 - 20.30

Registration

18.30 - 20.30

Welcome Reception

MONDAY MORNING SESSION

5 February, 2007

8.00

Early Morning Refreshments – Wrest Point Convention Foyer

Plenary Session 1

Plenary Hall

Chair: Assoc Prof Charles Young

9.00 Plenary Presentation

Prof KE Wieghardt

Coordination Chemistry of "Really" High Valent Iron
PL1

10.00

MORNING REFRESHMENTS

Concurrent
Session 1

Plenary Hall

Chair: Prof Peter Lay

10.30 Session Lecture

Assoc Prof PV Bernhardt

Electrochemically Driven Molybdoenzyme Catalysis
Bernhardt PV

CS-1A/1

11.00 Session Lecture

Dr SP Best

Dihydrogen Activation at [FeFe] Hydrogenase Structural
Models

CS-1A/2

Cheah MH, Best SP

11.30 Oral Presentation

Dr RJ Deeth

Modelling of Transition Metals Bound to Proteins: Ligand
Field Molecular Mechanics as a Fast Alternative to QM/MM
Deeth RJ

CS-1A/3

11.50 Oral Presentation

Dr R Codd

Survival of Antarctic Bacteria in an Iron Desert. Novel
Strategies in Biomolecular Capture

CS-1A/4

Eije N, Liu J, Pakchung AAH, Codd R

12.10 Oral Presentation

Prof A Ghosh

Nonheme {FeNO}^{6,7} landscapes: The first paramagnetic
{FeNO}⁶ complex

CS-1A/5

Ghosh A, Conradie J, Koch S, Lippard S, Harrop T

12.30 - 14.00

LUNCH

Tasman Room

Chair: Assoc Prof Barbara Messerle

Prof T Maschmeyer

Compartmentalised Nanoreactors and Dynamic Kinetic
Resolutions

CS-1B/1

Maschmeyer TH, Masters AF, Fols A

Prof KJ Cavell

N-Heterocyclic Carbenes: Reactivity and Catalysis
Cavell KJ

CS-1B/2

Dr HV Huynh

Hemilabile Behavior of Thioether-Functionalized N-Heterocyclic
Carbene Ligands

CS-1B/3

Huynh HV, Yeo CH, Ho JHHH

Dr DS McGuinness

Highly Selective Olefin Oligomerisation: Development of
Chromium Based Ethylene Tri- and Tetramerisation Catalysts

CS-1B/4

Tooze RP, Dixon JT, McGuinness DS

Prof ASK Hashmi

Gold Catalysis: Activity/Selectivity Profiles of Different Gold
Complexes

CS-1B/5

Hashmi ASK, Huck JA

MONDAY AFTERNOON SESSION

Plenary Session 2		Plenary Hall	
		Chair: Prof Keith Murray	
14.00	Plenary Presentation	Prof G Christou	PL2
		Single-Molecule Magnets: A Molecular Approach to Nanoscale Magnetic Materials	
	Concurrent Session 2	Plenary Hall	Tasman Room
		Chair: Prof Leone Spiccia	Chair: Dr Marcus Cole
15.00	Session Lecture	Prof KS Murray	Dr SA Macgregor
		Thermal and Photomagnetic Properties of New Iron(II) Spin-Crossover Materials	Acetate-Assisted Cyclometallation: A New Mechanism for C-H Activation?
		<u>Murray KS</u> , Leita B, Moubaraki B, Neville SM, Schneider C, Cashion JD, Letard JF	<u>Macgregor SA</u> , Davies DL, Al-Duaij O, Donald SMA, Poelleth M
15.30	Session Lecture	Dr G Koutsantonis	Assoc Prof MV Baker
		Molecularly Derived Nanomaterials	N-Heterocyclic Carbene Complexes Derived from Azolium-Linked Cyclophanes
		<u>Koutsantonis GA</u> , Buckley C, Douce L, Harrowfield JM, Kraatz B, Lengkeek A, Nealon GL, Orlowski G, Paskevicius M, Skelton BW, White AH	<u>Baker MV</u> , Brown DH, Haque RA, Hesler VJ, Simpson PV, Skelton BW, White AH
16.00	Oral Presentation	Dr CJ McAdam	Prof P Mastrorilli
		Ferrrocene Based Monomers for the Synthesis of Polyesters and Polyols	Synthesis of μ-Hydrido-μ-Phosphido Diplatinum Complexes by Protonation of a Dinuclear Phosphinito Complex of Pt(II)
		<u>McAdam CJ</u> , Robinson BH, Simpson J	Latronico M, <u>Mastrorilli P</u> , Nobile CF, Gallo V, Englert U, Polini F
16.20	Oral Presentation	Dr M Makha	Dr M Denney
		Towards Engineering Nanoporosity in Hybrid Organic - Metal Ionic Solids	Insertion of Molecular Oxygen into a Palladium(II) Hydride Bond
		<u>Makha M</u> , Sobolev AN, Raston CL	<u>Denney MC</u> , Smythe NA, Cetto KL, Kemp RA, Goldberg KI
16.40	Oral Presentation	Dr C Boskovic	Prof MG Humphrey
		New Families of Spin Clusters as Potential Molecular Nanomagnets	Metal Alkynyl Dendrimers with Switchable NLO Properties
		<u>Boskovic C</u> , Alley KG, Mukherjee A, Palmer AM, Mulyana Y, Abrahams BF, Moubaraki B, Murray KS, Bircher R, Guedel HU, Clerac R	<u>Humphrey MG</u> , Cifuentes MP, Samoc M
17.00	- 19.00	Poster Presentation	Boardwalk Gallery

MONDAY POSTER SESSION

Display Location	Abstract Number		
1	0012	A Large M_6L_4 Metallosupramolecular Assembly from a Flexible Hexadentate Tripodal Ligand	Zampese JA , Steel PJ
2	0017	Solid-State Copper and Silver NMR Spectroscopy of Copper(I) and Silver(I) Coordination Compounds	Bowmaker GA , Harris RK, Hanna JV
3	0020	Silver(I) Complexes of Linked Bis(pyrazolyl)methane Ligands: Formation of Discrete Metallacycles and Coordination Polymers based on Anion Coordinating Ability and Ligand Size, Rigidity, and Geometry	Reger DL, Watson RP , Smith MD
4	0021	Effect of Ring Substituents on Crystal Packing and H-bonding in a Series of Copper(II) Arylphosphonic Acid Complexes	Latham K , Coyle AM, White JM
5	0026	Direct and indirect electrochemistry of Dimethylsulfoxide Reductase	Chen KK , Bernhardt PV, McEwan AG
6	0027	Silver(I) Coordination Polymer Networks Formed with Multimodal Ligands	Argyle VJ , Hanton LR
7	0028	Synthesis, Reactivity and Stability of New Gold(III) Metallacyclic Systems	Henderson W, Kilpin KJ , Nicholson BK
8	0030	Polynuclear iron complexes containing redox-active ligands	Mulyana Y , Boskovic C, Abrahams BF, Mukherjee A, Moubaraki B, Murray KS
9	0032	Synthesis, Structure and Catalytic Studies of Palladium(II) Complexes with a sterically bulky, benzannulated N-heterocyclic Carbene Ligand	Han YH , Huynh HVH, Ho JHH, Tan GKT
10	0033	Calix[5]arenes: Molecular Recognition of Carboranes	Clark TE , Makha M, Raston CL, Sobolev AN
11	0034	Synthesis and Inclusion Phenomena of Phosphonated Calixarenes	Clark TE , Makha M, Raston CL, Sobolev AN
12	0037	Iron(II) Spin Crossover in a Series of 1-D Polymers using Di(2-pyridyl)amine Style Ligands	Neville SM , Moubaraki B, Murray KS, Chapman KW, Letard JF
13	0038	Electrospray Mass Spectra of Some Palladium(II) and Platinum(II) Complexes	Wimmer F
14	0043	Cold-Adapted Siderophores from Antarctic Bacteria	Pakchung AAH , Codd R
15	0044	New Bimetallic Copper and Zinc Thiosemicarbazonato Complexes for Diagnostic Imaging	Donnelly PS, Paterson BM , White AR, White JM
16	0045	4'-Hydrazone Substituted 2,2':6',2''-Terpyridine Ligands: Protonation and Metal Ion Complexation	Beves JE , Constable EC, Housecroft CE, Neuburger M, Schaffner S
17	0046	Where are the Metal Ions in Nucleic Acid Structures?	Clark GR
18	0047	Paramagnetic Complexes for Protein Structure Determination	Man B , Messerle BA, Otting G
19	0049	A Novel Entry to Diynyl Metal Complexes	Scoleri N , Bruce MI, Skelton BW, White AH, Nicholson BK
20	0051	Organometallic Carbonyl Tags for Infrared Imaging of Cells	Kong KV , Chew W, Lim L, Fan WY, Leong WK
21	0056	Acetylido- and Butenylnyl- Complexes of Ruthenium(II)	Magill AM , Field LD
22	0057	Insertion of CO ₂ and CS ₂ into Iron and Ruthenium-Carbon Bonds	Allen OR , Field LD

MONDAY POSTER SESSION

23	0061	Synthesis, Structure, and Reactions of New Cyclometallated Binuclear Gold Complexes containing the 2-C ₆ F ₄ PPh ₂ Ligand.	Mirzadeh N , Bhargava SK, Bennett MA, Priver SH, Byrnes M, Wagler J, Willis AC
24	0062	Transmetalation of Mononuclear and Dinuclear Phenylplatinum(II) Hydroxo Complexes with COD Ligand	Suzaki Y , Osakada KO
25	0066	Multi-Functional Framework Materials: Nanoporosity and Spin-Crossover	Sciortino NF , Halder GJ, Kepert CJ, Murray KS, Moubarak B
26	0068	An Unfortunate Way to Dye? Intercalation vs Groove-binding in DNA-Binding Studies	Spillane CB , Morgan JL, Smith JA, Keene FR
27	0070	Where it's AT: The Unexpected Affinity by Dinuclear Metal Complexes for the Minor Groove of AT-Rich Duplex Sequences of DNA	Smith JA , Collins JG, Keene FR
28	0075	Synthesis of Chromium N-Heterocyclic Carbene Complexes Using Chromium Fischer Carbenes as a Source of Chromium Carbonyls	Chung YK , Choi SY, Lee YT, Kim SJ
29	0076	Influence of Anions on Intervalence Charge Transfer (IVCT) in Mixed-Valence Dinuclear Ruthenium Complexes	Fellows EA, Keene FR
30	0077	Octahedral Nickel beta-Diketonate Complexes: Unexpected Stabilisation of Ni(III)	Harding P , Harding DJ, Phonsri W, Saithong S
31	0082	Novel Ferrocenyl-Naphthalimide and -Naphthaloyl Dyads with Ethenyl- and/or Ethynyl-Aromatic Spacer Groups	Tei WC , McAdam CJ, Robinson BH, Simpson J
32	0083	Applications of X-Ray Absorption Spectroscopy to the Speciation and Reactivity Studies of Transition Metal Complexes in Biological Systems	Levina A , Harris HH, Wu L, Mulyani I, Nguyen A, Gwee YY, Lay PA
33	0084	Framework Approaches to Polynuclear Spin-Crossover Systems	Price DJ , Kepert CJ
34	0088	Deracemisation of Chiral Phosphines by Asymmetric Transformation	Kilah NL , Wild SB
35	0089	Novel Phosphorus-Nitrogen Ligands and Their Metal Complexes	Zayza AI , Spencer JL
36	0094	Lanthanoid Pyridinecarboxylate and Naphthoate Complexes as Potential Green Corrosion Inhibitors	Ang D , Deacon GB, Junk PC, Forsyth M, Forsyth CM, Tuner D
37	0095	New and More Efficient Catalysts: The Role of Novel Si,P Ligands in Homogeneous Catalysis	Allan KM , Spencer JL
38	0098	Reduction Chemistry and Electrocatalysis by Site-Differentiated H-cluster Model Compounds	Cheah MH, Borg SJ, Tard C, Liu X, Pickett CJ, Best SP
39	0104	UV Resonance Raman Spectroscopic Studies of the Weak Interaction in Pseudoazurin M16Y Mutant and its Copper Complex Model	Kohzuma T , Uchida Y, Yajima T, Yamauchi O
40	0105	Isolated Octaiodide Anions In [Ba(dibenzo-18-crown-6) ₂] ₈	Walbaum C, Pantenburg I , Meyer G
41	0106	Ab Initio MO Studies of the Weak Interaction in Cu-Histamine-Tyrosine Complex as an Model of Pseudoazurin M16Y Mutant	Nagashima U , Watanabe T, Kohzuma T, Uchida Y, Yamauchi O
42	0107	XAFS Studies of the Heme Sites within NO and O ₂ Adducts of Heme Proteins	Lay PA
43	0108	Solid State Fullerene-Porphyrin Assemblies and Molecular Porphyrin Hosts for Fullerenes with 3,4,5-Trimethoxyphenyl Porphyrins.	Boyd PDW , Hosseini A
44	0112	Substituted Phosphazenes as Multimodal Polydentate Ligands	Ainscough EW, Brodie AM, Otter CA
45	0114	Synthesis and Reactivity of Ortho-Metallated Complexes of Nickel, Palladium and Platinum	Bennett MA, Bhargava SK, Priver SH , Willis AC

MONDAY POSTER SESSION

46	0115	Stabilisation of Copper(II) Thiosulfate and Thiosulfonate Coordination Complexes Through Cooperative Hydrogen Bonding Interactions	Fischmann AJ , Spiccia L
47	0116	Conformational Flexibility in Inorganic Rings: 2,2'-Dioxybiphenyl-chloro-cyclotetraphosphazenes	Brodie AM , Ainscough EW, Chaplin AB, Derwahl A, Harrison JA, Otter CA
48	0118	Alkynes on Gold Surfaces	McDonagh AM , Zareie MH, Ford MJ, Barton C
49	0119	Fluxional Behaviour of Metal-Bearing Phosphazenes	Kirk S , Ainscough EW, Brodie AM, Edwards PJB
50	0122	Chemistry of Hybrid Materials containing Organic Dye Cations and Polyoxometalate Anions	Xie J , Wedd AG
51	0123	Spin-crossover and Nanoporosity: Magnetic, Structural and Guest Exchange Studies	Sciortino NF , Halder GJ, Kepert CJ
52	0125	Tetrasulfidocopper(I) : A New Tetrahedral Building block	Robson R, Abrahams BF , Haywood MG
53	0126	The High Temperature Synthesis of Polynuclear Complexes	Bowden M, Kirchner A, Taylor JPH , Weatherburn DC
54	0128	Silica Attached Molecular Receptors	Hodgyl JAZ , Wainwright KP, Lincoln SF
55	0129	Coordination of One Versus Two Armed Pyridine/Pyrazine Based Ligands	Hellyer RM , Larsen DS, Brooker S
56	0130	Tethered Ru(II)enabenzenes, Osmabenzenes and Iridabenzenes	Bierstedt A, Johns PM, O'Neale TR, Roper WR, Tonei DM, Wright LJ
57	0134	Scaffolding Interconnect for Binding Fullerenes and Single Wall Carbon Nano-tubes	Makha M, Mickinnon JJ, Norret M, Raston CL , Sobolev AN, Spackman M
58	0138	Novel Quadrupole Alkynyl Ruthenium Compounds Featuring Extended -Delocalizable Systems	Dalton GT , Humphrey MG
59	0143	Selected Chemistry of Some High Nuclearity Ruthenium Clusters	Randles MD , Humphrey MG
60	0145	Electrochemical Investigation of Molecular Mimics of the Photosystem II Water Oxidation Complex	Brimblecombe R , Bond AM, Dismukes GC, Swiegers G, Spiccia L
61	0147	Novel Electro-, Photo-, and Photo- Switchable Organometallics	Green KA , Humphrey MG
62	0151	Extended Chain Dipolar Organometallics for Second Order Nonlinear Optical Applications. Syntheses of New Alkynyl Ru(II) Dipolar Compounds	Rigamonti L , Humphrey MG
63	0161	An Asymmetric Diamond Core Complex in the Mo Bis(thioethyl)pyridinate' (L-NS ₂) System	Gourlay C , Doonan CJ, White JM, Young CG
64	0164	Synthesis and DNA binding Studies of Flexible Bis-Intercalating Dinuclear Ruthenium(II) Complexes	Brodie CR , Aldrich-Wright JR
65	0167	Probing the Electronic Manifold of Tungsten(V) Monodithiolenes	Sproules S , McMaster J, Doonan CJ, George GN, Young CG
66	0173	Cages on Surfaces: Thiol Functionalisation of Co(III) Sarcophagine Complexes	Harrofield JM, Koutsantonis GA, Kraatz HB, Nealon GL , Orłowski G, Skelton BW, White AH
67	0175	Synthesis and Characterisation of New Water-soluble Lanthanide Carboxylates, beta-Diketonates and Tetrazolates	Andrews PC, Fraser BH, Junk PC, Massi M

MONDAY POSTER SESSION

68	0176	New Water Soluble Lanthanide Benzoates – Catalysts for Kinetic Resolution of Diastereomers: Epoxides	Fraser BH, Andrews PC, Junk PC, Tuck KL, Massi M, Blair M
69	0178	Applications of Cage Amines to Electrochemical and Photochemical Systems	Lengkeek NA, Koutsantonis GA, Harrowfield JM, Sauvage JP, Collin JP
70	0181	Studies of Amino Acid Pendant Arm Macrocyclic Metal Complexes	Baker C, Lincoln SF, Wainwright KP
71	0190	Application of CW and Pulsed EPR, MoSophe and DFT Calculations in Unravelling the Electronic Structure of the Molybdenum(V) Centre in Dimethylsulfoxide Reductase.	Noble CJ, Drew S, Lane I, Benson S, McEwan AG, Young CG, Hanson GR
72	0199	Preparation and Single Crystal EPR Studies of Oligonuclear Metal Aggregates	Elcoate CJ, Lee RA, McCool BJ, Davies MS
73	0204	Capillary Microreactor Catalysis Utilising Solid Organic Macroporous Monolith Supports	Bolton KF, Canty AJ, Devereil JA, Guijt RM, Hilder EF, Rodemann T, Smith JA
74	0212	Synthesis of new Metal Complex - Biomolecule Hybrids as Redox Sensors for Specific Nucleobases	Gasser G, Spiccia L, Bond AM, Kosowski Z
75	0225	The Assembly of Water-soluble Nanoscale Metallacycles as Potential DNA Nanoshuttles	Mulcahy C, Harding MM, Rendina LM
76	0234	Isomeric Oxo-Molybdenum(IV) Scorpionate Complexes	Evans DJ, Malarek MS, Doonan CJ, White JM, Young CG

TUESDAY MORNING SESSION

6 February, 2007

Early Morning Refreshments – West Point Convention Foyer

8.00

Plenary Session 3

Plenary Hall

Chair: Prof Glen Deacon

9.00 Plenary Presentation

Prof WJ Evans

PL3

The Rapidly Changing Nature of f Element Reduction Chemistry

10.00

MORNING REFRESHMENTS

Concurrent
Session 3

Plenary Hall

Chair: Prof Jim Simpson

10.30 Session Lecture

Dr MG Gardiner

CS-3A/1

Macrocyclic Control of Organolanthanide Chemistry

Gardiner MG

2005 Organometallic Award

11.00 Session Lecture

Prof J Okuda

CS-3A/2

Cationic Alkyl Complexes of the Rare Earth Metals: Synthesis, Structure, and Reactivity

Okuda J

11.30 Oral Presentation

Assoc Prof PC Junk

CS-3A/3

Subtle Steric Control in Organoamidolanthanoid Chemistry

Junk PC

11.50 Oral Presentation

Prof AJ Nielson

CS-3A/4

Determination of Linear Agostic Interactions in Early

Transition Metal Complexes

Lein M, Nielson AJ, Schwerdtfeger PA, Waters JM

12.10 Oral Presentation

Dr RP Watson

CS-3A/5

Discrete and Polymeric Fluoride-Bridged Metallacycles

Prepared from Linked Bis(pyrzoly)methane Ligands and

Fluoride Abstraction from Tetrafluoroborate Anion

Ruger DL, Watson RP, Gardinier JR, Smith MD, Pellechia PJ

12.30 - 14.00

LUNCH

Wellington Room

Chair: Prof Leonard Lindoy

Dr SR Batten

CS -3B/1

Scorpions and Crowns

Batten SR, Duriska M, Lu J, Turner DR, Chesman ASR, Turner P,

McKinnon JJ, Jensen P, Murray KS, Moubaraki B, Spiccia L,

Belousoff MJ

Dr T Söhnel

CS-3B/2

New Exciting Solid State Cluster Compounds

Söhnel T

Prof KAR Mitchell

CS-3B/3

Study of Catalysts Based on Non-Precious Metals for

Applications in PEM Fuel Cells

Bizzotto D, Campbell SA, Mitchell KAR, Parsons RR, Sode A,

Susac D, Teo M, Wong KC, Wong PC, Zhu L

Dr MS Thomas

CS-3B/4

Complexes of Thiophene Derivatives as Potential

Metallomesogens

Thomas MS, Lotz S, Landman M

Prof CL Raston

CS-3B/5

Fabricating Composite Hydrosols of Fullerene Nano-Whiskers

Shrouded by Silver

Iyer S, Raston CL, Saunders M

TUESDAY AFTERNOON SESSION

Plenary Session 4		Plenary Hall	
		Chair: Dr Lou Rendina	
14.00	Plenary Presentation	Prof G van Koten 'Pincer' Organometallics: Building Blocks with an Organic and an Organometallic Side	PL4
	Concurrent Session 4	Plenary Hall	Wellington Room
		Chair: Assoc Prof Lawrence Gahan	Chair: Prof Anthony Wedd
15.00	Session Lecture	Dr DP Arnold Metal-catalysed C-N and C-P Coupling on the Porphyrin Periphery	Prof SJ Berners-Price Targeting the Mitochondrial Cell Death Pathway with Gold(I) Complexes
		Atefi F, Basic B, Esdaile LJ, McMurtrie JC, Arnold DP	<u>Berners-Price SJ</u> , Baker MV, Barnard PJ, Hickey JL, Ruhayel RA, Wedlock LE
15.30	Session Lecture	Prof K Gloe A Comparative Study of the Structures of Silver(I) Complexes of 2,2'-Dipyridylamine Derivatives	Prof FR Keene Dinuclear Ruthenium(II) Complexes with Flexible Bridges as DNA Bulge-Selective Probes
		Antonoli B, Bray DJ, Clegg JK, Sumbly CJ, Wenzel M, Gloe K, Katajeva O, McMurtrie JM, Gloe K, Lindoy LF, Steel PJ	Morgan JL, Spillane CB, Smith JA, Collins JG, Keene FR
16.00	Oral Presentation	Dr LR Hanton Flexible Asymmetrical Ligands and Unusual Networks	Dr RK Hocking Fe L-edge XAS: A direct probe of covalency and back-bonding
		Black CA, <u>Hanton LR</u>	<u>Hocking RK</u> , Wasinger EC, Hodgson KO, Hedman B, Solomon EI
16.20	Oral Presentation	Prof KP Wainwright Fluorescent Metal-Ion Activated Molecular Sensors for Aromatic Anions	Dr PS Donnelly The Potential of Copper and Zinc Bis(thiosemicarbazonato) Complexes for the Treatment of Alzheimer's Disease
		<u>Wainwright KP</u> , Bradbury AJ, Hodyl JAZ	<u>Donnelly PS</u> , Barnham KJ, White AR
16.40	Oral Presentation	Prof J Spencer Control of Metal Reactivity with Designer Ligands	Prof R Stranger Resolving Differences in the Crystal Structures of Photosystem II through DFT Calculations
		<u>Spencer JL</u> , Zayya AI, Allan KM, Vagana RL, Matveenko M	Petrie S, <u>Stranger R</u> , Pace R, Gatt P
17.00	- 19.00	Poster Presentation	Boardwalk Gallery

TUESDAY POSTER SESSION

Poster Location	Abstract Number		
1	0013	Coordination Polymers of Various Bisphenol Derived Bridging Ligands	Cottam JRA, Steel PJ
2	0039	Iron Chelators as Anti-Cancer Drugs	Islam M, Sharpe P, Bernhardt PV, Richardson DR
3	0054	Stabilization and Surface Modification of Magnetite Nanoparticles By Chitosan and Calixarene Derivatives	Chin SF, Makha M, Raston C
4	0058	Ruthenium Complexes of Pincer and Tripodal Tridentate Ligands and Their Reactions with Ag(I)	Page MJ, Messerle BA, Field LD
5	0060	Synthesis and Complexes of Diaza-18-crown-6 Derivatives	Duriska MB, Batten SR
6	0065	Novel Hydrazine Chemistry of the Group 8 and 9 Metals	Dabb SL, Messerle BA, Field LD, Smith MK, Willis T
7	0069	RNA vs DNA: Comparing and Contrasting the Nucleic Acid-Binding Ability of a Dinuclear Polypyridyl Ruthenium(II) Complex	Spillane CB, Collins JG, Keene FR
8	0071	A Highly Efficient DNA-Affinity Based Chromatographic Method for the Separation of Metal Complex Stereoisomers	Smith JA, Keene FR
9	0078	Synthesis and Characterization of Sterically Hindered Tris(pyrazolyl)borate Ni Complexes	Harding DJ, Harding P, Adams H, Pakawatchai C, Tuntulani T
10	0087	Dinuclear SCO complexes of iron(II) featuring bridging 1,2,4-triazole moieties	Kitchen JA, Klingele MH, Moubaraki M, Murray KS, Grunert M, Gütllich P, Brooker S
11	0091	License to Kill (A Ligand) - Unexpected Nucleophilic Addition Products of Dicyanonitrosomethanide.	Chesman ASR, Turner DR, Deacon GB, Batten SR
12	0093	Meso-Porphyrinylphosphine Oxides: Ligands for Supramolecular Porphyrin Systems	Atefi F, Arnold DP
13	0099	Process Intensification Strategies for the Synthesis and Encapsulation of Metal Nanomaterials	Hartlieb KJ, Raston CL, Saunders M
14	0113	Asymmetric Syntheses of Chiral Diarsines Via Bis(Phosphine-Stabilised) Diarsenium Salts	Weir ML, Kilah NL, Willis AC, Wild SB
15	0121	Dinuclear Spin-Crossover Complexes	Amoore JJM, Neville SM, Kepert CJ, Murray KS, Letard JF, Moubaraki B, Guionneau P
16	0124	Molecular Characterisation of Metal Transporters in the Plant Arabidopsis Thaliana	Zimmermann M, Xiao Z, Wedd AG
17	0133	Alignment of Fullerene C ₇₀ within the Confines of Substituted Calix[5]arene Capsules	Makha M, Sobolev AN, Raston CL, McKinnon JJ, Spackman MA
18	0137	Vanadium Mixed-Valence Complexes with a Sulfur-Rich Coordination Sphere	Taylor MK, Evans DJ, Young CG
19	0139	Dendritic Alkynylmetal Complexes for Nonlinear Optics	Roberts RL, Humphrey MG
20	0141	Introducing Metals into Peptides: Derivatives of Macrocyclic Amino Acids and their Metal Complexes	Huth S, Spiccia L, Hearn MTW
21	0146	Synthesis and Reactivity of Molybdenum(IV) Complexes with Co-Ligands Containing Hydrogen-Bonding Groups	Ng VWL, Taylor MK, Young CG

TUESDAY POSTER SESSION

22	0148	Tuning and Functionalising Gold Nanoparticle Films	Bray DJ, Herrmann J, Lawrence GA, Lindoy LF, Müller KH, Wei G
23	0149	Water Soluble Aromatic Anion Receptors Involving a Tict Fluorophore	Kadidae LO, Wainwright KP, Lincoln SF
24	0155	Adsorption and Intercalation of Acid Blue 9 on Mg-Al Layered Double Hydroxides of Variable Metal Composition	Auxilio AR, Andrews PC, Junk PC, Spiccia L, Neumann D, Raverty W, Vanderhoeck N
25	0156	Synthesis, Characterization and Electrochemical Behaviour of Ortho-palladated Derivatives Containing (2-diphenylphosphino)phenyl	Kar G, Priver SH, Byrnes M, Guo SX, Wagler J, Bhargava SK, Bennett MA, Bond AM
26	0157	New M_2L_3 Helicates and M_4L_6 Tetrahedra Incorporating 5,5''-Dimethyl-2,2':5',5'':2'',2'''-Quaterpyridine and Extended Analogues.	Glasson CRK, Meehan GV, Lindoy LF, Clegg JK
27	0158	The Synthesis and Utility of Aluminochlorohydrates	Alexander SG, Cole ML
28	0162	One-Pot Tandem Hydroamination /Hydrosilylation, Catalyzed by Multiple Catalysts	Hodgson R, Messerle BA, Rumble SL
29	0163	Ruthenium Phthalocyanine Complexes: The Effect of Variation of Axial Ligand Substituents on Electrochemical and Spectroelectrochemical Properties	Rawling T, Xiao H, Lee S, Colbran S, McDonagh AM
30	0165	Spin Crossover and Nanoporous Framework Materials	Robertson MG, Kepert CJ, Murray KS, Moubaraki B, Letard J
31	0169	Transition Metal Allenylidene Complexes Incorporating a Terminal Coordination Site: Models for Molecular Wire Systems	Koutsantonis GA, Lengkeek NA, Sanford V, Schauer PA, Skelton BW, White AH
32	0170	Alkali Metal Amide Complexes: Metal Promoted Rearrangements and Their Impact on Organic Synthesis	Andrews PC, Bull SD, Minopoulos M
33	0171	A Study of the Directionality of Interstrand Cross-links Formed by Multinuclear Platinum Anticancer Compounds	Ruhayel RA, Zhang J, Moniodis JJ, Yang X, Berners-Price SJ, Farrell N
34	0174	A Novel Approach to the Synthesis of s-Block Metal Amides Directly from the Metals	MacLellan JG, Andrews PC, Deacon GB, Maguire M
35	0177	Fluorophores for Zinc(II) Detection in Biological Systems	Coleman H, Hendrickson K, Kimber MC, Lincoln SF, May BL, Ward AD
36	0179	Varying Molecular Polarity as a Tool for Tuning Non-Linear Optical Properties	Corkery TC, Humphrey MG
37	0182	A Preparative, Equilibrium and Kinetic Study of [2]-Pseudorotaxanes	Darcy R, Easton CJ, Lincoln SF, May BL
38	0187	Activation of $[PdCl_2(PPh_3)_2]$ via OH--Assisted Disproportionation: A Computational Study	Macgregor SA, Goodman J
39	0188	A Role for a Metallophosphorane Intermediate in C-F Activation at Iridium(I)	Macgregor SA, Erhardt S
40	0191	Potential Synthetic Routes to Pentaphenylcyclopentadienyl Complexes of Divalent Lanthanides	Deacon GB, Field LD, Forsyth CM, Junk PC, Kay DL, Masters AF, Maschmeyer TH
41	0197	Coupling Reactions between Organometallic and Thiazyl Radicals	Goh LY, Boeré RT, Lau HF, Ang PCY, Ng VWL, Kuan SL, Roemmele T
42	0198	Heteroleptic Macrocycles: Super (Protein) Models	Elcoate CJ, McCool BJ, Davies MS
43	0200	Reactivity of Cyclopentadienyl Ruthenium Carbonyl Complexes Towards Heterocyclic Disulfides	Kuan SL, Goh LY, Leong WK
44	0202	Self-supported Organometallic Rhodium Quinonoid Nanospheres for Catalytic Applications	Son SU, Park KH, Jang K

TUESDAY POSTER SESSION

45	0203	Synthesis and Reactivity of Platinum(IV) and Palladium(IV) Alkynyls	Canty AJ , Karpiniec S, Rodemann T, White AH, Skelton BW, Gardiner MG
46	0205	Kolbe-Schmitt: Can an Old Reaction Teach us New Tricks?	Stropin AAS, Cole ML
47	0206	Peptide Nucleic Acids (PNAs) Incorporating Novel Ruthenium (II) sensors	Nickita N , Bond AM, Gasser G, Spiccia L
48	0207	Impact of Phosphate and Geometric Isomerism on the Kinetics and Mechanism of the Formation of Interstrand Cross-links by a Dinuclear Platinum Complex.	Zhang J , Thomas DS, Berners-Price SJ, Farrell N
49	0210	Telluroether Complexes of Some Transition Metals	Oilunkaniemi R , Vigo L, Poropudas MJ, Laitinen RS
50	0213	Painting the Whole Picture: Combining Potentiometric and Spectrophotometric Titration Analysis to Determine Metal-Ligand Stability Constants	Norman SE , Maeder M, Lawrance G, Griggs B
51	0215	Binding and C-H Activation of Alkanes with the CpRe(CO)(PF ₃) Fragment: A Dynamic Equilibrium Between Alkane	Darwish TA, Ball GE , George MW
52	0216	Analysis and Simulation of the Thermodynamics and Kinetics of CO ₂ Absorption by Aqueous Amine Systems	McCann N , Maeder M, Attala M
53	0217	Application of 1-Alkyl-3-methylimidazolium Ionic Liquids and S-Containing Complexing Agents in the Oxidative Leaching of Gold and Silver	Zhang J , Whitehead JA, McCluskey A, Lawrance GA
54	0218	Combined FTIR, NMR and Computational Studies of Metal-Catalysed Addition of HX to Terminal Alkynes	Toh EC, Fan WY
55	0219	AAO Template Fabrication Of Copper Tetraaminonaphthalocyanine Nanowires By Electropolymerization	Ang SG , Xu GQ, Gu F
56	0220	Supramolecular mimic of an enzyme active site	Tapper S , Fry F, Tucker J
57	0221	Assembly Of Metallocyclic Architectures: Towards DNA Nanoshuttles	Schilter D , Rendina LM
58	0223	Crystal Structures Provide an Insight into the Catalytic Mechanism of Purple Acid Phosphatase	Leung EWW, Elliot TW, Mitic N, Gahan LR , Carrington LE, Shenk G, Guddatt LW
59	0224	Porphyrin-Appended Dendrimers: "Electronic Leaves and Molecular Trees"	D'Alessandro DM , Hambly AC, Khoury T, Crossley MJ
60	0226	Platinum(II) Derivatives of Dodecahydro-closo-dodecaborate as Potential BNCT Agents	Crossley EL , Rendina LM
61	0227	Hypercoordinate Silicon Complexes of the Dianion of Pyrrole-2-N-(o-hydroxyphenyl)-carbalimine	Wagler J , Gerlach D
62	0230	Electrocrystallization of the Semiconducting/Magnetic Co[TCNQ] ₂ (H ₂ O) ₂ : Towards Facile Morphology-Tunable Crystalline Materials	Nafady A , Bond AM
63	0231	Structural and Thermal properties of Polymer composites containing Manganese based Single Molecule Magnets	Johnson LP, Matisons JG
64	0232	Observation of Key Intermediates of Intermolecular Copper Transfer in Copper Resistance Protein PcoC from Escherichia coli	Djoko KY, Xiao Z, Wedd AG
65	0235	Synthesis and Characterisation of Chelating diamido {ArN(CH ₂) _n NAr'} ₂ (Ar = 2,6-Pr ₂ C ₆ H ₃) (n = 2, 3, and 4) Magnesium complexes and Reactivity Towards Lactides	Ashoor S , Cloke G, Hitchcock P
66	0236	Synthesis and Structures of Three, Four, and Six-Coordinate Monomeric Tin(II) and Tin(IV) Compounds Containing eta-2-Ketiminato Ligands	Huang JH , Kao HM, Chen IC, Lin CY, Lee GH
67	0237	Structural Developments in Lanthanoid(III) Amidinate Chemistry	Cole ML, Deacon GB, Forsyth CM, Junk PC, Konstas K

TUESDAY POSTER SESSION

68	0238	Synthesis and Structural Characterisation of Rare Earth 2,4,6-trimethylphenolate Complexes	Moxey GJ , Deacon GB, Junk PC
69	0239	Non-Chelate and Chelate Complexes of Palladium(II) With N-heterocyclic Carbenes Ligands of Amido Functionality	Lee HM , Liao C-Y, Kai-Ting C
70	0240	Multidentate Phosphine Ligands Containing the 2-Aminophenyl Moiety	Bennett J, Bennett K, Huang I, Lee H-Y, Lu D, Salem G , Tifan M
71	0241	Hexadentate Tertiary Phosphines	Bennett J, Doyle R, Salem G , Sheridan M, Walker L, Willis AC
72	0242	Telomerisation of Butadiene and Isoprene Using N-Heterocyclic Carbene Complexes of Palladium and Rhodium	Nielsen DJ , Cavell KJ
73	0243	Lanthanide Imides – A Synthetic Investigation	Gardiner MG, Stringer DN , Yates BF
74	0244	Structural Studies of Tethered Mixed Anion Lithium Complexes	Gardiner MG, Lockhart-Gillett B , Yates BF
75	0245	Lanthanide Imides - A Theoretical Investigation	Gardiner MG, Stringer DN , Yates BF
76	0246	Synthesis of Palladium and Platinum Heteroleptic Complexes and their Application in the Heck reaction	Jones RC , Canty AJ, Gardiner MG, Tolhurst V-A, White AH, Skelton BW
77	0247	Synthesis of Supported Heteroleptic Complexes for use in the Heck Reaction	Jones RC , Canty AJ, Gardiner MG
78	0248	C-C double bond activation by vanadium(IV) and molecular oxygen	Mohebbi S
79	0250	Novel Access to Monovalent Group 13 Metal Complexes: Synthetic and Theoretical Studies of the Thermal Decomposition of Metallocyclopent-3-enes	Gardiner MG, James AN , Yates BF
80	0251	The Synthesis & Structural Elucidation of 3,5-bis(2-pyridyl)-1,2,4-triazolate Bridged Dinuclear Iron(II) Spin Crossover Compounds	Schneider CJ , Cashion JD, Mobaraki B, Neville SM, Batten SM, Turner DR, Murray KS
81	0252	Ligand Influences on the Reduction Potentials of Platinum(IV) Complexes: comparison with quantum-chemical predictions of reduction potentials	Howard ST , Battle AR, Hambley TW

STRANKS AWARD POSTERS

84	0152	Dinitrogen Activation: A Comparison of the Laplaza-Cummins, Schrock and Fryzuk Systems using DFT	Christian G, Stranger R, Yates BF
85	0131	Structural Models of the CO Dehydrogenase Active Site	Gourlay C, Evans DJ, Nielsen DJ, White JM, Knottenbelt SZ, Kirk ML, Young CG
86	0101	Chiral Guest Sorption and Gas Storage in a Homochiral Nanoporous Framework Material	Iremonger SS, Kepert CJ
87	0092	α -Helix Induction In Short Peptides Using Metal Clips	Ma MT, Hoang HN, Bryant GK, Fairlie DP, Appleton TG
88	0111	Unusual Carbonate and Phosphate Co(III) Complexes	McClintock LF, Blackman AG
89	0120	Some Chemistry of the Ruthenium Ethynyl Complex, $\text{Cp}^*(\text{PP})\text{RuC}\equiv\text{CH}$, and Reactions of the Tricyanovinylethynyl Complex, $\text{Cp}^*(\text{PP})\text{RuC}\equiv\text{CC}(\text{CN})=\text{C}(\text{CN})_2$	Parker CR, Bruce MI, White AH, Skelton BW, Nicholson B

WEDNESDAY MORNING SESSION

7 February, 2007

8.00 Early Morning Refreshments – Wrest Point Convention Foyer

Plenary Session 5

Plenary Hall

Chair: Prof Allan Cauty

9.00 Plenary Presentation

Prof RR Shrock

PL5

Catalytic Reduction of Dinitrogen to Ammonia at Room Temperature and One Atmosphere with Protons and Electrons

10.00

MORNING REFRESHMENTS

Stranks Award Session

Plenary Hall

Chair: Prof Richard Keene

10.30 Oral Presentation

G Christian

SA1

Dinitrogen Activation: A Comparison of the Laplaza-Cummins, Schrock and Fryzuk Systems Using DFT

Christian G, Stranger R, Yates BF

10.45 Oral Presentation

C Gourlay

SA2

Structural Models of the CO Dehydrogenase Active Site

Gourlay C, Evans DJ, Nielsen DJ, White JM, Knottenbelt SZ, Kirk ML, Young CG

11.00 Oral Presentation

SS Iremonger

SA3

Chiral Guest Sorption and Gas Storage in a Homochiral Nanoporous Framework Material

Iremonger SS, Kepert CJ

11.15 Oral Presentation

MT Ma

SA4

 α -Helix Induction in Short Peptides Using Metal ClipsMa MT, Hoang HN, Bryant GK, Fairlie DP, Appleton TG

11.30 Oral Presentation

LF McClintock

SA5

Unusual Carbonate and Phosphate Co(III) Complexes

McClintock LF, Blackman AG

11.45 Oral Presentation

CR Parker

SA6

Some Chemistry of the Ruthenium Ethynyl Complex, $\text{Cp}'(\text{PP})\text{RuC}\equiv\text{CH}$, and Reactions of the Tricyanovinylethynyl Complex, $\text{Cp}'(\text{PP})\text{RuC}\equiv\text{CC}(\text{CN})=\text{C}(\text{CN})_2$ Parker CR, Bruce MI, White AH, Skelton BW, Nicholson B

12.00

FREE AFTERNOON or TOURS

19.00 for 19.30

Conference Dinner

Henry Jones Art Hotel, Hunter Street, Hobart

THURSDAY MORNING SESSION

8 February, 2007

Early Morning Refreshments – Wrest Point Convention Foyer

8.00

Plenary Session 6

Plenary Hall

Chair: Prof Graham Bowmaker

9.00 Plenary Presentation

Prof C Jones

PL6

Group 13 Metal(I) Heterocycles: Metal Donor Lewis Bases and N-heterocyclic Carbene Analogues

10.00

MORNING REFRESHMENTS

Concurrent
Session 6

Plenary Hall

Chair: Assoc Prof Leonard Wright

10.30 Session Lecture

Prof KO Osakada

Novel Multinuclear Pd and Pt Complexes Having Bridging

Silylene or Gemylene Ligands

Osakada KO, Tanabe MT

CS-6A/1

Tasman Room

Chair: Prof Stephen Lincoln

Prof AM Bond

Morphology Changes and Mechanistic Aspects of the

Electrochemically-Induced Reversible Solid-Solid

Transformation of Microcrystalline TCNQ into Co[TCNQ]₂-Based

Materials (TCNQ = 7,7,8,8-Tetracyanoquinodimethane)

Bond AM, Nafady A, O'Mullane AP, Neufeld AK

CS-6B/1

11.00 Session Lecture

Dr PC Andrews

Synthetic and Structural Chemistry of Bismuth Oxo-clusters

Andrews PC

CS-6A/2

11.30 Oral Presentation

Prof RS Laitinen

Ligand Chemistry of Chalcogen Diimides

Laitinen RS, Oilunkaniemi R, Risto M, Konu J, Chivers T

CS-6A/3

11.50 Oral Presentation

Dr PJ Brothers

Redox Chemistry in Boron Porphyrins

Brothers PJ, Boyd PDW, Albrett AM, Hodgson MC, Kohl U, Weiss A, Siebert W

CS-6A/4

12.10 Oral Presentation

Prof AM Brodie

Conformational Flexibility in Inorganic Rings: 2,2'-

Dioxybiphenyl-chloro-cyclotetraphosphazenes

Brodie AM, Ainscough EW, Chaplin AB, Derwahl A, Harrison JA, Offer CA

CS-6A/5

Dr S Iyer

Controlling the Size, Shape and Surface Morphology, Agglomeration, Phases and Defect of Inorganic Nano-Particles Under Continuous Flow Conditions

Iyer S, Raston CL, Saunders M

CS-6B/5

12.30 - 13.30

LUNCH

THURSDAY AFTERNOON SESSION

	Burrows Award Session	Plenary Hall Chair: Prof Richard Keene	
13:30	Burrows Award Lecture	Prof GB Deacon	BAL
		Some Recent Highlights in Rare Earth Chemistry	
14:30	Conference Close	Plenary Hall	
14:35	Division Meeting	Plenary Hall	

ORAL ABSTRACTS

Coordination Chemistry of “Really” High Valent Iron

K. E. Wieghardt

Max Planck Society, Muelheim, Germany

wieghardt@mpi-muelheim.mpg.de

The term “high-valent iron” implies the presence of a central iron ion in coordination compounds with d^n electron configuration with $n < 5$. The existence of Fe(IV) (d^4) or even Fe(V) (d^3) has been invoked in some metalloproteins. The coordination chemistry of Fe(IV), and – to a lesser degree – of Fe(V) has been developed in the past few years. Our efforts in this area will be presented with special emphasis on their spectroscopic features. Synthesis and spectroscopic characterization of the first genuine, octahedral Fe(VI) (d^2 ; diamagnetic) complex will be presented.

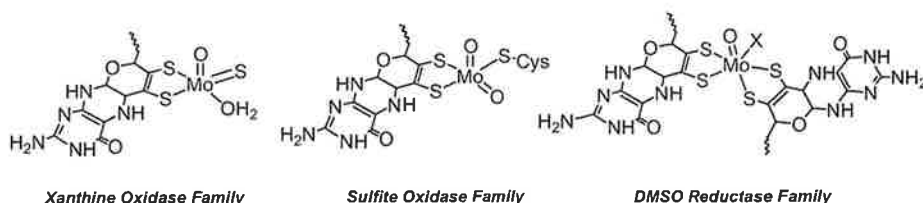
Electrochemically Driven Molybdoenzyme Catalysis

P V Bernhardt

University of Queensland, Brisbane, Australia

p.bernhardt@uq.edu.au

Mononuclear molybdenum enzymes are found in all forms of life. In all known cases the Mo ion at the active site is bound by either one or two bidentate pterin-dithiolene ligands. The mononuclear Mo-enzymes fall into three distinct groups comprising the xanthine oxidase, sulfite oxidase and DMSO reductase families (below). The ligand 'X' in the DMSO reductase family is provided by a serine, aspartate, cysteine or selenocysteine residue (or no protein ligand in some cases).



We have been successful in obtaining voltammetric responses from a number of Mo-enzymes under particularly in the presence of their natural substrate where the electrochemical working electrode plays the part of the enzyme's natural electron partner. [1-3]. This presentation will include some of our most recent results with Mo enzymes from each of the above families.

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- [1] K.-F. Aguey-Zinsou, P.V. Bernhardt, U. Kappler and A.G. McEwan, *J. Am. Chem. Soc.*, **2003**, *125*, 530.
 - [2] K.-F. Aguey-Zinsou, P.V. Bernhardt and S. Leimkuehler, *J. Am. Chem. Soc.*, **2003**, *125*, 15352.
 - [3] P.V. Bernhardt and J.M. Santini, *Biochemistry*, **2006**, *45*, 2804.

Dihydrogen Activation at [FeFe] Hydrogenase Structural ModelsM.-H. Cheah, S.P. Best*University of Melbourne, Melbourne, Victoria, Australia*

spbest@unimelb.edu.au

This paper is concerned with the integration of theory and experiment with view to establishing a well grounded approach to the delineation of reaction paths for electrocatalytic reactions. The vehicle is dihydrogen activation by [FeFe]-hydrogenase; a reaction of profound technological and environmental importance. Two different viable DFT-charted paths for dihydrogen activation at the [FeFe] hydrogenase active site have been reported [1,2]. These involve either heterolytic cleavage at the “so called” vacant site of the Fe atom remote from the 4Fe4S fragment of the H-cluster [1], the other involves binding to the 2Fe subsite opposite the dithiolate bridge [2]. Our studies focus on delineation of the reduction products and reaction path of simple diiron compounds that are structural and/or compositional models of the diiron subsite of the H-cluster. A combination of electrochemical, spectroscopic, EXAFS and DFT studies of linked thiolato and phosphido-bridged diiron carbonyl compounds following reduction and during electrosynthesis provide an experimental precedent for predominant dihydrogen evolution through formation of dihydride species in cases where the coordination environment about the two iron atoms is similar [3]. In this case the Fe-Fe distance and core geometry are crucial to the kinetics of the system. While differentiation between the coordination environments of the two Fe atoms, possible involvement of hydrogen bonding via a dithiomethylamine bridge and the influence of the protein environment may result in a change in reaction path the chemical precedent needs to be established. In a related poster (Cheah, Tard, Pickett and Best) the results obtained from site differentiated diiron compounds are reported.

- 1 Cao, Z.; Hall, M. B. *J. Am. Chem. Soc.* **2001**, 123, 3734-42; Liu, Z.-P.; Hu, P. *J. Chem. Phys.* **2002**, 117, 8177-80.
- 2 Zhou, T.; Mo, Y.; Liu, A.; Zhou, Z.; Tsai, K. R. *Inorg. Chem.* **2004**, 43, 923-30; Bruschi, M.; Fantucci, P.; De Gioia, L. *Inorg. Chem.* **2002**, 41, 1421-9.
- 3 Borg, S. J.; Behrsing, T.; Best, S. P.; Razavet, M.; Liu, X.; Pickett, C. J. *J. Am. Chem. Soc.* **2004**, 126, 16988-99; Borg, S. J.; Tye, J. W.; Hall, M. B.; Best, S. P. *Inorg. Chem.* **2006**, in press; Cheah, M. H.; Borg, S. J.; Best, S. P. *submitted*.

**Modelling of Transition Metals Bound to Proteins:
Ligand Field Molecular Mechanics as a Fast Alternative to QM/MM**

R J Deeth

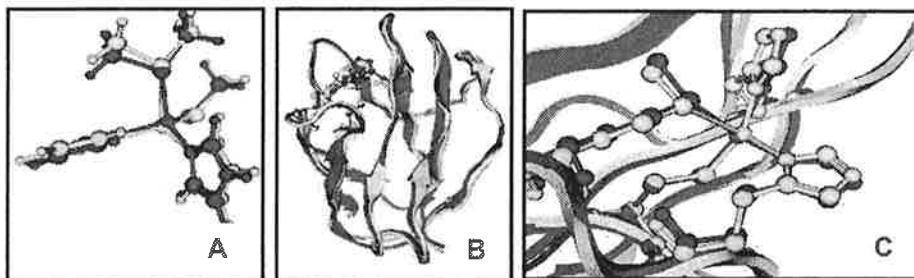
University of Warwick, Coventry, United Kingdom

r.j.deeth@warwick.ac.uk

Computer modelling of proteins containing electronically challenging metal centres like d^9 Cu(II) presents significant challenges for conventional molecular mechanics (MM). One is forced either to develop a highly specialised, highly specific force field which works for a particular active site (and no other) or, more usually, abandon MM altogether in favour of hybrid QM/MM methods.

While the quantum part of QM/MM implicitly handles the all-important electronic effects arising from the d electrons, compared to purely classical methods, QM/MM is relatively slow. Our response, therefore, has been to enhance MM by adding an empirical d -electron energy term based on ligand field theory – ligand field molecular mechanics (LFMM). The LFMM approach delivers quantum accuracy at MM prices for a range of copper(II) complexes and provides a detailed and accurate treatment even of the complex structural and energetic consequences of the Jahn-Teller effect.

It has now been applied to the Type I site of blue copper proteins and gives excellent results compared both to DFT calculations of models systems and the X-ray crystal structures of complete proteins. The critical feature of the LFMM is that the FF parameters are not restricted to a particular, specific coordination. For example, the model works equally well for the Cu-N bond of an isolated imidazole as the Cu-N bond of an imidazole which also happens to be part of a histidine attached to some protein backbone. The LFMM thus retains the same flexibility around the metal centre as a fully quantum approach but executes three to four orders of magnitude faster.



DFT (blue) and LFMM (yellow) structures for A: isolated Type I model complex $[\text{Cu}(\text{imid})_2(\text{SMe})(\text{Me}_2\text{S})]^+$; B: LFMM (blue) and X-ray crystal structure (yellow) of amicyanin (PDB 1AAC); C: Active site detail of amicyanin.

**Survival of Antarctic Bacteria in an Iron Desert.
Novel Strategies in Biomolecular Capture**

N Ejje, J Liu, A. A. H. Pakchung, R Codd

School of Chemistry, The University of Sydney, NSW 2006, Australia

r.codd@chem.usyd.edu.au

Siderophores are small organic molecules with high iron(III) affinities ($K_{\text{aff}} \sim 10^{40} \text{ M}^{-1}$) produced by marine and terrestrial bacteria in response to the poor availability of soluble iron(III), which, in an aqueous, oxic and pH-neutral environment, exists at concentrations (10^{-18} M) significantly below that required for viable microbial growth. Due to the low Aeolian iron influx in the Southern Hemisphere, Antarctic waters are the most iron-deficient on Earth. Coupled with the extreme cold (which might further depress the K_{sp} for $\text{Fe}(\text{OH})_3$), Antarctic bacteria will have evolved aggressive iron scavenging mechanisms, relative to other marine bacteria resident in more temperate waters. We have identified the production of hydroxamate-based siderophores from select strains of Antarctic bacteria when cultured in iron-deficient media at refrigerated conditions. Relative to phylogenetically-related bacteria adapted to middle-range temperatures ('mesophiles'), the yields of siderophores from cold-adapted (psychrophiles; 'psychros' from the Greek for 'cool') Antarctic bacteria are low, which has prompted us to develop a novel biomolecular capture technique for these targets. While over 500 siderophores have been documented, relatively few have been isolated in quantities required for spectroscopic and/or crystallographic characterization. Our biomolecular capture technique will enable a more complete molecular-level inventory of siderophores be built, which has significant implications to both the environment and human health. Furthermore, Antarctic bacteria have adapted the suite of membrane-bound and soluble proteins associated with iron-siderophore uptake and downstream processing to function at sub-zero temperatures. Here, we will also detail our novel chemical proteomics approach toward the isolation of iron-siderophore receptor proteins.

Pakchung, A.A.H., Simpson, P.J.L. and Codd, R. (2006). Life on Earth. Extremophiles Continue to Move the Goal Posts. *Environ. Chem.* 3: 77-93.

Nonheme {FeNO}^{6,7} landscapes: The first paramagnetic {FeNO}⁶ complex

A Ghosh, J Conradie, S Koch, S Lippard, T Harrop

¹University of Tromsø, N-9037 Tromsø, Norway, ²University of the Free State, Bloemfontein, South Africa, ³SUNY Stony Brook, New York, United States, ⁴Massachusetts Institute of Technology, Cambridge, MA, United States, ⁵Massachusetts Institute of Technology, Cambridge, MA, United States
abhik@chem.uit.no

We have carried out a comprehensive experimental and DFT study of nonheme {FeNO}^{6,7} complexes with trithiolate, trithiolatoamine (NS₃), and trithiolatophosphine (PS₃) supporting ligands. The tetrahedral S = 3/2 [Fe(*St*Bu)₃(NO)]⁻ complex exhibits a nearly linear FeNO group, while the analogous NS₃ complex exhibits a strongly bent FeNO unit. Use of the tripodal PS₃ ligand permits the isolation of a stable S = 1 {FeNO}⁶ complex, Fe(PS₃)(NO), with a linear FeNO group.

According to the DFT calculations, *trans* effects play a significant part in determining the ground states and potential energy surfaces of these complexes. Thus, the *trans* effect of the amine nitrogen of the NS₃ ligand appears to play a key role in shaping the bent FeNO unit of the [Fe(NS₃)(NO)]⁻ complex, while the even stronger *trans* effect of the phosphorus in the PS₃ ligand destabilizes the d_{z2} orbital (assumed to be aligned with the Fe-P vector) so much that the d_{z2} electron is lost altogether to generate the {FeNO}⁶ complex, Fe(PS₃)(NO).

Compartmentalised Nanoreactors and Dynamic Kinetic Resolutions

TH. Maschmeyer, A.F. Masters, A Fois

The University of Sydney, Sydney, Australia

th.maschmeyer@chem.usyd.edu.au

The fabrication and properties of polymer nanocapsules using Layer-by-Layer (LBL) self-assembly¹ represent an exciting area of research with widespread applications. The selective permeability of these capsules² has allowed for encapsulation of a variety of macromolecular catalysts (both chemical³ and enzymatic⁴) to form catalytic nanoreactors that are impermeable to macromolecules while allowing small molecular substrates and products to cross the membrane. Such nanoreactors have clear application to the protection of catalysts (particularly sensitive species such as enzymes⁴) from inhibitors, allowing the incorporation of many mutually-interfering catalysts into a single system by *compartmentalisation*. Dynamic Kinetic Resolution requires the combination of a selective catalyst (commonly an enzyme) with an *in situ* racemisation catalyst. These two types of catalyst are often incompatible.^{5,6,7}

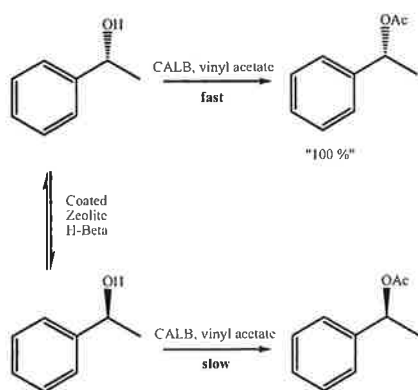


Figure 1 . Dynamic Kinetic Resolution of a typical secondary alcohol using coated Zeolite H-Beta nanoreactors and CALB, with vinyl acetate the acyl donor.

Herein we describe the encapsulation of the solid acid Zeolite H-Beta using polyelectrolytes and the combination of the resulting nanoreactors with the pH sensitive enzyme *Candida Antarctica* lipase B (CALB) for the Dynamic Kinetic Resolution of secondary alcohols, cf. Figure 1. The system using the encapsulated zeolite was shown to give much higher yields and enantiomeric excesses than were observed for that using a standard zeolite, illustrating the protective capabilities of the capsule and its benefits.

Encapsulation of the zeolite was confirmed in each case by fluorescence microscopy. Due to the basicity of the calcium carbonate template, only the directly coated zeolite was found to retain its acidic activity, but the templated method may be useful for applications requiring basic zeolites.

The zeolite nanoreactors were combined with lyophilised CALB and Dynamic Kinetic Resolution was attempted using several different solvents, substrate/catalyst ratios and substrates. The best results were achieved in octane, yielding a successful Dynamic Kinetic Resolution (~70 % yield of chiral products with >80% ee's)

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N-Heterocyclic Carbenes: Reactivity and Catalysis

K. J. Cavell

School of Chemistry, Cardiff University, Cardiff, United Kingdom

cavellkj@cf.ac.uk

N-heterocyclic carbenes (NHCs) are now well established as valuable ligands for a number of purposes. However, their application in catalysis has met with mixed success. Successes, such as the Grubbs metathesis catalyst, are rare at present. A reason for this is that many metal-NHC complexes are prone to decomposition via reductive elimination, leading to loss of the NHC ligand as imidazolium salt, and hence consequent loss of catalytic effectiveness.¹ Careful design of the NHC ligand and a selection of appropriate catalytic reactions may help reduce this problem.²

The reductive elimination step may be incorporated into a catalytic reaction in which the NHC/imidazolium salt becomes the substrate rather than a spectator ligand. Such a reaction provides a route into the catalytic formation of substituted heterocyclic rings, which represent valuable building blocks in the synthesis of pharmaceuticals.³

This lecture will look at aspects of the structure and reactivity of NHCs, and their applications in catalysis. New aspects of ligand development and catalyst design will be described.

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Hemilabile Behavior of Thioether-Functionalized N-Heterocyclic Carbene Ligands

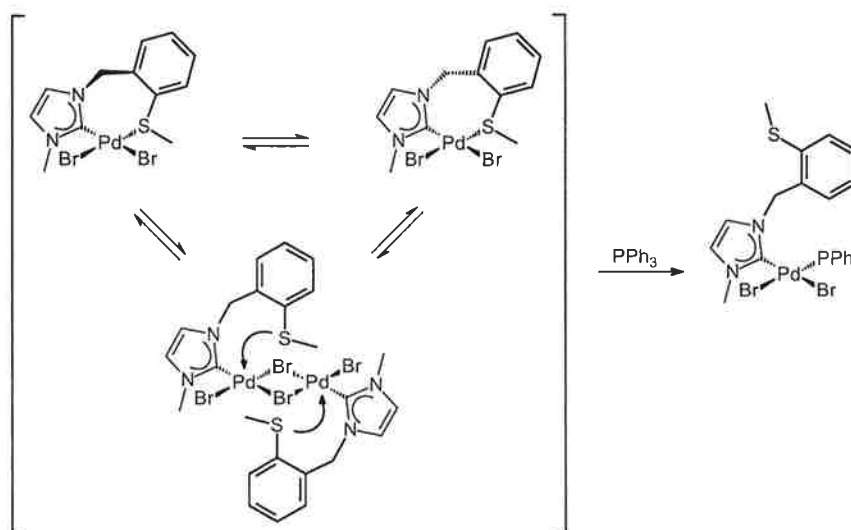
Han Vinh Huynh, Chun Hui Yeo, Joanne Hui Hui Ho

National University of Singapore, Singapore, Singapore

chmhhv@nus.edu.sg

N-heterocyclic carbenes (NHCs) have been the focus of intense research in organometallic chemistry and catalysis due to their unique properties. Of particular interest is a donor-functionalization of NHC ligands at their nitrogen atoms, since it offers both the possibility for hemilabile coordination as well as the opportunity to immobilize the resulting catalysts on polymer resins. To this point, several complexes with *N*-, *O*- and *P*-donor functionalized NHCs have been investigated. Examples of NHCs functionalized with a softer sulfur atom are surprisingly rare, and to the best of our knowledge, limited to two thiolate-NHCs and only one thioether-NHC. Although many of the above examples are potentially hemilabile ligands, no such behavior has been reported to date.

Here we present a versatile synthetic route to thioether-functionalized imidazolium salts and a study on the hemilabile coordination behavior of their corresponding NHC ligands in palladium(II) complexes.



**Highly Selective Olefin Oligomerisation:
Development of Chromium Based Ethylene Tri- and Tetramerisation Catalysts**

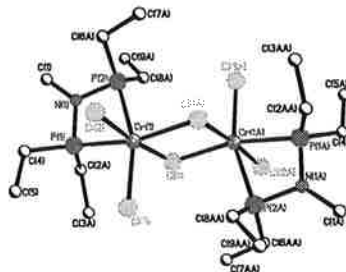
DS McGuinness¹, RP Tooze², JT Dixon³

¹University of Tasmania, Hobart, Tasmania, Australia, ²Sasol Technology UK, St Andrews, Fife, United Kingdom, ³Sasol Technology, Sasolburg, South Africa

david.mcguinness@utas.edu.au

The oligomerisation of ethylene is predominantly carried out in industry using transition metal catalysts that produce a geometric distribution of linear alpha olefins (LAOs). While the C₆-C₂₀ range is used on a large global scale as comonomers, as surfactant precursors, and in synthetic lubricant production, such distributions of LAOs do not closely match market demand. In particular, 1-hexene and 1-octene are in high demand due to their use as comonomers for polyethylene production (LLDPE). This has led to considerable recent interest in the selective oligomerisation of ethylene, particularly trimerisation to 1-hexene and tetramerisation to 1-octene.

A series of highly active and selective catalysts for ethylene trimerisation have been developed within the research laboratories of Sasol Technology.¹⁻² Additionally, we have recently disclosed the unprecedented tetramerisation of ethylene to yield 1-octene with selectivities up to ca 80%.³⁻⁴ This presentation will cover aspects of the development of these systems.



Gold Catalysis: Activity/Selectivity Profiles of Different Gold ComplexesA. S. K. Hashmi, J. A. Huck

Universität Stuttgart, Stuttgart, Germany

hashmi@hashmi.de

Gold complexes have recently become a hot topic in homogeneous catalysis.¹ In the initial publications for gold(III)² mainly AuCl₃ (occasionally AuBr₃) and for gold(I)³ mainly Ph₃PAuX were used as pre-catalysts. The process of exploring the catalytic activity and the catalytic selectivity of other gold complexes⁴ has just begun. On the other hand a broad variety of gold-catalyzed reactions are known today, but not only a large number of ligands but also different types of reactivity have to be explored.

We will report the selection of representative reaction types for a catalyst screening kit and show why the choice of the individual test substrates is critical. The setup for an efficient preparation and screening of different gold complexes by IR-thermography will be discussed. Interesting gold catalysts could be obtained this way. Coordination chemists preparing new gold complexes are invited to submit samples and thus to participate in this kind of screening process.

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Single-Molecule Magnets: A Molecular Approach to Nanoscale Magnetic MaterialsG. Christou*University of Florida, Gainesville, Florida, United States*

christou@chem.ufl.edu

Many present and future specialized applications of magnets require monodisperse, nanoscale magnetic particles, and the discovery that individual molecules can function as nanoscale magnets was therefore a significant development. Such a single-molecule magnet (SMM) functions as a single-domain magnetic nanoparticle that, below its blocking temperature (T_B), exhibits the classical macroscale property of a magnet, namely magnetization hysteresis. SMMs thus represent a molecular (or ‘bottom up’) approach to new nanoscale magnetic materials, offering all the advantages of molecular chemistry, particularly crystallinity, monodispersity, and solubility. SMMs are also true mesoscale particles, straddling the interface between classical and quantum behaviour by also exhibiting quantum tunnelling of magnetization (QTM). As a result, SMMs have potential applications in high-density information storage, with each molecule storing one bit, as well as in quantum computing as quantum bits (qubits), since the QTM allows each molecule to exist in a quantum superposition of states.

The first SMMs were the $[\text{Mn}_{12}\text{O}_{12}(\text{O}_2\text{CR})_{16}(\text{H}_2\text{O})_4]$ family with a spin ground state of $S=10$. Another well-studied SMM family are the $[\text{Mn}_4\text{O}_3\text{X}(\text{O}_2\text{CR})_4(\text{dbm})_4]$ compounds with $S=9/2$. These two families have been particularly rich sources of data on the sensitivity of the magnetic properties and the QTM to small structural perturbations, the environment and site-symmetry of the molecules within the crystal, the effect of adding extra electrons one at a time, and exchange interactions with neighbouring molecules. The latter can in some cases be a problem for certain studies or potential applications, and in other cases be beneficial in providing a means to modulate the magnetic properties in desirable ways. More recent work has extended the field to very large SMMs, either in terms of molecular size or magnitude of S , or both. This talk will overview our work in this area.

Thermal and Photomagnetic Properties of New Iron(II) Spin-Crossover Materials

KS Murray¹, B Leita¹, B Moubaraki¹, SM Neville¹, C Schneider¹, JD Cashion³, JF Letard²

¹*School of Chemistry, Monash University, VIC, Australia,* ²*ICMCB, Bordeaux, France,* ³*School of*

Physics, Monash University, VIC, Australia

keith.murray@sci.monash.edu.au

Enormous strides have been made in recent years in both fundamental and applied aspects of iron(II) compounds displaying spin switching properties derived from their bistable properties [1]. In collaborative work with Kepert and coworkers, we have studied dinuclear, covalently bridged Fe(II)Fe(II) compounds (at Monash University) and extended network materials, some displaying porosity and guest induced switching (in Sydney). Here the syntheses, structural, magnetic, Mossbauer spectral and LIESST (light induced excited state spin trapping) properties of new mononuclear, dinuclear and 1D chain Fe(II) crossover materials are discussed. The results are analysed in terms of the relevant mechanism of the spin transition occurring, involving, for example in dinuclear cases, the spin states [HS-HS], [LS-LS] and the elusive [HS-LS] 'ordered' state, the latter found in 2-step transitions.

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Molecularly Derived Nanomaterials

GA Koutsantonis¹, Buckley C², Douce L³, Harrowfield JM⁴, Kraatz B⁵, Lengkeek N¹,

Nealon G¹, Orlowski G⁵, Paskevicius M², Skelton BW¹, White AH¹

¹*Chemistry, BBCS, University of Western Australia, Perth, WA, Australia,* ²*Department of Applied Physics, Curtin University of Technology, Perth, WA, Australia, 6845,* ³*IPCMS-GMO23, Strasbourg, France,* ⁴*Institut de Science et d'Ingénierie Supramoléculaires, Université Louis Pasteur 8, Strasbourg, France,* ⁵*Department of Chemistry, University of Saskatchewan, Saskatoon, Canada.*

gak@chem.uwa.edu.au

Metal ion coordination is one of the most powerful mechanisms for the spatial ordering of organic ligands (being almost ubiquitous in Nature) and that macrobicyclic ligand molecules, and cage amines in particular, offer a platform of enormous versatility for the construction of functional supermolecules, the present work is offered as one which is both timely and likely to produce a range of new materials suitable for use in molecular electronics, analytical sensing, medical therapy, molecular machines and electrocatalysis, to mention but some of the possibilities.

We have utilised a range classical organometallic and inorganic complexes as viable scaffolds for the construction of metal containing surfactants, polymers, molecular wires, magnetic materials and catalysts.

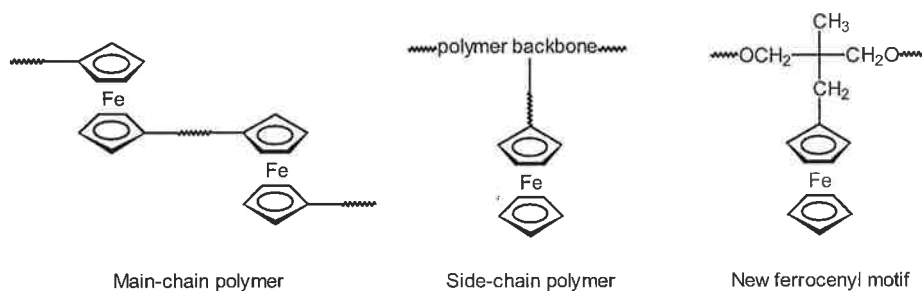
Specifically, conjugated organometallic molecules with additional coordination tectons are being investigated as tectons for the production of molecular wires. Cage amines are being incorporated into polymers for sensing applications and similar cage amines containing surfactant tails have been arranged into complex three dimensional arrangements on the nanoscale.

The nature of the study is long term but potential applications are starting to present themselves.

Ferrocene Based Monomers for the Synthesis of Polyesters And NylonsCJ McAdam, BH Robinson, J Simpson*University of Otago, Dunedin, New Zealand*

mcadamj@alkali.otago.ac.nz

The two main architectures available for ferrocenyl containing polymers are main-chain polymers, in which the metallocene is incorporated into the backbone, and side-chain polymers, where it is attached in some means to a polymer backbone [Manners, Hudson]. Of these, the latter offers the best opportunities for conventional macroscopic properties of the polymer and economic viability. Numerous ferrocenyl polyesters are reported in literature, but these are almost exclusively main-chain 1,1'-ferrocenecarboxylic acid / aromatic diol derivatives. This paper reports a new ferrocenyl substituted propylene glycol suitable for polyester synthesis via condensation or co-condensation. The monomer is also easily modified and provides a versatile building block for small molecule ferrocenyl assemblies.



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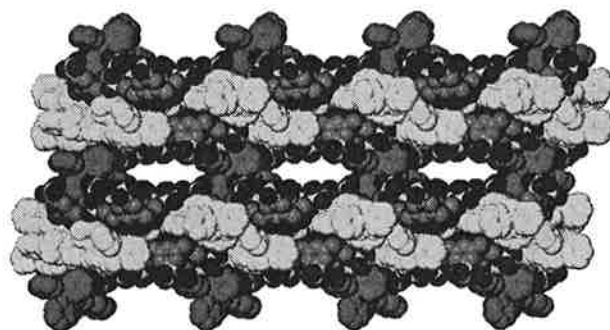
Towards Engineering Nanoporosity in Hybrid Organic - Metal Ionic Solids

M Makha, A. N. Sobolev, C. L. Raston

The University of Western Australia, Perth, Australia

mmakha@chem.uwa.edu.au

Nanoporosity in self assembled molecular framework are gaining prominence and offering potential solutions to many current problems involving molecular separation, sensing, heterogeneous catalysis and stabilization or ordering of nanoparticles. The paper will focus on water soluble calixarenes and will present recent work on the use of macrocyclic calixarenes sulfonates as molecular platform in conjunction with metal and organic ions of various spatial geometries to construct molecular assemblies of nano dimensions. Molecular assemblies of organic ions can contain large channels or voids as suitable environments for controlled chemical transformations, ie 'nanoreactors' or as materials for ion exchange chromatography.¹ We have recently demonstrated the accessibility of such molecular assemblies via the interaction of polyanionic calixarene sulfonate with phosphonium cations and others guest species.² Ionic solids based on organic ions posses properties with potential applications in separation science and biological membrane mimics, and, in addition, specific pore sizes are in demand for nanofiltration of gaseous mixtures and in catalysis. Functionalisation and balance of the hydrophobicity/hydrophilicity of the inner lining of these channels will also be discussed.



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New Families of Spin Clusters as Potential Molecular Nanomagnets

C Boskovic¹, KG Alley¹, A Mukherjee¹, AM Palmer¹, Y Mulyana¹, BF Abrahams¹, B Moubaraki², KS Murray², R Bircher³, HU Guedel³, R Clerac⁴

¹*School of Chemistry, University of Melbourne, Vic, Australia,* ²*School of Chemistry, Monash University, Vic, Australia,* ³*Department of Chemistry and Biochemistry, University of Berne, Berne, Switzerland,* ⁴*Centre de Recherche Paul Pascal, CNRS, Pessac, France*

c.boskovic@unimelb.edu.au

New families of spin clusters have been obtained following the reaction of simple transition metal salts or preformed polynuclear complexes with polydentate proligands that feature polyalcohol and amine or imine functionalities. These polynuclear $\{M_n\}$ complexes ($n = 2-12$) of paramagnetic d and f block transition metals incorporate multiple ligands that simultaneously chelate and bridge the metal centres, giving rise to complex and unusual structures (Figure 1). This includes two and three dimensional coordination polymers where discrete spin clusters act as the constituent building blocks. Diverse magnetic behaviour results from these novel structures, which has been investigated in detail by conventional and low temperature SQUID magnetometry and inelastic neutron scattering.

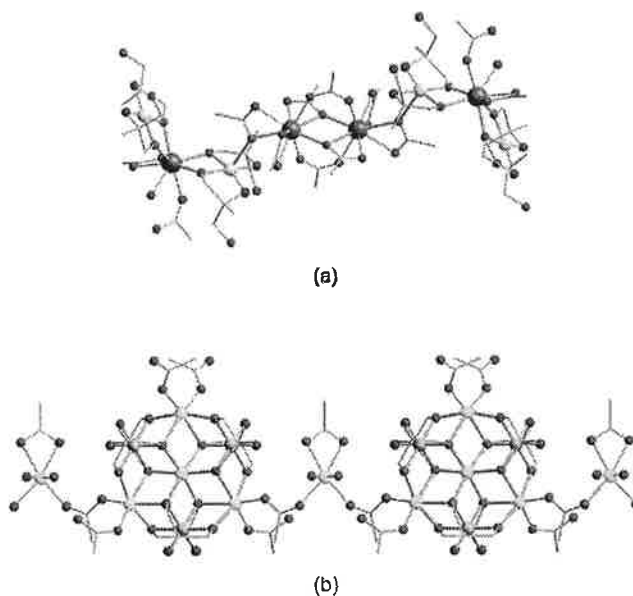


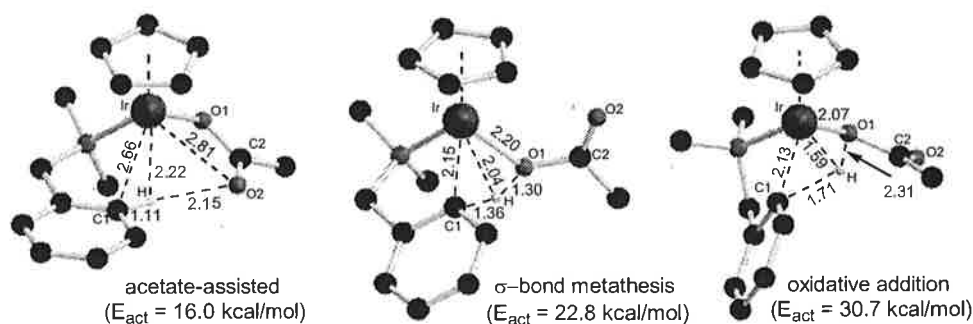
Figure 1. Structures of (a) a $\{Cu_4Tb_4\}$ spin cluster and (b) a coordination polymer of $\{Co_7\}$ spin clusters

Acetate-Assisted Cyclometallation: A New Mechanism for C-H Activation?SA Macgregor¹, DL Davies², O Al-Duaij², SMA Donald¹, M Poelleth¹¹Heriot-Watt University, Edinburgh, United Kingdom,²University of Leicester, Leicester, United Kingdom

s.a.macgregor@hw.ac.uk

Dimethylbenzylamine undergoes cyclometallation under mild conditions when treated with $[\text{Pd}(\text{OAc})_2]$ ¹ or with $[\text{IrCl}_2\text{Cp}^*]_2$ in the presence of NaOAc.² The acetate may play a number of roles in (i) protecting a vacant site by chelation (ii) making the metal more electrophilic (iii) directing the C-H activation by H-bonding or (iv) acting as an intramolecular base.

We have studied the mechanism of these reactions by DFT methods.^{3, 4} For the iridium complex, calculated transition states for an acetate-assisted electrophilic activation, a σ -bond metathesis and oxidative addition pathway are shown below.⁴ Related cyclometallations of N-donor ligands with $[\text{MCl}_2\text{Cp}^*]_2$ (M = Rh, Ir) and $[\text{RuCl}_2(p\text{-cymeme})]_2$ in the presence of acetate have also been studied and give further insight into the mechanism.



We will discuss the mechanism of these reactions particularly with respect to the role of the metal and acetate and the implications for finding new systems for C-H activation.

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N-Heterocyclic Carbene Complexes Derived from Azolium-Linked Cyclophanes

M V Baker, D H Brown, R A Haque, V J Hesler, P V Simpson, B W Skelton, A H White

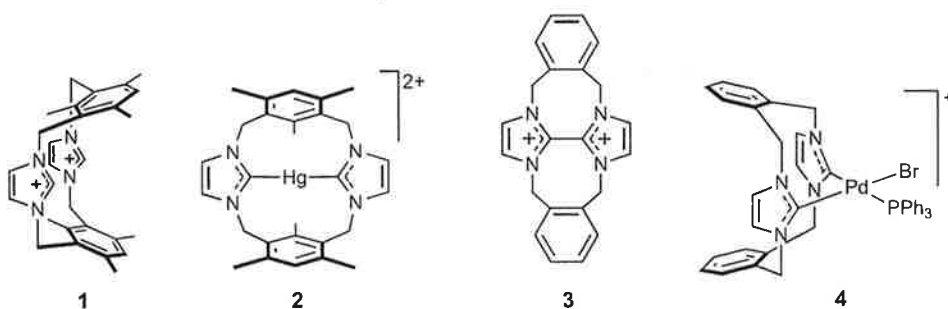
Chemistry M313, The University of Western Australia, Crawley, WA, Australia

mvb@chem.uwa.edu.au

This presentation will describe recent studies of metal complexes of chelating *N*-heterocyclic carbene (NHC) ligands, in which the NHC groups are part of a cyclophane structure.

Typically, the NHC ligands are derived from azolium cyclophanes (e.g. **1**). The cyclophane framework imposes geometric constraints on NHC ligands that result in interesting metal coordination environments and we have found unprecedented structures amongst, for example, Ag(I) and Hg(II) complexes (e.g. **2**). In some cases, the cyclophane framework is amenable to functionalisation at its periphery, to alter properties such as solubility of NHC complexes or electron donating ability of the NHCs, without changing the geometry of the metal coordination site.

As an alternative to established routes to NHC complexes, we have explored oxidative addition of biimidazolium salts (e.g. **3**) to low-valent metals to yield cyclophane NHC complexes (e.g. **4**). Recent studies of catalytic activity of complexes such as **4** will be discussed.



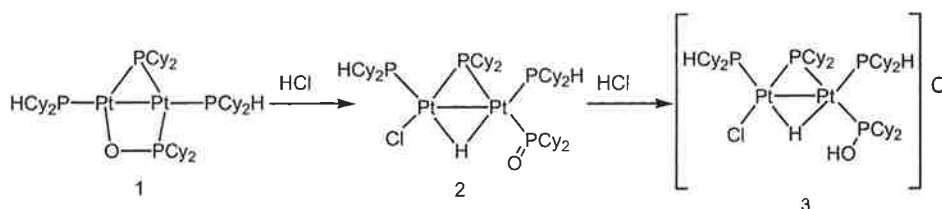
Synthesis of μ -hydrido- μ -phosphido Diplatinum Complexes by Protonation of a Dinuclear Phosphinito Complex of Pt(I)

M. Latronico¹, P. Mastrorilli¹, C.F. Nobile¹, V. Gallo¹, U. Englert², F. Polini¹

¹*Dept of Water Engineering and of Chemistry, Polytechnic of Bari, Bari, Italy,* ²*Institut of Inorganic Chemistry, Technical University of Aachen, Aachen, Germany*

p.mastrorilli@poliba.it

We deemed it worthwhile to study the protonation reaction of the Pt(I) complex $[(\text{Cy}_2\text{PH})\text{Pt}(\mu\text{-PCy}_2)(\mu^2\text{P},\text{O}-\mu\text{-Cy}_2\text{PO})\text{Pt}(\text{Cy}_2\text{PH})]$ (*Pt-Pt*) (**1**) due to the site selectivity potentially associated with this molecule. In principle, in fact, the attack of an acidic proton may occur onto one of the metals, on the metal-metal or the metal-phosphorus bond, or onto the oxygen atom of the phosphinito bridge.

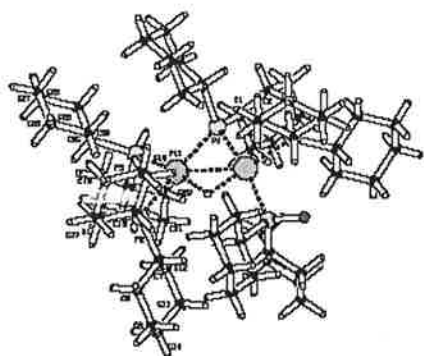


Reacting **1** with excess HCl resulted in the quantitative transformation into the cationic complex **3**, the product of the uptake of two molecules of acid. Monitoring the reaction by multinuclear NMR spectroscopy showed the intermediacy of an adduct **1**·HCl, and of the diplatinum species **2**.

The possible structure of the intermediate **1**·HCl and a plausible reaction mechanism will be presented.

The results obtained in the reactions of **1** with different protic sources such as HBF₄, PhOH and Cy₂POH will also be discussed. In particular, reactions with the strong acid HBF₄, having a poorly coordinating anion, gave complexes structurally analogous to **2** and **3**, but with the solvent (CH₃CN)

coordinated to one platinum in place of Cl; the reactions with the weak acids PhOH and Cy₂POH gave the bridging hydride species $[(\text{Cy}_2\text{PH})\text{Pt}(\mu\text{-PCy}_2)(\mu\text{-H})\text{Pt}(\text{X})(\kappa\text{P-Cy}_2\text{PO})]$ (*Pt-Pt*) (X = OPh or Cy₂PO) with incorporation of only one molecule of acid. The product obtained with Cy₂POH was crystallised as water adduct and its structure, featuring a short Pt-Pt distance of 2.8502(6) Å, determined by XRD.



Insertion of Molecular Oxygen into a Palladium(II) Hydride Bond

MC Denney¹, NA Smythe¹, KL Cetto¹, RA Kemp², KI Goldberg¹

¹*University of Washington, Seattle, Washington, United States,* ²*University of New Mexico and Sandia*

National Laboratory, Albuquerque, New Mexico, United States

Melanie.Denney@csiro.au

Insertion of molecular oxygen into a palladium(II) hydride bond has been observed to form an (η^1 -hydroperoxo)palladium(II) complex. The hydroperoxo palladium(II) product has been crystallographically characterized. A second-order rate law (first-order in palladium and first-order in oxygen) is observed for the reaction, and a large kinetic isotope effect implicates Pd-H bond cleavage in the rate-determining step. The results of studies with radical inhibitors and light suggest that the reaction does not proceed by a radical chain mechanism. In solution, the palladium(II) hydroperoxide is slowly converted to a palladium(II) hydroxide complex.

Metal Alkynyl Dendrimers with Switchable NLO Properties

M.G. Humphrey, M.P. Cifuentes, M. Samoc

ANU, ACT, Australia

Mark.Humphrey@anu.edu.au

Organometallic dendrimers are of interest because the metal may imbue the dendritic material with specific optical, electronic, magnetic, catalytic, and other properties. Nonlinear optical (NLO) materials with a dendritic construction may have large nonlinearities, coupled to favorable transparency and processing characteristics, because the branching points in arylalkynyl dendrimers may permit extensive π -delocalization without appreciable red-shift of the important linear optical absorption band(s). This presentation will summarize synthetic procedures to bis(diphosphine)ruthenium-containing arylalkynyl dendrimers containing 18 electron metal centers, including systematically-varied dendrimer examples peripherally functionalized by electron-donating (NEt_2) or electron-withdrawing (NO_2) substituents, together with studies of their electrochemical, linear and nonlinear optical properties. In particular, facile interconversion of alkynyl/vinylidene complex pairs (by protonation/deprotonation sequences) and Ru(II)/Ru(III) complex pairs (by oxidation/reduction sequences) affords the possibility of dendritic materials with switchable NLO properties.

The Rapidly Changing Nature of f Element Reduction Chemistry

W. J. Evans

Univ Of California, Irvine, Irvine, California, United States

wevans@uci.edu

For nearly 90 years, reductive divalent lanthanide chemistry was thought to be available only from three ions, Eu^{2+} , Yb^{2+} , and Sm^{2+} . The existence of such well-established boundaries is typical of fundamental, heavily-studied reactions like reduction. However, in the past several years, four new ways of accomplishing divalent lanthanide reduction chemistry have been discovered. These involve the discovery of new molecular divalent oxidation states and several methods of achieving reductive chemistry from complexes containing redox-inactive trivalent ions. This lecture will survey these changes and present the latest methods for extending divalent reductive lanthanide chemistry to the entire lanthanide series including diamagnetic La^{3+} , Y^{3+} , and Lu^{3+} . In addition, the utility of combining the new methods of reduction with traditional redox couples will be discussed as an approach to multi-electron reduction. Molecular species that deliver from 2 to 8 electrons per mole will be described. These relatively rapid changes in this old fundamental reaction demonstrate how much new chemistry is still waiting to be developed in "mature" areas of basic chemistry.

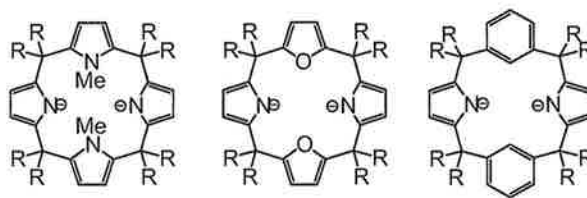
Macrocyclic Control of Organolanthanide Chemistry

MG Gardiner

School of Chemistry, University of Tasmania, Hobart TAS, Australia

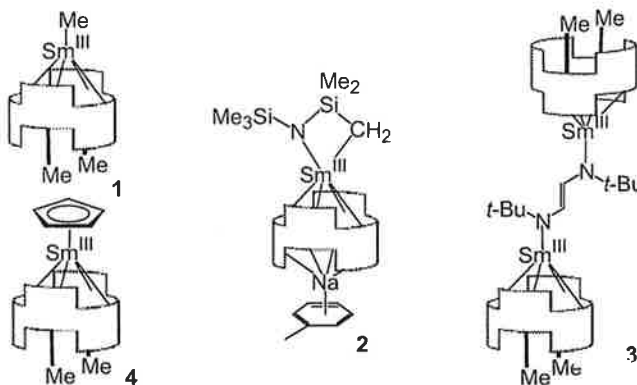
mgg@postoffice.utas.edu.au

We have been studying lanthanide complexes derived from various modified calix[4]pyrroles with the view to realising their utility as alternatives to the ubiquitous bis(pentamethylcyclopentadienyl) ligand set. I will present a summary of the structural features of each complex type, the pros and cons of the different systems, as well the unusual reactivities and applications that we are pursuing.



As a taster, we have observed all extremes of reactivity in these systems, ranging from;

- “ought to be reactivity species” that are dead in the water due to steric congestion **1**,
- to “ought to be inert functionalities” that undergo reactions due to effects of the macrocycle **2**,
- to an almost unheard of *reversible* Sm(II)/Sm(III) redox process **3**,
- to Sterically Induced Reduction chemistry (a new form of ligand-based reduction chemistry) **4**,



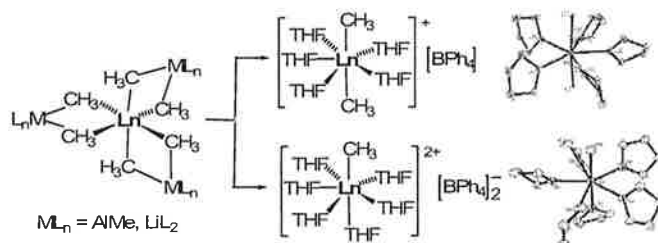
Cationic Alkyl Complexes of the Rare Earth Metals: Synthesis, Structure, and Reactivity

J. Okuda

Institute of Inorganic Chemistry, RWTH Aachen University, Aachen, Germany

jun.okuda@ac.rwth-aachen.de

Alkyl cations of trivalent rare-earth metals have recently been shown to play an important role as active species in the rare-earth metal catalyzed homogeneous ethylene, 1-hexene, and 1,3-diene polymerization.[1] These highly Lewis acidic species combine an electrophilic metal center with a nucleophilic alkyl group. In general, cationic rare-earth metal alkyl complexes are formed by reacting neutral $[\text{LnR}_3\text{L}_n]$ complexes with Brønsted or Lewis acids. In the presence of suitable neutral donors such as THF and crown ethers,[2] robust cationic alkyl complexes can be isolated and structurally characterized. Methyl cations have become available through the use of formally anionic intermediates, previously isolated as $[\text{LiL}_2]_3[\text{LnMe}_6]$, but which also contains derivatives such as $[\text{LiL}_2]_3[\text{Ln}_2\text{Me}_9]$. Efficient ethylene [3a] and stereoselective 1,3-diene polymerization [3b] can be achieved in solution by controlling the size of the cationic lanthanide center and the nature of the cocatalysts consisting of aluminum trialkyl and $[\text{NMe}_2\text{HPh}][\text{B}(\text{C}_6\text{F}_5)_4]$. Model studies suggest that novel mono(alkyl) dications $[\text{Ln}(\text{CH}_2\text{X})(\text{THF})_n]^{2+}$ ($\text{X} = \text{H}, \text{SiMe}_3$) are also generated.[3] Synthesis, structural, and reactivity studies of alkyl cations such as $[\text{Ln}(\text{CH}_2\text{X})_n(\text{THF})_{7-n}]^{(3-n)+}$ ($n = 1, 2$) will be presented.



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- [2] (a) Arndt, S.; Spaniol, T. P.; Okuda, J. *Chem. Commun.* **2002**, 896. (b) Elvidge, B. R.; Arndt, S.; Zeimentz, P. M.; Spaniol, T. P.; Okuda, J. *Inorg. Chem.* **2005**, 44, 6777.
- [3] (a) Arndt, S.; Spaniol, T. P.; Okuda, J. *Angew. Chem. Int. Ed.* **2003**, 42, 5075. (b) Arndt, S.; Beckerle, K.; Zeimentz, P. M.; Spaniol, T. P.; Okuda, J. *Angew. Chem. Int. Ed.* **2005**, 44, 7473.

Subtle Steric Control in Organoamidolanthanoid Chemistry

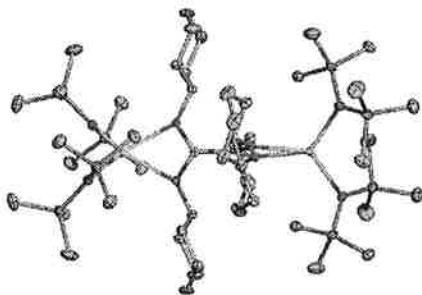
P.C. Junk

Monash University, Clayton, Vic, Australia

peter.junk@sci.monash.edu.au

New chemistry involving rare earth complexes of the formamidinato ligands will be discussed. Synthetic methods involving classical metathesis reactions, redox transmetallation/ligand exchange, high temperature metathesis and high temperature solvent-free methods will be presented and the differences in products from these reactions will be highlighted.

The β -dinitrogen ligands of interest are the formamidinates where the steric bulk of the ligands can be varied sufficiently to allow for optimization of bulkiness to subtly engineer unusual chemistry and structures. Structures and reactivity of the interesting rare earth compounds arising from this variety of synthetic approaches will be presented.



References

Steric Engineering of C-F Activation with Lanthanoid Formamidinates

ML Cole, GB Deacon, PC Junk and K Konstas, *Chem. Comm.*, **2005**, 1581-3. HOT PAPER

The synthesis of a sterically hindered samarium(II) bis(amidinate) and conversion to its homoleptic trivalent congener

ML Cole and PC Junk, *Chem. Comm.*, **2005**, 2695 - 2697

Determination of Linear Agostic Interactions in Early Transition Metal Complexes

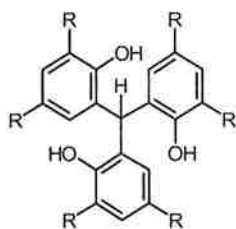
M. Lein, A.J. Nielson, P.A. Schwerdtfeger, J.M. Waters, J.A. Harrison

Massey University at Auckland, Auckland, New Zealand

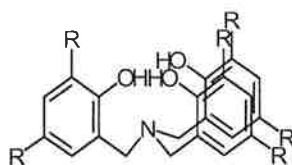
a.j.nielson@massey.ac.nz

Crystal structure determinations show that the coordination mode for the tris(hydroxyphenyl)methane ligand $[\text{CH}(\text{ArOH})_3]$ (ligand type **I**) in the anion $[\text{CH}(\text{ArO})_3\text{TaCl}_3]^-$ and the complex $[\text{CH}(\text{ArO})_3\text{Ti}(\text{NEt}_2)]$ is such that the trityl C-H hydrogen lies on the inside of a cage and makes a close approach to the metal. A crystal structure determination shows that on reaction of the tris(hydroxybenzyl)amine ligand, $[\text{N}(\text{ArOH})_3]$ (ligand type **II**) with $[\text{Zr}(\text{O}^n\text{Bu})_4]$, the nitrogen atom becomes protonated giving the di-zwitterionic complex $\{[\text{NH}^+(\text{ArO})_3]_2\text{Zr}^{2-}\}$ in which the N-H hydrogen lies on the inside of a cage and points directly at the metal. Density functional (DFT) calculations at the B3LYP level show full models of these complexes are in good agreement with the crystal structures. The interaction of the C-H or N-H bonding electron density with metal orbitals were studied using NBO and Bader analyses. Other d^0 zirconium and hafnium complexes of these ligands as well as d^2 molybdenum complexes were studied using theoretical methods as reactions of the ligands with the various metals can not be guaranteed to produce the required trityl or benzylammonium hydrogen in the required inside position. The results show that the trityl C-H bonding electron density interacts significantly with an unfilled metal orbital resulting in a linear agostic interaction while the benzylammonium N-H bonding interaction with the metal is insignificant.

I



II



**Discrete and Polymeric Fluoride-Bridged Metallacycles Prepared from Linked
Bis(pyrazolyl)methane Ligands and Fluoride Abstraction from Tetrafluoroborate Anion**

D. L. Reger¹, R. P. Watson¹, J. R. Gardinier², M. D. Smith¹, P. J. Pellechia¹

¹*University of South Carolina, Columbia, South Carolina, United States,* ²*Marquette University,*

Milwaukee, Wisconsin, United States

watson@mail.chem.sc.edu

Reactions of the arene-linked bis(pyrazolyl)methane ligand 1,3-bis[bis(1-pyrazolyl)methyl]benzene (*m*-[CH(pz)₂]₂C₆H₄, **L_m**) with BF₄[−] salts of late d-block metals result in fluoride abstraction from BF₄[−] and formation of compounds comprising discrete fluoride-bridged metallacyclic cations. Treatment of M(BF₄)₂·*x*H₂O (M = Fe, Co, Cu, Zn; *x* = 5–6) with **L_m** leads to the complexes [M₂(μ-F)(μ-**L_m**)₂](BF₄)₃ in which a single fluoride ligand and two **L_m** molecules bridge the two metal centers. The reaction of Ni(BF₄)₂·6H₂O or [Cd₂(thf)₅](BF₄)₄ with **L_m** yields [M₂(μ-F)₂(μ-**L_m**)₂](BF₄)₂ (M = Ni, Cd), which contains dimeric metallacyclic cations in which two fluoride and two **L_m** ligands bridge the metal centers. Similarly, equimolar amounts of the mesitylene-based ligand 1,3,5-tris[bis(1-pyrazolyl)methyl]benzene (1,3,5-[CH(pz)₂]₃C₆H₃, **L³**) and Zn(BF₄)₂·5H₂O react to give the related monofluoride-bridged complex [Zn₂(μ-F)(μ-**L³**)₂](BF₄)₃, in which one bis(pyrazolyl)methane unit on each ligand remains unbound. The more flexible, ethylene-linked ligand 1,1,4,4-tetrakis(1-pyrazolyl)butane (CH(pz)₂(CH₂)₂CH(pz)₂, **L2**) also reacts with Zn(BF₄)₂·5H₂O to afford a fluoride-bridged complex, but in this compound, the F[−] ligands bridge in an *exo*-manner and link adjacent zinc metallacycles into infinite chains. Preliminary magnetic studies carried out on the iron compound indicate antiferromagnetic coupling between the metal centers.

Scorpions and Crowns

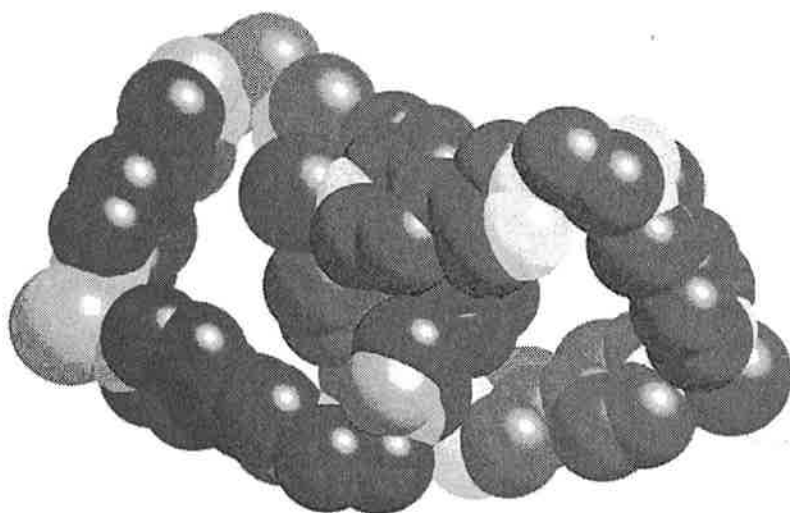
S.R. Batten, M. Duriska, J. Lu, D.R. Turner, A.S.R. Chesman, P. Turner, J. McKinnon, P. Jensen, K.S. Murray, B. Moubaraki, L. Spiccia, M.J. Belousoff

Monash University, Clayton VIC Australia, University of Sydney, Sydney NSW Australia,

University of Western Australia, WA Australia

stuart.batten@sci.monash.edu.au

We have designed and synthesised a variety of new bridging ligands based on scorpionates (polypyrazolylborates), azacrowns, and other related ligands. Our ultimate aim is to synthesise new coordination polymers and supramolecules which are chemically active after assembly. In pursuit of this aim, we have unearthed some fascinating new chemistry and numerous interesting structures. Aspects of this work to be discussed include homogeneous catalysis, heterogeneous catalysis, coordination polymers, hydrogen bonded networks, hollow nanometer sized molecular spheres ('nanoballs'), porous structures containing only weak C-H...N intermolecular interactions, coordination polymers containing channels lined with uncoordinated pyridyl groups, a new category of bridging ligands in which the bridge length is controlled by the presence and nature of included cations, and a [2]-catenane.



New Exciting Solid State Cluster Compounds

Tilo Söhnel

Department of Chemistry, The University of Auckland, Auckland, New Zealand

t.soehnel@auckland.ac.nz

The search for novel compounds with interesting electrical and magnetic properties is one of the most exciting areas of current inorganic solid state chemistry. Mixed main group metal - transition metal cluster compounds seem to be especially promising but have not been studied extensively in the past.

First results have been obtained in the systems M/Sn/O (M = Ru, Os, Ir), Ru/M/Sn/O (M = Si, Al, Mn, Fe, Co, Zn, Mg), Fe/Si/Sn/O and Ir/M/Sn/O (M = Fe, Co, Ru). The central and most striking structural feature of all these oxidic clusters is the formation of Sn₆-octahedra, which are filled with the different transition metals. These [MSn₆]-octahedra are either isolated or condensed via common corners and edges forming one-dimensional endless chains or three-dimensional networks. With the decrease of metal to oxygen ratio the coordination state of the condensation of the [MSn₆]-octahedra increases systematically from compound to compound. Compounds which are not showing condensation of the [MSn₆]-octahedra are [RuSn₆](M_xO₄)₂ (M = Si, Al) and the very recently discovered [RuSn₆](MO₄)O₄ (M = Mn, Fe, Co, Zn, Mg), respectively (Fig. 1). The condensation of the [MSn₆]-octahedra via vertices has been observed in such compounds as M₃Sn₁₅O₁₄ (M = Ru, Os), Ir₁₀Sn₄₅O₄₄, Ru₂Ir₂Sn₁₉O₁₈ and Ir₄FeSn₁₈O₁₉. The first example of a partly side-linkage is the incommensurably modulated compound Ir₃Sn₈O₄. This paper gives an overview about the preparation, crystallographic and spectroscopic characterisation of this new group of cluster compounds.

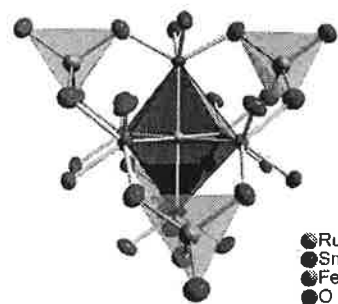


Fig. 1 Crystal structure of RuSn₆(FeO₄)O₄

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- [3] T. Söhnel, F. E. Wagner; *Proceedings of the IXth European Conference on Solid State Chemistry*, September, 2003, Stuttgart, Germany, 238.
- [4] T. Söhnel; In: M. Lein, P. Schwerdtfeger (eds.), *Proceedings of the First German / New Zealand Workshop on Heavy and Superheavy Elements*, Palmerston North, New Zealand, Massey University Press, 2005, 135.

Study of Catalysts Based on Non-Precious Metals for Applications in PEM Fuel Cells

D. Bizzotto¹, S.A. Campbell², K.A.R. Mitchell¹, R.R. Parsons¹, A. Sode¹, D. Susac¹, M. Teo¹, K.C. Wong¹, P.C. Wong¹, L. Zhu¹

¹*University of British Columbia, Vancouver, BC, Canada,*

²*Ballard Power Systems, Burnaby, BC, Canada*

karm@chem.ubc.ca

The search continues for catalysts, based on non-precious metals, that can act as cathodes in proton exchange membrane (PEM) fuel cells. This is motivated by the cost of Pt for the mass production of automobiles using currently available technology. Key challenges for the development of new catalytic materials for this application concern activity for oxygen reduction, stability in acidic environment, and open circuit potential (OCP). Our research focuses on thin-film materials prepared by magnetron sputtering, and formed from Fe, Co and/or Ni in combination with S or Se. A fundamental approach is emphasized in which performances of the model catalysts are evaluated against a Pt standard. This paper will review the new information gained so far by characterizing these catalysts with such techniques as scanning Auger microscopy, X-ray photoelectron spectroscopy, micro-Raman spectroscopy and X-ray diffraction, before and after application of electrochemical tests. Thin films have been produced with OCP values approaching 0.9 V (vs. reversible hydrogen electrode).

Complexes of Thiophene Derivatives as Potential Metallomesogens

M. S. Thomas, S Lotz, M Landman

¹*University of Limpopo, Sovenga, South Africa*, ²*University of Pretoria, Pretoria, South Africa*

maryt@ul.ac.za

The study involved the synthesis and structural characterization of new transition metal complexes of thiophene derivatives that have (potential) liquid crystalline properties. Thiophene has been selected because of its stability and versatility in lending itself to synthetic modification and hence forms links in chain structures for rod-like metallomesogens. Thiophene, when compared with 1,4-disubstituted benzene units, can change considerably the polarity, polarizability and also the geometry of the compounds, altering the types of mesophases, phase transition temperatures, dielectric constants and other properties of mesogens.

The reactions of a series of 5-alkyl-2-thiophenedithiocarboxylates with nickel(II) chloride formed two types of complexes: (i) blue mononuclear nickel(II) complexes with two terminal dithiocarboxylate ligands, $[\text{NiS}_2\text{CTR}]_2$ (T = 2,5-disubstituted thiophene); and (ii) violet mononuclear nickel(II) complexes with perthio- and dithiocarboxylate ligands, $[\text{Ni}(\text{S}_3\text{CTR})(\text{S}_2\text{CTR})]$ (R = alkyl groups).

The blue monomers are preferred for the shorter alkyl chains (C_4 and C_6), and the violet compounds for the longer chains (C_8 , C_{12} and C_{16}).

The thermal properties of the complexes were studied by using differential scanning calorimetry (DSC) and polarising optical microscopy (POM). Nickel complexes of the violet type with longer alkyl chains (C_8 and C_{12}) showed liquid crystalline properties.

Zinc(II) complexes analogous to nickel(II) complexes were prepared similarly. A crystal structure determination of one of those complexes revealed the fusion of two monomers to give a dimeric structure with bridging sulfur atoms, $[\text{Zn}_2((\mu)\mu\text{-S}_2\text{CTR})_2(\text{S}_2\text{CTR})_2]$. Although an irregular melting pattern was observed, the complexes did not show any liquid crystalline properties.

The results of this study will be presented in the conference.

Fabricating Composite Hydrosols of Fullerene Nano-Whiskers Shrouded by Silver

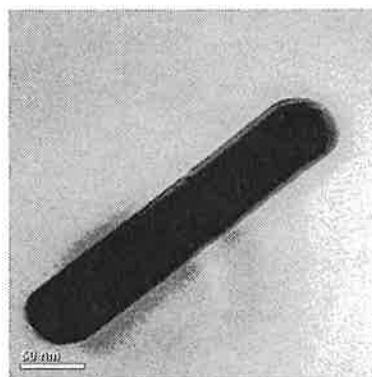
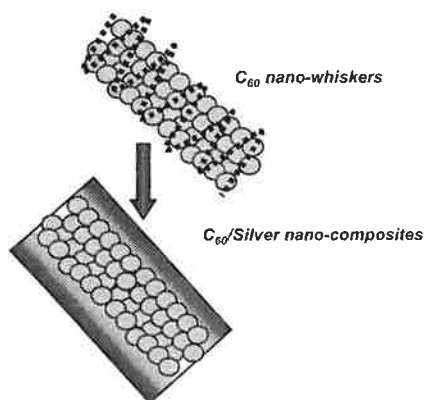
S. Iyer, C. L. Raston, M. Saunders

The University of Western Australia, Perth, Australia

clraston@chem.uwa.edu.au

Gaining control over the interplay of fullerenes is a paradigm in building up new material.^{1,2} Cavitands and related molecules can form host-guest complexes with C_{60} and C_{70} , and at the same time the solid state structures can involve fullerene...fullerene interactions, with the fullerenes in chains and sheets, and arrays of higher complexity. We have embarked on the use of biopolymers as potential receptor for fullerenes in aqueous media, in the first instance focusing on C_{60} .

Reaction of the classical starch iodine complex with solid C_{60} results in uptake of the fullerene by starch. Addition of ascorbic acid consumes the iodine (as tri-iodide) resulting in the formation of a brown solution after removing excess fullerene by centrifugation. TEM shows the fullerenes are assembled into quasi-crystalline nano-whiskers approximately 7 nm in diameter and > 120 nm in length. There is no iodine in the fibres. Addition of silver nitrate under spinning disc processing (SDP) affords silver coated nano-fibres, with the thickness of the silver variable, depending on the SDP parameters. The silver in these fibres is hexagonal closed packed rather than the cubic form which is found in bulk silver metal.

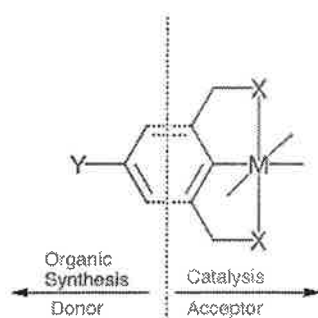


1. Makha, A. Purich, C. L. Raston, and A. N. Sobolev, *Eur. J. Inorg. Chem.*, **2006**, 507 - 517.
2. M. Makha, A. N. Sobolev, C. L. Raston, and P. Turner, *Crystal Growth & Design*, **2006**, 6, 224 - 228.

'Pincer' Organometallics: Building Blocks With An Organic And An Organometallic SideG Van Koten*Dept. Of Organic Chemistry and Catalysis, Utrecht, Netherlands*

g.vankoten@chem.uu.nl

In recent years we explored the synthesis of “pincer” metal complexes of ever increasing complexity and applicability¹. In retrospect these complexes can be seen as small, multifunctional devices comprising an arene C₆ ring as a scaffold to which various functionalities are connected; i.e. a covalently bound metal center with either catalytic, sensor or non-covalent binding properties, one or two ortho-chelating functionalities and a reactive, functional group para to the M-C bond. This group can either modulate the metal-center properties by mesomeric and inductive effects² or is amenable to further functionalization (onto dendrimers³, lipases⁴, peptide chains⁵, etc.). In this lecture the organic and inorganic syntheses involved will be discussed as well as the novel materials- and physico-chemical properties.



Their use as biosensors^{5, 6}, biomarkers and anchored nanosize organometallic catalysts⁷ will be demonstrated.

¹*Inorg. Chim. Acta*, **300-302** (2000) 1094-1098, ²*Organometallics*, **16** (1997) 4985, *Chem. Eur. J.*, **10** (2004) 1331-1344, ³*Nature*, **372** (1994) 659, ⁴*J. Organom. Chem.*, **668** (2003) 3-7, ⁵*Chem. Eur. J.*, **8** (2002) 5368-5376, *Org. Letters*, **12** (2003) 2021-2024, ⁶*Can. J. Chem.*, **79** (2001) 709-718, ⁷*Adv. Synth. Catal.*, **345** (2003) 364-369, ⁸*Chem. Eur. J.*, **10** (2004) 1267-1273, ⁹*Organometallics*, **23** (2004) 1525-1532.

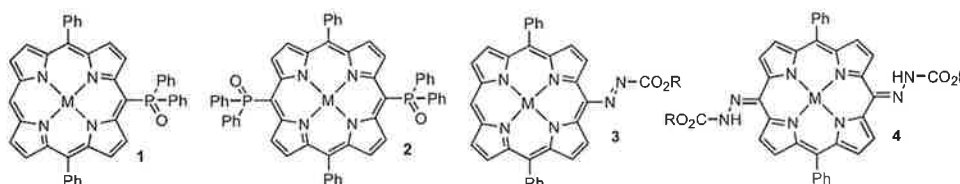
Metal-catalysed C-N and C-P Coupling on the Porphyrin Periphery

F. Atefi, B. Basic, L.J. Esdaile, J.C. McMurtrie, D.P. Arnold

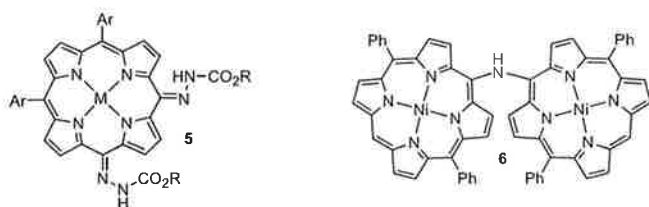
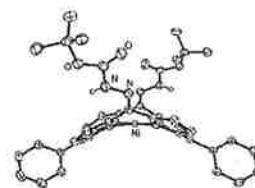
School of Physical and Chemical Sciences, Queensland University of Technology, Brisbane, Australia

d.arnold@qut.edu.au

Metal-catalysed C-X bond formation has become a vital reaction in organic chemistry, and we have used C-N and C-P couplings to prepare a range of new porphyrinoids. The reactions of bromoporphyrins and –metalloporphyrins with secondary phosphine oxides led to a range of mono- and bis-phosphine oxides, e.g. **1** and **2**, and we are currently studying these systems as ligands for supramolecular chemistry.¹



C-N couplings with hydrazine and carbazates yielded a range of novel azo-substituted porphyrinoids and diporphyrins, including azocarboxylates (**3**), “deconjugated” diiminoporphodimethenes [**4** (see ORTEP structure) and **5**] and a bis(porphyrinyl) secondary amine (**6**).² The structures, reactivity, spectra, and potential applications of a selection of these macrocycles will be discussed.



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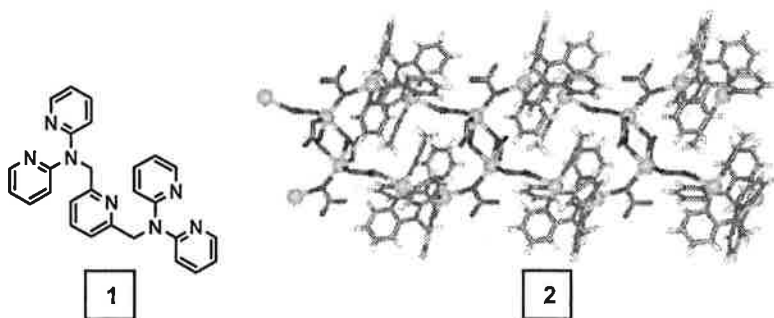
A Comparative Study of the Structures of Silver(I) Complexes of 2,2'-Dipyridylamine Derivatives

Bianca Antonioli¹, David J. Bray², Jack K. Clegg², Christopher J. Sumby³, Marco Wenzel¹, Kerstin Gloe¹, Olga Katajeva⁴, John M. McMurtrie², Karsten Gloe¹, Leonard F. Lindoy², Peter J. Steel³

¹TU Dresden, Department of Chemistry, Dresden, Saxony, Germany, ²University of Sydney, School of Chemistry, Sydney, NSW, Australia, ³University of Canterbury, Department of Chemistry, Christchurch, New Zealand, ⁴A.E. Arbusov Institute of Organic Chemistry, Kazan, Russia

karsten.gloe@chemie.tu-dresden.de

The coordination chemistry of 2,2'-dipyridylamine and its derivatives has now been the focus of a considerable number of investigations. Similarly due to its coordination flexibility, the d^{10} ion Ag(I) has received increasing attention; it has been demonstrated to form a range of metal complex and supramolecular materials, especially with nitrogen donor ligands.



We have undertaken a comparative solid state and solution investigation of the interaction of six linked 2,2'-dipyridylamine ligand systems with Ag(I). Apart from changes reflecting the variation of ligand structure, the results indicate that the nature of the anion, the solvent and the ratio of ligand/metal employed can all influence the architecture achieved. The resulting complexes contain a number of interesting structural features and range from linear polymers to metallamacrocycles and two-dimensional arrangements based on different coordinate binding and π -interactions (involving Ag(I), the ligand, anion and solvent molecules).

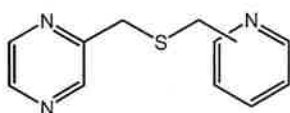
As an example, the interaction of ligand 1 and AgNO₃ leads to the formation of the one-dimensional ladder structure 2 which contains an unprecedented tetra-bridging [Ag₂(NO₃)₆]⁴⁻ anion and the doubly-bridging [Ag(1)(MeCN)]²⁺ cation. These ladders interact with their neighbours via π - π interactions giving infinite two-dimensional sheets.

Flexible Asymmetrical Ligands and Unusual NetworksC. A. Black, L. R. Hanton*Department of Chemistry, University of Otago, Dunedin, New Zealand*

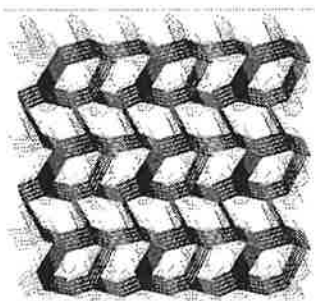
lhanton@alkali.otago.ac.nz

The use of flexible ligands presents various challenges when used to engineer coordination polymer networks. These ligands tend to produce less predictable network structures that do not readily fit into a current paradigm. The use of flexible and asymmetrical ligands compounds these issues. Coordination polymers formed through the use of asymmetrical ligands are more likely to produce a diverse range of structures through an assortment of different binding sites. These binding sites can produce a variety of binding modes and coordination geometries resulting in interesting and novel architectures. The use of asymmetrical ligands in coordination polymer chemistry is rare. This is perhaps because there is a desire to create reproducibly one type of architecture and symmetrical ligands are less likely to result in structural ambiguity.

We shall describe the results of using flexible asymmetrical pyrazine–pyridine thioether ligands with various metal salts, typically Ag(I) and Cu(I). The ligands differ by varying the location of the N(pyridine) donor in the 2, 3, or 4 positions. This seemingly simple variation has a significant effect on the resulting architecture and in particular the resulting dimensionality. Topological analysis will be presented for all two and three dimensional structures. A case will be made for the use of asymmetric ligands in coordination polymer chemistry.



asymmetrical pyrazine–
pyridine thioether ligand



A rare example of non-interpenetrated
10,3-d networks formed with 4 substituted
ligand and AgX (X=BF₄, PF₆, ClO₄).

Fluorescent Metal-Ion Activated Molecular Sensors for Aromatic Anions

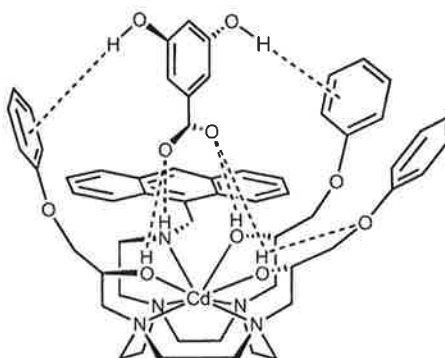
K. P. Wainwright, A. J. Bradbury, J. A. Hodyl

School of Chemistry Physics & Earth Sciences, Flinders University,

Adelaide, South Australia, Australia

Kevin.Wainwright@flinders.edu.au

Complexation of tetrakis(2-hydroxyethyl) pendant arm macrocycles, derived from cyclen, with Cd(II) leads to eight-coordinate complexes. If the pendant arms have aromatic appendages, and providing the complexes are produced as their perchlorate salts, an anion binding cavity, devoid of any guest molecule, becomes a structural feature of the complex. This has been verified by X-ray crystallography and is known to persist in solution from conductivity and NMR data. Subsequently, on reaction with various different aromatic oxoanions, inclusion complexes containing the aromatic oxoanion can be formed where the included anion is retained by complementary hydrogen bonding to the four hydroxy groups that are present at the base of the cavity. We have now found that by substituting a pendant anthracene moiety for one of the 2-hydroxyethyl arms in these molecular receptor complexes, as shown in the structure below,



that we can convert them to sensors in which the fluorescence of the anthracene responds to the entry and egress of guest anions within the binding cavity. The retention of a series of hydroxy-benzoates will be discussed in the context of their ability to form O-H hydrogen bonds to the aromatic cavity walls, as well as its base, and the effect that this has both on the binding constant for the anion and on the fluorescence response that signals the event.

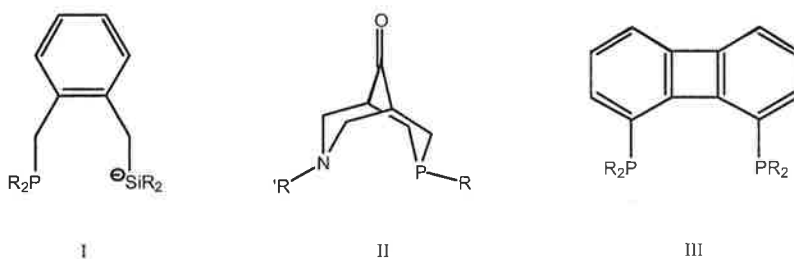
Control of Metal Reactivity with Designer Ligands

J L Spencer, A I Zayya, K Allan, R L Vagana, M Matveenko

Victoria University of Wellington, Wellington, New Zealand

john.spencer@vuw.ac.nz

The reactivity of a transition metal centre is frequently determined by the environment created by the associated ligands. This has been used to great effect, for example in the design of highly specific homogeneous catalysts. We have designed several new chelating bidentate ligand systems that afford considerable control of the metal environment. We have synthesized novel heterobidentate PN and PSi ligands with specific electronic and steric properties and controlled bite angles. These new ligands have afforded unique reactivity at the metal.



The coordination chemistry of the ligands with Group 10 and 11 metals has been examined. An interesting aspect of the chemistry of **II** is the propensity of the nitrogen arm of the ligand to dissociate from the metal if the metal is in low oxidation state (hemilability). This has particular significance in catalytic cycles that involve the metal in oxidative addition reactions. In the lower oxidation state the nitrogen is labile, creating a vacant coordination site, whereas in the higher oxidation state the ligand tends to be fully bidentate.

In contrast the very high trans influence and effect of the silyl group in **I** has a significant influence on the behaviour of the other ligands in the coordination sphere. Ligand **III** potentially has a very large bite angle but presents an interesting synthetic challenge.

Targeting the Mitochondrial Cell Death Pathway with Gold(I) ComplexesSJ Berners-Price, MV Baker, PJ Barnard, JL Hickey, RA Ruhayel, LE Wedlock*University of Western Australia, Perth, WA, Australia*

sbp@chem.uwa.edu.au

There is considerable interest in targeting the mitochondrial cell death pathway in the development of new chemotherapeutic agents. Two distinct classes of Au(I) phosphine compounds exhibit antitumour activity that may depend on different antimitochondrial mechanisms: neutral, linear two-coordinate Au(I) phosphine complexes typified by the tetraacetylthioglucose derivative, Auranofin, and lipophilic-cationic 1:2 Au(I)diphosphine complexes, such as pyridylphosphine analogs of $[\text{Au}(\text{dppe})_2]^+$. The latter exhibit a degree of selectivity for cancer cells over normal cells that is tuned by changing the lipophilicity.¹ We are investigating a variety of neutral and cationic Au(I) complexes of *N*-heterocyclic carbenes (NHCs), as analogs of these two classes of Au(I) phosphines.² All these compounds exhibit antimitochondrial activity showing that phosphine ligands are not essential for the activity. Some of the dinuclear Au(I) NHC complexes display interesting luminescent properties attributable to aurophilic interactions. By manipulating the Au-Au distance the excitation wavelength can be tailored, enabling study of the intracellular distribution of the Au(I) NHC complex in single cancer living cells using fluorescence microscopy.³

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3. P. J. Barnard, L. E. Wedlock, M. V. Baker, S. J. Berners-Price, D. A. Joyce, B. W. Skelton and J. H. Steer, *Angew. Chemie. Int. Ed.*, (2006), in press.

Dinuclear Ruthenium(II) Complexes with Flexible Bridges as DNA Bulge-Selective Probes

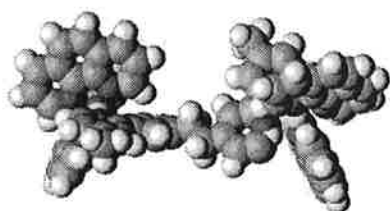
J.L. Morgan¹, C.B. Spillane¹, J.A. Smith¹, J.G. Collins², F.R. Keene¹

¹James Cook University, Townsville, Qld., Australia, ²ADFA, University of New South Wales,

Canberra, A.C.T., Australia

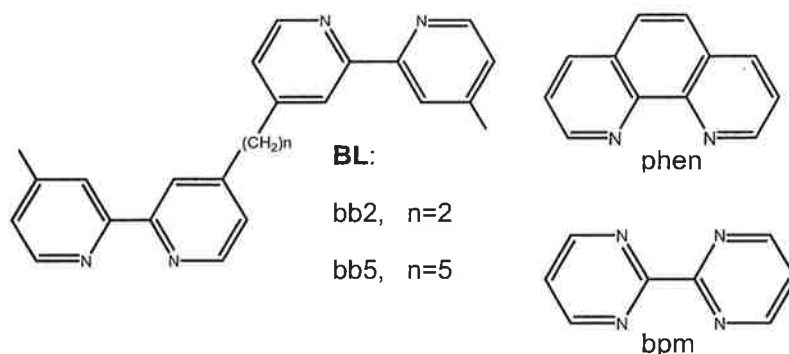
richard.keene@jcu.edu.au

Small changes in ligand substitution patterns of dinuclear ruthenium(II) complexes, and variations in stereochemistry, can lead to large differences in their DNA binding affinities. For example *meso*-[$\{\text{Ru}(\text{phen})_2\}_2(\mu\text{-bpm})\}^{4+}$ has a particularly high affinity ($1 \times 10^6 \text{ M}^{-1}$) and selectivity for an adenine bulge site in the sequence d(CCGAGAATTCCGG)₂, compared to the $\Delta\Delta$ and $\Lambda\Lambda$ forms.



A series of dinuclear ruthenium complexes with flexible bridges of the form $[\{\text{Ru}(\text{phen})_2\}_2(\mu\text{-BL})]^{4+}$ (see structures below) has been stereoretentively synthesized to give three stereoisomers of each of four complexes.

Preliminary DNA binding studies of these twelve complexes to a variety of DNA oligonucleotides including duplexes, bulge-containing and hairpin sequences have been undertaken. From these surveys it was found that the bb7-bridged complexes gave the highest apparent binding affinity to the single adenine bulge-containing sequence {d(CCGAGAATTCCGG)₂}, and detailed NMR studies were subsequently conducted on $\Delta\Delta$ - and $\Lambda\Lambda$ -[$\{\text{Ru}(\text{phen})_2\}_2(\mu\text{-bb7})\}^{4+}$ complexes with the bulge sequence to elucidate their particular efficacy. Modelling studies have also been conducted using NOE interactions, and these results along with the NMR and initial DNA binding surveys, will be presented.



Reference:

1. J.L. Morgan, D.P. Buck, A.G. Turley, J.G. Collins, F.R. Keene, *Inorg. Chim. Acta*, **2006**, 359, 888-898.

Fe L-edge XAS: A Direct Probe of Covalency and Back-bonding

RK Hocking¹, EC Wasinger¹, KO Hodgson¹, B Hedman², EI Solomon¹

¹*Department of Chemistry, Stanford University, Stanford, United States,* ²*Stanford Synchrotron*

Radiation Laboratory, Stanford, United States

rhocking@stanford.edu

A new methodology involving Fe L-edge XAS has been developed which allows us to directly probe both the covalency of the different Fe d-orbitals and back-bonding. An Fe L-edge, $2p \rightarrow 3d$ transition, is similar to an Fe K pre-edge, $1s \rightarrow 3d$ transition, in that both techniques probe the Fe d manifold. However, the metal L-edge is dipole allowed, whereas the metal K pre-edge is dipole forbidden. This means that Fe L-edge spectra have greater intensity, better resolution, and more detailed spectroscopic structure than metal K pre-edge spectra. Further, since the 2p orbital is localized on the Fe the total intensity is proportional to the total metal character in the unoccupied and $\frac{1}{2}$ occupied orbitals. The Fe L-edge spectral shape has three major contributions: ligand field splittings, multiplet effects and covalency. The sensitivity of spectral shape to ligand field and covalency means that once multiplet effects have been accounted for, changes in spectral shape can be quantified in terms of differential orbital covalency (DOC); the differences in delocalization of the different d orbitals into the ligand. Back-bonding to Fe causes additional transition pathways to π^* orbitals increasing the L-edge intensity and causing further, sometimes dramatic, changes to spectral shape. The new technique has been applied to provide new insights into a number of different areas including to characterise the π delocalisation in heme.

The Potential of Copper and Zinc Bis(thiosemicarbazonato) Complexes for the Treatment of Alzheimer's Disease

P. S. Donnelly¹, K. J. Barnham², A. R. White³

¹*School of Chemistry, Bio21 Institute, University of Melbourne, Melbourne, Australia,* ²*Department of Pathology, Bio21 Institute, University of Melbourne, Melbourne, Australia,* ³*Department of Pathology, University of Melbourne, Melbourne, Australia*

pauld@unimelb.edu.au

Alzheimer's disease (AD) is the most common form of neurodegenerative dementia. Onset of the symptoms of the disease is associated with formation of senile plaques that are a pathological marker of the disease. The core constituent of the plaques is the aggregated peptide amyloid beta ($A\beta$), a 40-42 amino acid peptide derived from the amyloid precursor protein (Fig 1). $A\beta$ is generally accepted as being neurotoxic and, as such, is a therapeutic target as well as a diagnostic marker.

An important factor in controlling accumulation of $A\beta$ in the brain is the activity of protein degrading enzymes such as matrix metalloproteases (MMP). We have been investigating the use of membrane permeable copper(II) and zinc(II) bis(thiosemicarbazonato) complexes (Fig. 1) for controlled delivery of metal ions to cell cultures over expressing the precursor protein for $A\beta$. The release of copper from the ligand intracellularly can be controlled by manipulation of the Cu(II)/Cu(I) reduction potential. The increased intracellular concentrations of bio-available copper or zinc activate cell-signalling pathways that stimulate the production of MMP enzymes that degrade $A\beta$. These results suggest that copper(II) and zinc(II) bis(thiosemicarbazonato) complexes have potential in Alzheimer's disease therapy.

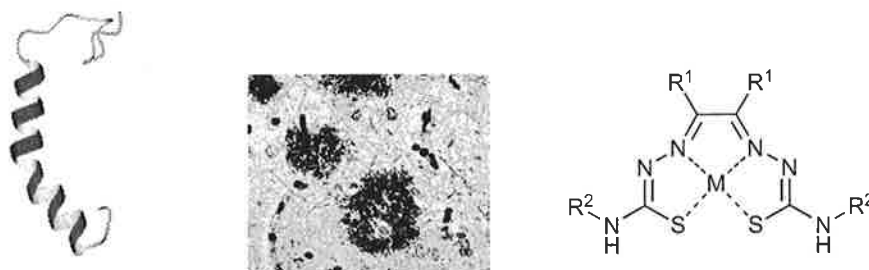


Fig 1. The $A\beta$ peptide (left) forms insoluble aggregates (centre) in the brains of Alzheimer's disease patients. The structure of metal bis(thiosemicarbazonato) complexes (right), $M = \text{Cu(II)}$ or Zn(II) .

Resolving Differences in the Crystal Structures of Photosystem II through DFT Calculations

S Petrie, R Stranger, R Pace, P Gatt

Australian National University, Canberra, ACT, Australia

rob.stranger@anu.edu.au

Isomerism and hydration in a model of the Mn_4 active centre of photosystem II (PSII), $[\text{Mn}_4\text{C}_9\text{N}_2\text{O}_{16}\text{H}_{10}]^-\cdot(\text{H}_2\text{O})_n$ ($n = 0-5$), has been investigated using density functional theory (DFT). Our calculations reveal several tantalising trends, which appear to account for the major structural differences between the Berlin and London X-ray crystal structures of PSII. These calculations also suggest pathways through which the oxidation of water to O_2 might be achieved.

Our calculations show that several structures on the variously hydrated potential energy surfaces are prone to tautomerization, involving proton transfer from ligated H_2O to μ_2 -oxo bridges between Mn atoms. More dramatic structural modification is also observed in several instances, with the formation of new oxo- or hydroxo-bridging interactions being driven by dehydration of the model complex. Most remarkably, our calculations suggest that interconversion between a 'Berlin-like' and a 'London-like' structure, involving the formation of a second μ_3 -oxo bridge, may be dependent on no more than the reorientation of a pendant carboxylate ligand. The respective 'Berlin-like' and 'London-like' structures, which are comparable in total energy, are among the lowest-energy structures of many isomers explored. It therefore appears that the sometimes heated debate concerning the validity and mechanistic relevance of the competing crystal structures can be resolved as reflecting a plausible structural modification during the pre-crystallographic workup for one or other crystal structure.

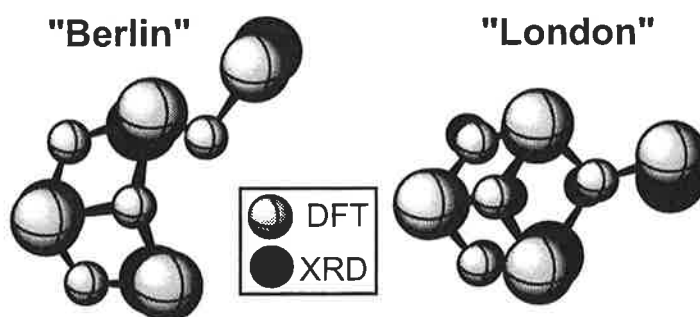


Diagram highlighting agreement between computed and crystalline structures of the Mn_4 core of PSII. For clarity, only Mn and bridging O atoms are shown.

"Catalytic Reduction of Dinitrogen to Ammonia at Room Temperature and One Atmosphere with Protons and Electrons"

R.R. Shrock

We have been able to reduce dinitrogen selectively and catalytically to ammonia at 1 atm and room temperature with protons and electrons. Reduction takes place at a single molybdenum center that is sterically protected against bimetallic decomposition reactions with *meta*-terphenyl-substituted triamidoamine ligands such as $[(\text{HIPTNCH}_2\text{CH}_2)_3\text{N}]^{3-}$ where HIPT is hexaisopropyl-metaterphenyl. The proton source is $(\{2,6\text{-lutidinium}\}\{\text{BAR}'_4\})$; $\text{Ar}' = 3,5\text{-(CF}_3)_2\text{C}_6\text{H}_3$ and the reductant is decamethyl chromocene. The reducing equivalents make either ammonia (~60% from dinitrogen) or dihydrogen. All evidence suggests that N_2 is being reduced at a single Mo center in which the oxidation state of the metal varies between Mo(III) and Mo(VI). Recent studies concern complexes that contain a variety of "Hybrid" ligands, $(\text{HIPTNHCH}_2\text{CH}_2)_2\text{NCH}_2\text{CH}_2\text{NHAr}$, where $\text{Ar} = 3,5\text{-Me}_2\text{C}_6\text{H}_3$, $3,5\text{-(CF}_3)_2\text{C}_6\text{H}_3$, $3,5\text{-(MeO)}_2\text{C}_6\text{H}_3$, $3,5\text{-Me}_2\text{NC}_5\text{H}_3$, $3,5\text{-Ph}_2\text{NC}_5\text{H}_3$, $2,4,6\text{-i-Pr}_3\text{C}_6\text{H}_2$, or $2,4,6\text{-Me}_3\text{C}_6\text{H}_2$. [Hybrid]Mo=N-NH species could be observed as a consequence of protonation of $\{[\text{Hybrid}]\text{MoN}_2\}^-$ species, but they could not be isolated as a consequence of a facile decomposition to yield dihydrogen and [Hybrid]MoN₂ species. Attempts to reduce dinitrogen catalytically led to little or no ammonia being formed from dinitrogen. The cause is likely to be a rapid decomposition of intermediate [Hybrid]Mo=N-NH species, a decomposition that was shown to be accelerated dramatically by 2,6-lutidine, the conjugate base of the acid employed in the attempted catalytic reduction. $[(\text{HIPTNCH}_2\text{CH}_2)_3\text{N}]^{3-}$ complexes of tungsten, chromium, and vanadium all failed to yield any catalytic turnover of dinitrogen to ammonia.

SA1

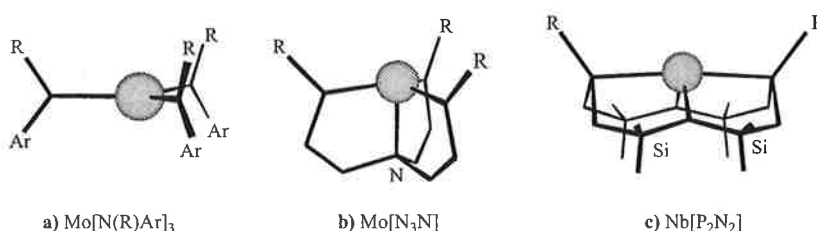
**Dinitrogen Activation: A Comparison Of The Laplaza-Cummins,
Schrock And Fryzuk Systems Using DFT**

G Christian, R Stranger, BF Yates

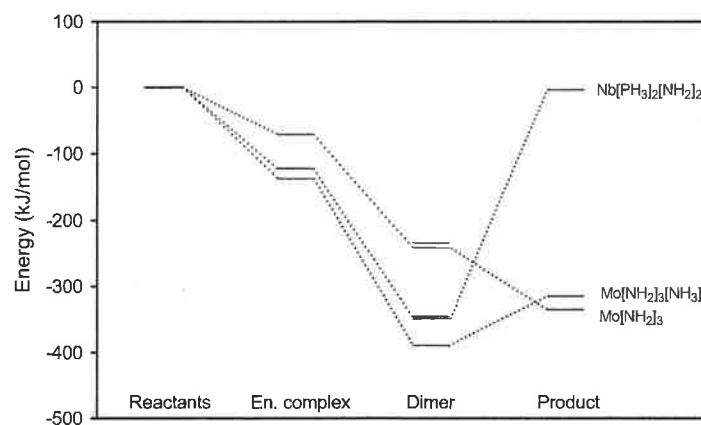
¹*Australian National University, Canberra, ACT, Australia,*

²*University of Tasmania, Hobart, TAS, Australia*

Three systems have been intensely studied in the pursuit of catalytic dinitrogen cleavage: a) Laplaza and Cummins' three-coordinate complex $\text{Mo}[\text{N}(\text{R})\text{Ar}]_3$, b) Schrock's three-coordinate trigonal-capped complex $\text{Mo}[\text{N}_3\text{N}]$, and c) Fryzuk's four-coordinate complex $\text{Nb}[\text{P}_2\text{N}_2]$.



DFT calculations on model complexes are used to compare dinitrogen cleavage in the experimental systems assuming a similar mechanism: coordination of dinitrogen to form the encounter complex $\text{L}_n\text{M}-\text{N}_2$, coordination of a second ML_n unit to form the intermediate dimer $\text{L}_n\text{M}-\text{N}_2-\text{ML}_n$, and N_2 cleavage to form the nitride product $\text{L}_n\text{M}-\text{N}$. The calculations highlight the importance of the coordination environment, d^n configuration, donor atoms, and constraints due to the ligand backbone structure on the reaction energetics and resulting products.



Structural Models of the CO Dehydrogenase Active Site

C Gourlay¹, D J Evans¹, D J Nielsen¹, J M White¹, S Z Knottenbelt², M L Kirk², C G Young¹

¹*School of Chemistry, The University of Melbourne, Victoria, Australia,* ²*Department of Chemistry, The University of New Mexico, Albuquerque, New Mexico, United States*

The carbon monoxide dehydrogenase (CODH) present in the eubacterium *Oligotrophia carboxidovorans* is responsible for catalysing the oxidation of CO to CO₂ through a bimetallic (MCD)Mo(=O)(OH)(□-S)Cu(S-Cys) active site.^[1] The active site has also been confirmed by Mo- and Cu- K-edge X-ray absorption spectroscopy.^[2] This molybdoenzyme differs from other members of the xanthine oxidase family in possessing a bridging rather than a terminal sulfido group. We report here a range of [Tp^{iPr}MoO(OAr)(□-S)Cu(Me₃tcn)] (Tp^{iPr} = hydrotris(3-isopropylpyrazolyl)borate; Ar = substituted aryl group; Me₃tcn = 1,4,7-trimethyl-1,4,7-triazacyclononane) complexes which exhibit similar structural properties to that of the enzyme.^[3] Spectroscopic experiments have also revealed four line EPR spectra drawing similarities with the spectrum of the enzyme, exhibiting Mo hyperfine features consistent with delocalisation of an unpaired electron over the Mo-S-Cu active site.

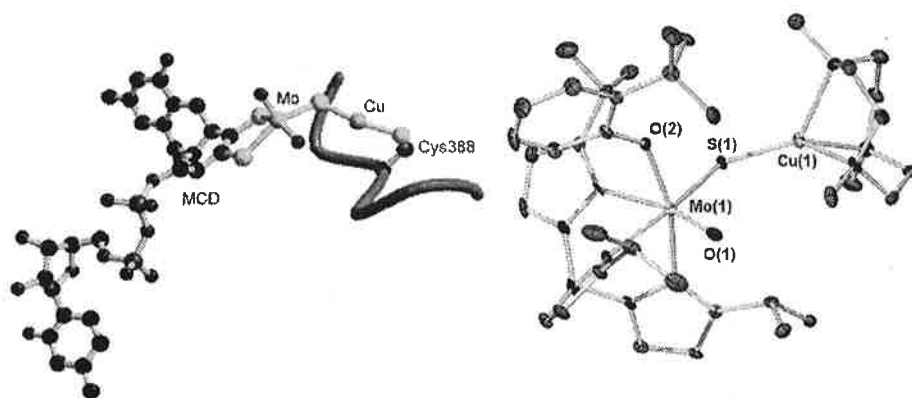


Figure 1. a) Active site of *O. carboxidovorans* CODH. **b)** The crystal structure of [Tp^{iPr}MoO(OC₆H₄^tBu-2)(μ-S)Cu(Me₃tcn)]

[1] Dobbek, H; Gremer, L; Kiefersauer, R; Huber, R; Meyer, O; *PNAS*, 2002, **99**,15971

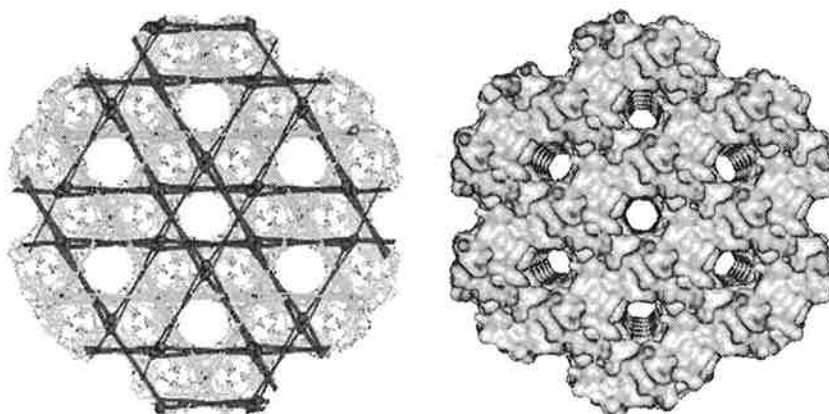
[2] Gnida, M; Ferner, R; Gremer, L; Meyer, O; Meyer-Klauke, W; *Biochemistry*, 2003, **42**, 222

[3] Gourlay C, Nielsen D. J., White J. M., Knottenbelt S. Z., Kirk M. L., and Young C. G; *J. Am. Chem. Soc.*, 2006, **128**, 2164-2165.

Chiral Guest Sorption and Gas Storage in a Homochiral Nanoporous Framework MaterialS S Iremonger, C J Kepert*School of Chemistry, University of Sydney, Sydney, NSW, Australia*

Metal-organic frameworks have received much attention not only because of their numerous potential applications in catalysis, small molecule separation and gas storage, but also because of their intriguing variety of architectures and topologies. Use of a enantiopure ligand and hence formation of a homochiral framework may allow the above processes to be carried out enantioselectively.^[1]

A number of new enantiomerically pure ligands have been synthesised and incorporated into metal-organic frameworks. Of particular interest is a porous and robust 3D framework based on a 1,2,4-triazole ligand that has a triply interpenetrating (4,6) net topology. The framework features large 1D (12 Å) helical pores, the chiral alcohol groups of the ligand also line the pore creating a highly chiral environment. We are currently investigating the ability of the framework to separate racemic mixtures of small molecules. The framework has also shown the ability to store significant quantities of hydrogen gas.



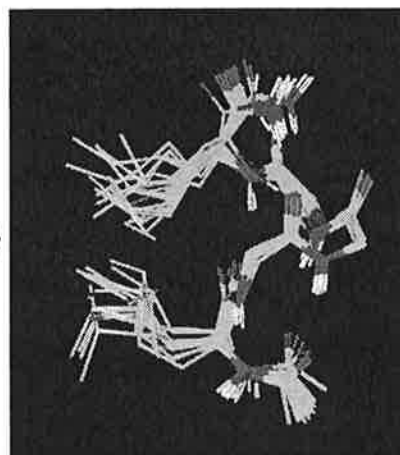
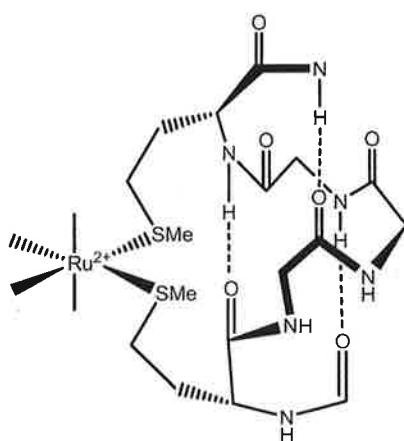
[1] B. Kesanli, W. Lin, *Coordination Chemistry Reviews* **2003**, 246, 305.

α -Helix Induction in Short Peptides Using Metal Clips

M.T. Ma¹, H.N. Hoang², G.K. Bryant¹, D.P. Fairlie², T.G. Appleton¹

¹*School of Molecular and Microbial Sciences, The University of Queensland, Brisbane, Queensland, Australia,* ²*Institute of Molecular Bioscience, The University of Queensland, Brisbane, Queensland, Australia*

Short α -helical segments account for approximately 40% of protein structure and are critical in mediating important biological processes as molecular recognition motifs and as scaffolds in proteins such as metalloenzymes. However, short peptide sequences (less than fifteen residues) corresponding to these regions do not form thermodynamically stable α -helices in solution. Here we show that the metal clip $[\text{Ru}(\text{NH}_3)_4(\text{solvent})_2]^{2+}$ can induce α -helicity in a five residue peptide through binding to methionine residues at the i and $i+4$ amino acid positions, with helical content in aqueous solution estimated at over 80%. This species exhibits the most stable α -helical turn reported for a metalloprotein to date. We are examining the effects of varying the nature and position of the metal ion clip and the donor atom side chains of the peptides of the macrocycle on the stabilisation of α -helical structure.



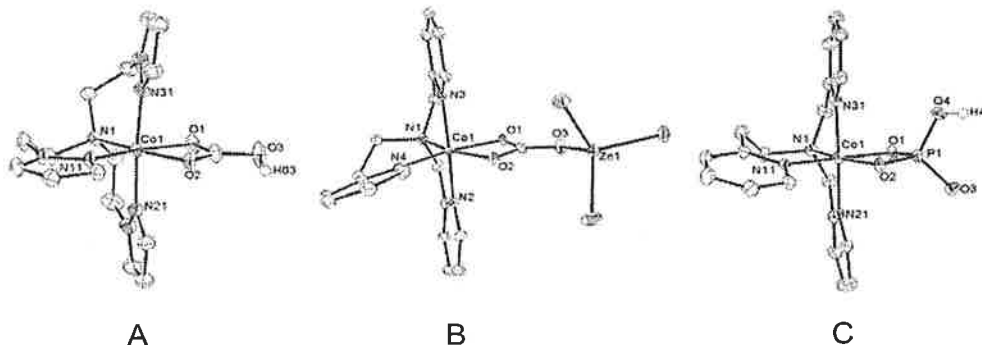
Unusual Carbonate and Phosphate Co(III) Complexes

L F McClintock, A G Blackman

University of Otago, Dunedin, New Zealand

Previously we have shown that Co(III) carbonate complexes containing tripodal ligands with pyridyl donors are very resistant to acid hydrolysis.^{1, 2} We have extended this work by showing that similar ligands based on pyrazole behave in the same manner. This has led to the isolation of chelated bicarbonate complexes (eg [Co(trpyn)O₂COH]⁺, Figure A). We have also synthesised complexes where the chelated carbonate acts as a bridge to a zinc atom (eg [Co(pmea)O₂COZnCl₃], Figure B), a rarely observed carbonate coordination mode.

Phosphate esters are of particular interest as they constitute the backbone of DNA and RNA. It has been hypothesised that four membered ring metal-phosphate ester chelates play an important role in enzymic systems responsible for phosphate ester hydrolysis. However, all attempts to prepare and structurally characterise complexes containing a chelated phosphate ester have thus far been unsuccessful. We have managed to prepare the first example of a chelated hydrogen phosphate complex, [Co(pmea)O₂PO₂H]⁺² (Figure C). With this in mind we have attempted to isolate previously uncharacterised chelated monophosphate ester complexes and the results of this work will be reported.



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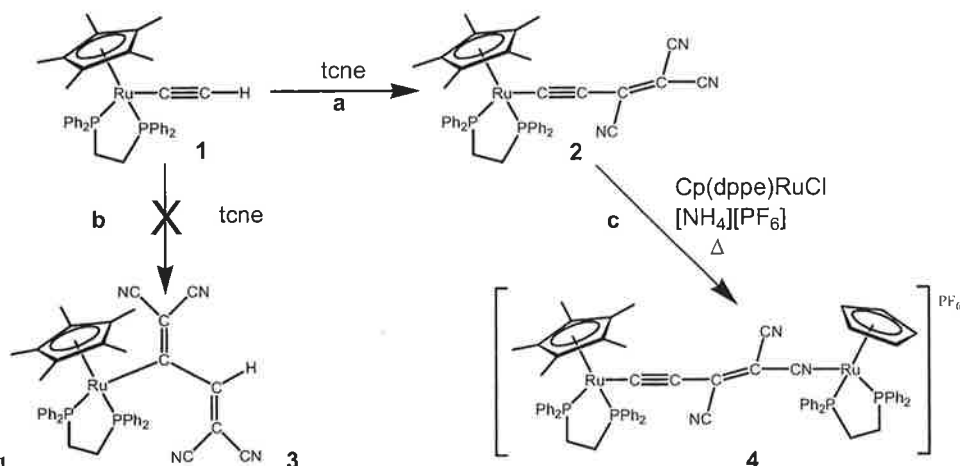
2. Cheyne, S. E.; McClintock, L. F.; Blackman, A. G., *Inorganic Chemistry* **2006**, *45*, 2610-2618.

**Some Chemistry of the Ruthenium Ethynyl Complex, $\text{Cp}'(\text{PP})\text{RuC}\equiv\text{CH}$, and Reactions of the
Tricyanovinylethynyl Complex, $\text{Cp}'(\text{PP})\text{RuC}\equiv\text{CC}(\text{CN})=\text{C}(\text{CN})_2$**

C. R. Parker¹, M. I. Bruce¹, A. H. White², B. W. Skelton², B. Nicholson³

¹*The University of Adelaide, Adelaide, SA, Australia,* ²*The University of Western Australia, Perth, WA, Australia,* ³*University of Waikato, Hamilton, New Zealand*

In the field of material science, conjugated organometallic compounds have attracted much attention for their optical and electronic properties. Our interest in this field has focused on the electron-rich ruthenium metal centres, $[\text{Ru}(\text{PP})\text{Cp}']$ (where $\text{PP} = (\text{PPh}_3)_2$ or dppe and Cp' is either $\text{Cp} = \text{C}_5\text{H}_5$ or $\text{Cp}^* = \text{C}_5\text{Me}_5$). The ruthenium ethynyl complex, $\text{Cp}^*(\text{dppe})\text{RuC}\equiv\text{CH}$ (**1**), has displayed unexpected nucleophilic behaviour with respect to tetracyanoethene, tcne , to give the substitution product $\text{Cp}^*(\text{dppe})\text{RuC}\equiv\text{CC}(\text{CN})=\text{C}(\text{CN})_2$ (**2**) (**Scheme 1a**) rather than the expected cycloadduct $\text{Cp}^*(\text{dppe})\text{RuC}[\text{C}(\text{CN})_2]\text{CH}[\text{C}(\text{CN})_2]$ (**3**) (**Scheme 1b**). In contrast $\text{Cp}(\text{PPh}_3)_2\text{RuC}\equiv\text{CH}$ gives both the cycloadduct and the substitution products. The scope of this chemistry will be described in more detail. The intensely purple coloured compound $(\text{Cp}'(\text{PP})\text{Ru})\text{C}\equiv\text{CC}(\text{CN})=\text{C}(\text{CN})_2$ (**2**) has displayed some interesting reactivity. The nitrile groups on **2** react with other $[\text{ML}_n]\text{X}$ to produce bi-, tri- and tetra-metallic systems (**Scheme 1c**). Formation of the bimetallic complex (**4**) allows the electrochemistry of this system to be examined and to assess the conductivity of the new bridging motif, $\text{C}\equiv\text{CC}(\text{CN})=\text{C}(\text{CN})\text{CN}$.



Scheme 1

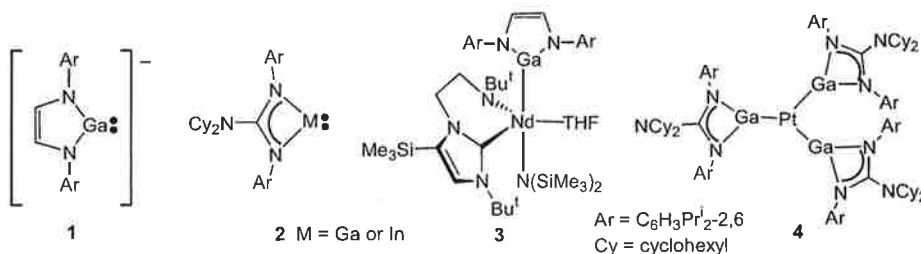
Group 13 Metal(I) Heterocycles: Metal Donor Lewis Bases and N-heterocyclic Carbene Analogues

C Jones

School of Chemistry, Cardiff University, Cardiff, United Kingdom

jonesca6@cf.ac.uk

Since the isolation of the first thermally stable N-heterocyclic carbene (NHC) in 1991, this class of ligand has become ubiquitous in the formation of p-, d- and f-block metal complexes, many of which have found wide application in synthesis and catalytic processes. Through our work in low oxidation state p-block chemistry we have become interested in stabilising heavier main group element "carbenoid" analogues of these ligands and investigating their coordination and further chemistry. Most success has been achieved in group 13 with the 5-membered anionic, and 4-membered neutral metal(I) heterocycles, **1** and **2**. We have shown these to be versatile metal donor Lewis bases that can stabilise unusual complexes with metal fragments from across the periodic table, e.g. **3** - **4**.^{1,2} Throughout this work a number of similarities, but also differences, between the coordination chemistry of these heterocycles and NHCs have been identified and investigated by reactivity and theoretical studies. In addition, similarities between d-block metal complexes of **1** and transition metal-boryl complexes have been identified and are beginning to be exploited in the development of organic and organometallic synthetic methodologies. This lecture will discuss our recent work in the area.



1. R.J. Baker and C. Jones, *Coord. Chem. Revs.*, 2005, **249**, 1857.
2. C. Jones, P.C. Junk and A. Stasch, *J. Am. Chem. Soc.*, 2006, **128**, 2206.

Novel Multinuclear Pd and Pt Complexes Having Bridging Silylene or Germylene LigandsKO Osakada, MT Tanabe*Tokyo Institute of Technology, Yokohama, Japan*

kosakada@res.titech.ac.jp

This paper presents preparation, structures, and chemical properties of new tetranuclear Pd and Pd-Pt complexes having bridging SiPh₂ or GePh₂ ligands. Reaction of a chelating diphosphine ligand with a dinuclear complexes with bridging diphenylsilyl or diphenylgermyl ligands, Pd₂(PCy₃)₂(μ-SiPh₂)₂, at elevated temperature produces the tetranuclear complexes having a planar Pd₄E₃ (E = Si, Ge) core. Pd₃Pt type complex with bridging SiPh₂ ligands is obtained by using a similar reaction with the heterodinuclear complex, PdPt(PCy₃)₂(μ-SiPh₂)₂. X-ray crystallography and DFT calculation of the Pd₄ complexes indicate the structure containing four Pd(0) centers and three Si atoms bonded with Pd-Pd and Pd-Si bonds.

Mononuclear bis(diphenylsilyl)palladium and bis(diphenylgermyl)palladium complexes with a chelating phosphine ligand are also converted into the Pd₄Si₃ and Pd₄Ge₃ complexes upon heating, respectively. An intermediate dinuclear Pd complex with bridging organogermeryl ligands was isolated from the reaction mixture, and was characterized by X-ray crystallography and NMR spectroscopy. Plausible pathway for formation of the tetranuclear Pd complex is mentioned.

The Pd₄ and Pd₃Pt tetranuclear complexes with bridging silylene ligand reacts with CuI to form a complex with Pd-Cu bonds. Details of the reaction as well as relevance of chemical reactivity of the complexes with the structure and bonding are discussed.

Synthetic And Structural Chemistry Of Bismuth Oxo-Clusters

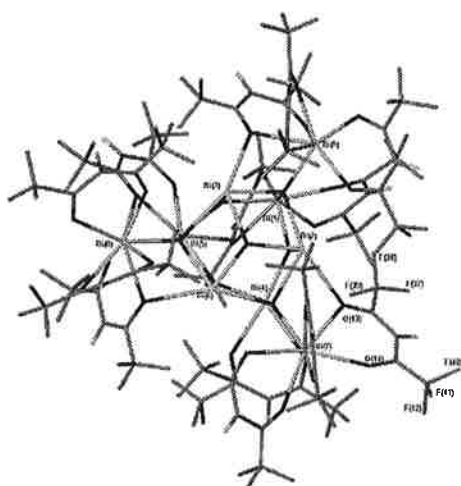
P. C. Andrews

Monash University, Melbourne, Australia

phil.andrews@sci.monash.edu.au

The inorganic and organometallic chemistry of bismuth has been plagued by many physical and chemical problems, mostly stemming from high levels of insolubility and a tendency the compounds have for undergoing facile hydrolysis and/or reactions with available solvent. These factors can result in polymer formation, ligand lability and thermodynamic instability. The end product is often compounds which prove difficult to comprehensively characterise. However, while this has meant difficulties in isolating homogenous compounds and caused some problems with synthetic reproducibility, it has not prevented them from finding application as common therapeutic agents, as antimicrobials, as precursors

for oxide-based materials containing Bi_2O_3 , as heterobimetallic catalysts, and as catalysts and reagents in organic synthesis in their own right. The generally accepted low toxicity of bismuth compounds has meant a recent surge in interest in their application in 'green chemistry'.



Molecular structure of bismuth oxo-hexafluoroacetylacetonate

In this presentation I will discuss our recent work on solvent-free and solvent based approaches to the synthesis of bismuth alkoxides, carboxylates and di-ketonates using Ph_3Bi ,¹ and will explore the formation of bismuth-oxo-clusters, including our recent characterisation of the Bi_{138} cluster at the heart of

bismuth subsalicylate (BSS), the well known antiulcer drug.²

1. P. C. Andrews, G. B. Deacon, P. C. Junk, I. Kumar and M. Silberstein. *Dalton Trans*, 2006, In Press.
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Ligand Chemistry of Chalcogen Diimides

R.S. Laitinen¹, R. Oilunkaniemi¹, M. Risto¹, J. Konu¹, T. Chivers²¹University of Oulu, Oulu, Finland, ²University of Calgary, Calgary, Canada

risto.laitinen@oulu.fi

Monomeric sulfur diimides have an extensive coordination chemistry, as might be anticipated from the availability of three potential donor sites and two π -bonds.¹ The bonding mode is dependent on the nature of the metal centre as well as the steric or electronic properties of the imido substituent. For example, the $M(CO)_5$ unit in the $\sigma(N)$ -trigonal complex $[W(CO)_5\{S(NMe)_2\}]$ undergoes a 1,3-shift between the two nitrogen donors, whereas the *tert*-butyl forms a N,N' -chelated $[W(CO)_4\{S(N^tBu)_2\}]$ complex, as is also observed with main-group metal halides, *e.g.*, $[SnCl_4 \cdot \{E(N^tBu)_2\}]$ ($E = S, Se$).²

The coordination chemistry of selenium and tellurium diimides has seen much slower progress. *Tert*-butyl selenium diimide forms an N,N' -chelated adduct with $SnCl_4$ ² and the reaction of dialkyl selenium diimides with bis(amino)stannylenes produces a four-membered $SnNSeN$ ring systems.³ The dimeric tellurium diimides can also act as chelating or bridging ligands *e.g.*, with $HgCl_2$,⁴ $Ag(CF_3SO_3)$, or $Cu(CF_3SO_3)$.⁵

The present contribution is concerned with the stereochemistry of the transition metal complexes containing selenium diimide and tellurium diimide ligands. We report the preparation and structural characterization of $[CoCl_2\{N^tBu)Te(N^tBu)_2Te^tBuN\}]$ from $CoCl_2$ and *tert*-butyl tellurium diimide and discuss the structural similarities and differences in the complexes formed in the analogous reaction between selenium diimides and $CoCl_2$. The preparation and structures of coinage metal complexes of *tert*-butyl selenium diimide are also reported and compared with those of *tert*-butyl tellurium diimide.

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- [2] J. Gindl, M. Björgvinsson, H. W. Roesky, C. Freire-Erdbrügger, and G. M. Sheldrick, *J. Chem. Soc., Dalton Trans.* **1993**, 811.
- [3] B. Wrackmeyer, C. Köhler, W. Milius, and M. Herberhold, *Z. Anorg. Allg. Chem.* **1995**, 621, 1625.
- [4] T. Chivers and G. Schatte, *Can. J. Chem.* **2003**, 81, 1307.
- [5] T. Chivers, M. Parvez, and G. Schatte, *Angew. Chem., Int. Ed. Engl.* **1999**, 38, 2217.

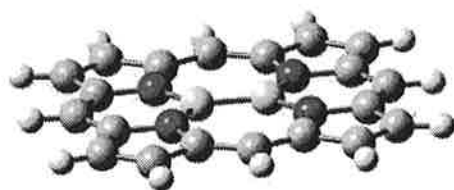
Redox Chemistry in Boron Porphyrins

P J Brothers¹, P D W Boyd¹, A M Albrett¹, M C Hodgson¹, U Kohl¹, A Weiss², W Siebert²

¹*University of Auckland, Auckland, New Zealand*, ²*University of Heidelberg, Heidelberg, Germany*

p.brothers@auckland.ac.nz

Over recent years we have investigated the chemistry of boron porphyrins, which are unique in containing two boron atoms per porphyrin ligand. Although the direct products of the reactions of BF_3 or BCl_3 with free base or lithiated porphyrins are the diboryl porphyrin complexes $(\text{BX}_2)_2(\text{Por})$, we have recently discovered that the corresponding reactions with BBr_3 or BI_3 lead to the diboranyl species $(\text{BX})_2(\text{Por})$ which contain a B-B single bond and are the result of a spontaneous reductive coupling reaction. Further reduction of $(\text{BX})_2(\text{Por})$ gives a product $\text{B}_2(\text{Por})$ (see figure), formally at the oxidation level boron(I), although experimental and computational evidence suggests the additional electrons reside on the macrocycle rather than the boron centres. These results have been supported by extensive DFT calculations. Recent experimental results will be described, along with potential applications of the boron porphyrin complexes.



**Conformational Flexibility in Inorganic Rings:
2,2'-Dioxybiphenyl-chloro-cyclotetraphosphazenes**

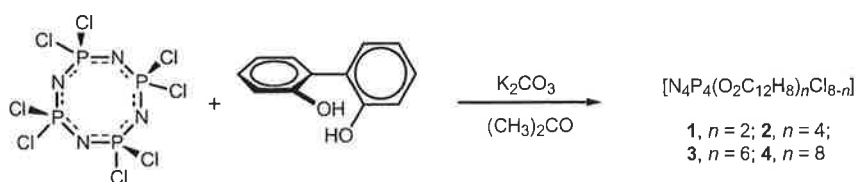
A. M. Brodie¹, E. W. Ainscough¹, A. B. Chaplin², A. Derwahl¹, J. A. Harrison³, C. A. Otter¹

¹Massey University, Palmerston North, New Zealand, ²Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland, ³Massey University, Auckland, New Zealand

A.Brodie@massey.ac.nz

Phosphazenes, particularly polyphosphazenes, continue to receive considerable commercial interest owing to their diverse range of material properties. Cyclic or short-chain linear phosphazenes are valuable small molecule models for the polymeric systems, which are often difficult to characterise owing to their higher molecular weight and structural complexity. Of these model systems, the cyclotriphosphazenes, $[\text{N}_3\text{P}_3\text{R}_6]$, are the most prevalent, although the less common cyclotetraphosphazenes, $[\text{N}_4\text{P}_4\text{R}_8]$, may be better structural analogues primarily owing to the flexible nature of the ring in contrast to the trimers which are generally planar.

In this paper we describe the synthesis of partially substituted 2,2'-dioxybiphenyl-cyclotetraphosphazenes and their characterisation using ^{31}P nmr spectroscopy, single crystal X-ray crystallography and DFT calculations.



In the context of the solid state structures, it is concluded that the presence of π -stacking is a factor that modifies the nature of the potential energy surface between the different conformers. The flexibility of the phosphazene ring is supported computationally, through the calculated low energy barriers, and experimentally, through the highly disordered phosphazene ring conformations observed in the solid state.

Morphology Changes and Mechanistic Aspects of the Electrochemically-Induced Reversible Solid-Solid Transformation of Microcrystalline TCNQ into Co[TCNQ]₂-Based Materials (TCNQ = 7,7,8,8-Tetracyanoquinodimethane)

AM Bond¹, A Nafady¹, AP O'Mullane¹, AK Neufeld²

¹Monash University, Clayton, Victoria, Australia, ²BlueScope Steel Limited, Port Kembla,

New South Wales, Australia

Alan.Bond@sci.monash.edu.au

The chemically reversible solid-solid phase transformation of a TCNQ-modified glassy carbon, indium tin oxide or metal electrode into Co[TCNQ]₂(H₂O)₂ material in the presence of Co²⁺_(aq) containing electrolytes has been induced and monitored electrochemically. Voltammetric data reveal that the TCNQ/Co[TCNQ]₂(H₂O)₂ interconversion process is independent of electrode material and identity of cobalt electrolyte anion. However, a marked dependence on electrolyte concentration, scan rate and method of electrode modification (drop casting or mechanical attachment) is found. Cyclic voltammetric and double potential step chronoamperometric measurements confirm that the formation of Co[TCNQ]₂(H₂O)₂ occurs through a rate-determining nucleation and growth process that initially involves incorporation of Co²⁺_(aq) ions into the reduced TCNQ crystal lattice at the TCNQ/electrode/electrolyte interface. Similarly, the reverse (oxidation) process, which involves the transformation of solid Co[TCNQ]₂(H₂O)₂ back to parent TCNQ crystals, also is controlled by nucleation-growth kinetics. The overall chemically reversible process that represents this transformation is described by the reaction: $2\text{TCNQ}^0_{(s)} + 2e^- + \text{Co}^{2+}_{(aq)} \rightleftharpoons [\text{Co}(\text{TCNQ})_2(\text{H}_2\text{O})_2]_{(s)}$. *Ex situ* SEM images illustrated that this reversible TCNQ/Co[TCNQ]₂(H₂O)₂ conversion process is accompanied by drastic size and morphology changes in the parent solid TCNQ. In addition, different sizes of needle-shaped nanorod/nanowire crystals of Co[TCNQ]₂(H₂O)₂ are formed depending on the method of surface immobilization.

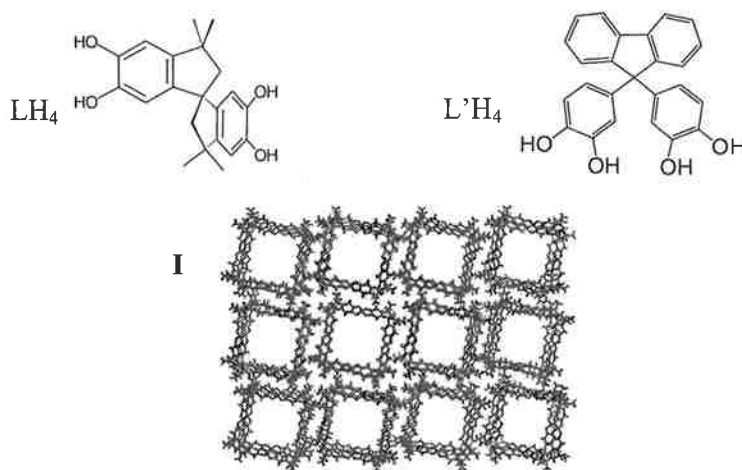
Bis-catecholate Ligands as Molecular Building Blocks in Crystalline Supramolecular Systems

B. F. Abrahams, N. J. FitzGerald, D. J. Price, R. Robson

University of Melbourne, Parkville, Victoria, Australia

bfa@unimelb.edu.au

In recent times we have been interested in using multi-catecholate units, such as LH_4 and $L'H_4$, as bridging ligands in large macrocycles. When L is combined with trimethylborate, square anionic macrocycles of formula $B_4L_4^{4-}$ are formed. Within the crystalline state these units stack on top of each other to generate parallel nanotubes of the type indicated in **I**. In this structure ionic interactions play a key role in the stacking process.¹



In the case of Mo^{VI} and Sn^{IV} , 2:2 macrocycles are formed when L' is used as a bridging ligand. In this case the macrocycles are arranged in a highly symmetrical manner that leaves vast regions of isolated solvent (nanodroplets) within the crystal. The remarkable aggregation of 12 fluorene units ($C_{13}H_8$) which participate in complementary edge-to-face interactions appears to be a dominant structural influence in the generation of a broad series of very unusual crystalline materials.

In systems involving each of the ligands, L and L' , we have successfully expanded the range of the series following careful consideration of the interactions which appear to be controlling the arrangement of the macrocycles.

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**Porphyrin-Appended Dendrimers:
“Electronic Leaves and Molecular Trees”**

D. M. D'Alessandro, A. C. Hambly, T Khoury, M. J. Crossley

Molecular Electronics Group, School of Chemistry, The University of Sydney, Sydney, NSW, Australia

deanna@chem.usyd.edu.au

Energy and electron transfer are ubiquitous in biological, chemical and physical systems: the phenomena are fundamental in natural processes such as photosynthesis, and in materials science applications such as catalysis and photochemical molecular devices. The elegance and efficiency of energy and electron transfer in nature has motivated considerable multidisciplinary research efforts into model systems with mimic aspects of the photosynthetic apparatus.

Porphyrin-appended dendrimers based on non-interacting dendritic support architectures such as the polypropylene imine (DAB-Am) and polyamido amine (PAMAM) cores constitute ideal model systems to elucidate the complex interplay of factors which govern the structure, function and efficiency of natural systems. The development of a general synthetic methodology for the construction of five generations of mono-disperse dendritic systems based on DAB-Am and PAMAM cores containing 4, 8, 16, 32, 64 and 128 porphyrin units will be described, in addition to structural characterisation techniques such as diffusion NMR. Modifications of the free-base porphyrin-appended dendrimers by metallation with Zn(II), Pd(II) and Mg(II), and through solvent mediated conformational changes in the dendritic cores were investigated as a means to fine-tune their electrochemical, spectral and photophysical properties.

New applications of the dendrimers have been found in surface-based sensing, olefin catalysis and solar cells that mimic the photosynthetic process.

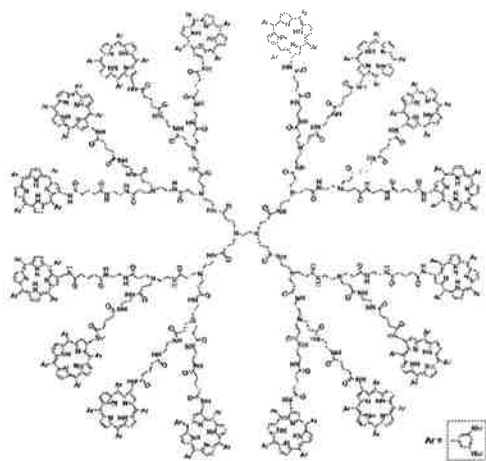


Figure 1

The third generation
porphyrin-appended
PAMAM
dendrimer.

Metal Complexes of Graphene-based Ligands

NT Lucas¹, T Darwish¹, K Müllen²

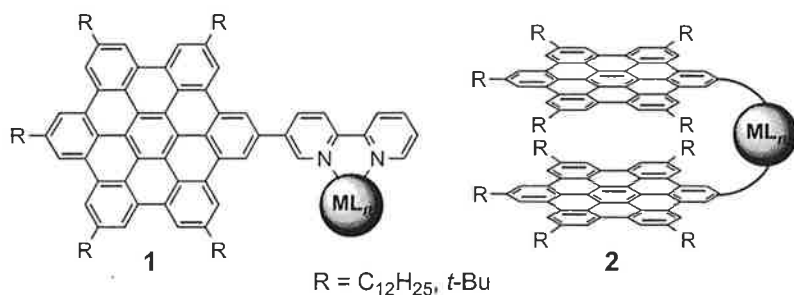
¹*School of Chemistry, The University of Sydney, NSW, Australia,* ²*Max Planck Institute for Polymer*

Research, Mainz, Germany

n.lucas@chem.usyd.edu.au

Polycyclic aromatic hydrocarbons (PAHs) are of interest because of their electronic and optoelectronic properties, and especially as they can be formally regarded as two-dimensional fragments of graphite known as graphenes.¹ Recent synthetic advances allow selective experimental entry to PAHs under mild conditions and of a size previously not thought possible.¹ When functionalized with long alkyl chains, these soluble disc-like molecules self-assemble into columnar liquid crystalline mesophases that have shown promise as semiconductor materials.^{1,2} In contrast, the incorporation of bulky rigid groups, such as *t*-butyl, impede the formation of extended columns while still exhibiting significant π - π interactions in the crystalline state. Large PAHs are also useful precursors for the pyrolytic preparation of new types of graphitic carbon nanotubes.^{1,3}

Strong arene-arene interactions are one attribute that has prompted us to investigate such molecules (and their functionalized derivatives) as ligands for metal complexation (e.g., **1**, **2**). The graphene moiety typically drives the arrangement of the ligand and its metal complexes in the bulk states, usually resulting in long range order; however, aggregation of the complexes when in solution can make characterisation challenging. Recent results on the binding of metal centres at the periphery of large PAHs will be presented.



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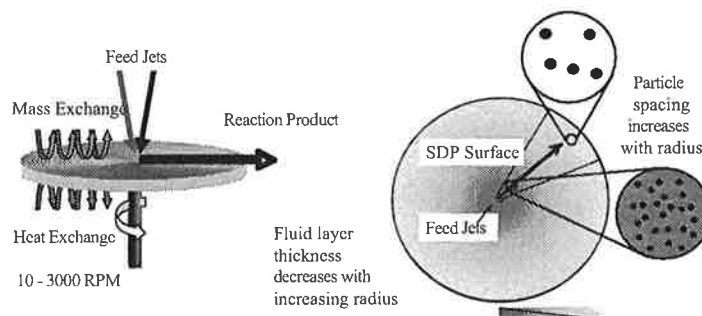
Controlling the size, shape and surface morphology, agglomeration, phases and defect of inorganic nano-particles under continuous flow conditions

S. Iyer, C. L. Raston, M. Saunders

The University of Western Australia, Perth, Australia

clraston@chem.uwa.edu.au

Spinning disc processing (SDP), is an instantaneously scalable, continuous flow and high throughput flash nano-fabrication technology. SDP can be applied to the fabrication of nano-particles of organic molecules (including drugs), inorganic material (including metals), and composites. Previous use of SDP has focused on particles > 100 nm. We have developed SDP for generating truly nano-particles, ie particles < 100 nm, for a range of materials including β -carotene, fullerenes, superparamagnetic magnetite, and metals. The work on silver nano-particles alone highlights the power and versatility of SDP. Nano-particles of silver can be prepared with remarkable control in size (5 – 200 nm), shape (spheroidal, acicular or agglomerate rosettes), surface characteristics, and phase (cubic versus hexagonal), along with imparting defects for particles > 10 nm diameters. The control is associated with changing the nature of the stabilising surfactant (starch, polyethylene glycol and poly(4-vinylpyridine)), the concentration of the reactants, and flow rates. Variation in surface features of the disc and temperature on the nature of the particles will also be presented.



The use of SDP in generating nano-particles is also of interest in incorporating green chemistry metrics into nano-technology at the inception rather than using the 20th century approach of dealing with unforeseen negative impact issues at a later date. The use of SDP in fabricating nano-particles is a paradigm shift in developing nano-technologies which can address nano-toxicology issues, scalability, effluent treatment and hazardous work environment. SDP comes under the umbrella of process intensification whereby all molecules are exposed to the same conditions.

BAL

Some Recent Highlights in Rare Earth Chemistry

G B Deacon

Monash University, Victoria, Australia

glen.deacon@sci.monash.edu.au

Snapshots of some recent highlights of our investigations of rare earth chemistry will be given. These include:

- Syntheses of rare earth organometallics, organoamides, and aryloxides from rare earth metals, as an alternative to metathesis.
- Lanthanoid fluorocarbon complexes and C-F activation.
- Low coordinate complexes and organometallic intermediates from redox transmetallation/ligand exchange syntheses.
- Supracyclopentadienyl lanthanoid complexes.
- Lanthanoid tetraphenylborates (from counter ions to pseudo metallocene complexation) and C-H activation.

As a diversion from air- and water-sensitive compounds:

- Lanthanoid carboxylates as green corrosion inhibitors.
- New lanthanoid pseudohalides – 12 coordination.

With elevated temperature syntheses, we return to high reactivity compounds.

- Elevated temperature metathesis reactions as a source of pyrazolate complexes with novel binding modes.
- Bimetallic aryloxides and pyrazolates formed directly from the metals

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