

PART 1

Conference organisation/Lecture abstracts

Joint Meeting
of the Inorganic Division of the

Royal Australian Chemical Institute

and the
Inorganic and Organometallic
Specialist Group
of the

New Zealand Institute of Chemistry



WELLINGTON, NEW ZEALAND

31 January – 4 February 1999

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ABSTRACTS:

Burrows Lecture
Plenary Lectures
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Session Lectures
Posters

ADDRESS LIST OF PARTICIPANTS

ACKNOWLEDGEMENTS

The Organising Committee wishes to thank the following sponsors who have assisted IC'99:

The Royal Society of New Zealand

The Royal Society of Chemistry

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Victoria's Centennial

This year, 1999, Victoria University of Wellington celebrates its centennial. The university today is a far cry from 1899, when only 115 students attended Arts classes at Wellington Girls' High School, in Pipitea Street and Science classes in the Technical School in Victoria Street. The university then was known as Victoria College, affiliated to the University of New Zealand. After a few years the Hunter Building, now a centrepiece of the university, was built but it was not long before that was bursting at the seams, as student numbers rose from 254 in 1905 to 547 in 1912.

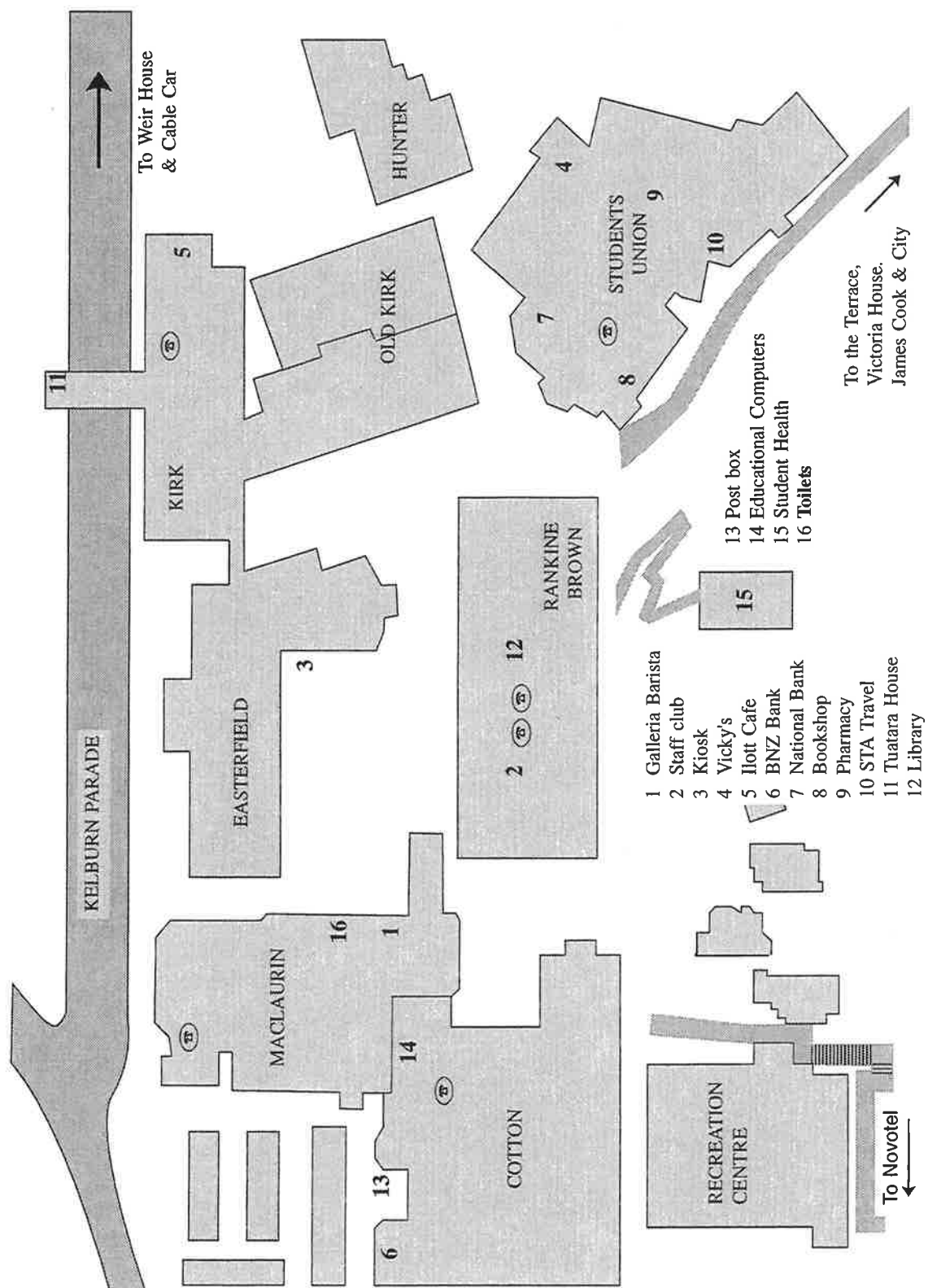
The college and its site grew steadily until the 1960s. In 1962 Victoria College became Victoria University, and in the same decade student numbers doubled, buildings proliferated and the university started to take on its modern appearance. Now, some 15,000 students attend a much larger, more diverse and vibrant university

..... and one that is still changing the lives of staff and students.

The first Professor of Chemistry was T H Easterfield who took up his appointment in 1899 as one of the four foundation professors. Easterfield was an idealist, much influenced by his experience of the German academic system where he had worked under Emil Fischer at Wurzburg. As an educator he was scornful of a system heavily focussed on examination performance. He was a committed advocate of a research-based training as the most effective means of developing a student scientifically and "culturally", but his inaugural lecture *Research as the Prime Factor in a Scientific Education* was delivered to a colonial audience unwilling or unable to grasp the message. However, Easterfield established a strong research ethos at Victoria which has been maintained over the last hundred years.

Easterfield is remembered through the prominent campus building that bears his name, and which, until recently, housed the Department of Chemistry.

CAMPUS MAP



GENERAL INFORMATION

The Inorganic Division of the Royal Australian Chemical Institute and the Inorganic Specialist Group of the New Zealand Institute of Chemistry jointly support IC '99. The scientific sessions will be held in the Maclaurin Building of Victoria University of Wellington, Kelburn Parade.

Registration and Information

On Sunday 31 January, a Registration and Information Desk will be open from 2.00 pm until 7.00 pm in the University Staff Club, Floor 3, Rankine Brown Building. For the remainder of the week the Conference Desk will be located in the Foyer of the Maclaurin Building and will be open from 8.30 am to 4.00 pm for registration and general information.

Location of Conference Sessions

Plenary and Conference Lectures, Maclaurin Building, Theatre MCLT103

Session 1 Lectures, Maclaurin Building, Theatre MCLT101

Session 2 Lectures, Maclaurin Building, Theatre MCLT102

Welcoming Reception (Sunday 31 January 8.30 pm), University Staff Club, Floor 3, Rankine Brown Building.

Poster Sessions, Foyer, Maclaurin Building

Morning and afternoon tea, Foyer, Maclaurin Building

Conference Dinner, Te Papa, Cable Street.

Scientific Programme

The nomenclature used is as follows:

PLENARY LECTURES: **PL**

CONFERENCE LECTURES: **CL**

SESSION LECTURES: **L**

POSTERS MONDAY: **M**

POSTERS WEDNESDAY: **W**

Instructions for Speakers

All lecture theatres are equipped with a normal slide projector, overhead projector, microphone and remote slide control.

Lecturers are responsible for loading and checking their own slides. Facilities for loading and previewing slides will be available in Cotton LT122. Loaded and labelled carousels should be given to the projectionist in the lecture theatre during the interval immediately before the session in which the talk is to be given.

In the parallel sessions it is important that the lecture timing is controlled. Session lecturers are asked to keep to their allocated time of 15 minutes.

Poster Sessions

Posters for *Session M* should be put up before 9 am on Monday 1 February and remain in place until noon on Tuesday 2 February. Posters for *Session W* should be put up before 9 am on Wednesday 3 February and remain in place until noon on Thursday 4 February.

Posters should be 1m x 1m. Attachments for mounting the posters to the boards will be available from the conference desk. Pins are not suitable for mounting posters and should *not* be used.

There will be prizes awarded to the two best student posters from each session and these will be presented at the conference dinner.

Messages and Information

Messages and information will be posted on a notice board adjacent to the Registration and Information Desk in the Maclaurin Foyer. Fax messages for delegates to the conference may be directed to +64 4 495 5241.

On-Campus Food and Beverage Services

Light meals and refreshments are available on campus. However, all cafes and restaurants have limited capacity and delegates are advised to seek out the less crowded locations.

Galleria-Barista Cafe, above the Maclaurin Foyer.
Staff Club, Floor 3 Rankine Brown Building.
Vicky's Restaurant, Student Union Building.
Ilott Cafe, Level 3 Foyer, Kirk Building.
Quad Kiosk, northwest corner of the Quadrangle.

Other On-Campus Facilities

Medical: the Student Health clinic offers a service to conference delegates. The clinic is open from 8.30 am to 5.00 pm weekdays. Telephone 471 5308 (internal 5308) for an appointment. There is a consultation charge. For emergency after-hours service, see below.

Banking: the Bank of New Zealand has a branch in the Cotton Building approximately 50 metres from the Maclaurin Foyer. There is a branch of the National Bank at the entrance to the Student Union Building. Banks will exchange foreign currency for NZ dollars and are open from 9.00 or 9.30 am to 4.30 pm.

Post: there is no post office on campus. However, stamps and stationery are available at the Victoria Book Centre, in the top entrance to the Student Union Building, where letters may be left for collection. There is also a post-box at the entrance to the Cotton Building adjacent to the BNZ Bank.

Telephones: several telephones are situated around the campus adjacent to the conference area and are marked on the map. Telephones require a Telecom NZ Phonecard which may be purchased from Educational Computers in the Cotton Building next to the Maclaurin Foyer, or from the Victoria Book Centre. The international access code is 00.

Pharmacy: there is a pharmacy, which also sells films and toiletries, on the lower level of the Student Union Building.

Travel agent: STA Travel is situated on the lower level of the Student Union Building.

Newspapers and magazines: a limited selection is available from the Victoria Book Centre in the upper level of the Students Union Building.

Transport

Kelburn Parade is on several bus routes – ask at the Conference Desk for details.

The Cable Car provides easy up-hill transport from Lambton Quay and the main shopping area. University station gives access to Weir House and the University. However, for the Maclaurin Building you may prefer to ride to the Botanical Gardens at the top of the Cable Car and walk down the hill to the University.

Conference dinner: buses will collect delegates from Weir and Victoria Houses and the Novotel Wellington at 6.00 and 6.30 pm. After dinner, buses will return delegates to the principal hotels and to Weir and Victoria Houses.

Restaurants and Entertainment in Wellington

Wellington offers a large variety of restaurants to suit every taste and pocket. Many of them are situated in the streets around Courtenay Place, Manners Street (Manners Mall) and Cuba Street (Cuba Mall). There are also several theatres and cinema complexes in the centre of Wellington close to the Civic Centre. Additional information is provided in the conference satchel.

Emergency Services

Fire, Ambulance or Police, telephone 111 from a Cardphone (no card required) or 1-111 from an internal university phone.

24 Hour Medical Centre and Pharmacy, 17 Adelaide Road, Newtown, telephone 384 4944.
No appointment is necessary.

IC'99 PROGRAMME

	Sunday 31 January	Monday 1 February	Tuesday 2 February	Wednesday 3 February	Thursday 4 February
9.00 am		Plenary - PL2	Plenary - PL4	Plenary - PL5	Plenary - PL7
10.00 am		Lectures Parallel Sessions A1 & A2	Morning Tea	Lectures Parallel Sessions D1 & D2	Morning Tea
10.30 am			Lectures Parallel Sessions C1 & C2		Morning Tea Posters Session - W
11.05 am		Morning Tea Posters Session - M		Lunch	
12.00 pm		Lunch	TRIPS		Lunch
1.00 pm				Plenary - PL3	
2.00 pm	Registration	Afternoon Tea		Afternoon Tea	Afternoon Tea
3.00 pm		Lectures Parallel Sessions B1 & B2		Lectures Parallel Sessions E1 & E2	Burrows Lecture Inorg Division AGM
3.30 pm					
Evening	Opening (7.00 pm) Plenary - PL1 Mixer	Conf Lecture CL1 (7.30 pm) Social		Conf Lecture CL2 (7.30 pm) Social	Conference Dinner (8.00 pm)

Plenary and Conference Lectures
Session Lectures
Poster Session M
Poster Session W

45 minutes duration
15 minutes duration
Posters to be up *before* 9 am Mon
Posters to be up *before* 9 am Wed

CONFERENCE PROGRAMME

SUNDAY 31 JANUARY 1999

- 2.00 pm** **Staff Club, Rankine Brown Building**
REGISTRATION COMMENCES
- 7.00 pm** **Lecture Theatre MCLT 103, Maclaurin Building**
CONFERENCE WELCOME
John Spencer, Victoria University of Wellington
Michael Irving, Vice-Chancellor, Victoria University of Wellington
PLENARY LECTURE 1
William Tolman, University of Minnesota
Insights into the Chemistry of Copper Protein Active Sites From Studies of Synthetic Complexes
Chairperson: Andrew Brodie, Massey University
- 8.30 pm** **Staff Club, Rankine Brown Building**
CONFERENCE MIXER

MONDAY 1 FEBRUARY 1999

- 9.00 am** **Lecture Theatre MCLT 103, Maclaurin Building**
PLENARY LECTURE 2
John Bercaw, California Institute of Technology
Hydrocarbon Hydroxylation with Electrophilic Platinum Complexes
Chairperson: John Spencer, Victoria University of Wellington
- 10.05 am** **CONCURRENT SESSION LECTURES**
- | | Session A1
Lecture Theatre MCLT 101
Chairperson: Anthony Burrell | Session A2
Lecture Theatre MCLT 102
Chairperson: Graham Bowmaker |
|-----------------|---|---|
| 10.05 am | L1 Gregory Kubas, Los Alamos National Laboratory
<i>Activation of H₂ and Other Small Molecules on Cationic Platinum and Rhenium Complexes</i> | L4 Lars Kloo, Royal Institute of Technology, Stockholm
<i>LEGO Chemistry Practised: Polyiodides in the Liquid and Solid State</i> |
| 10.25 am | L2 Graham Ball, University of New South Wales
<i>Observation and Characterisation of Alkane Complexes using NMR Spectroscopy</i> | L5 Hubert Schmidbaur, Technischen Universität München
<i>Phosphinic and Phosphinous Acids and their Thio Analogues as Ligands in Gold Chemistry</i> |
| 10.45 am | L3 Eric Wenger, Australian National University
<i>Insertion Reactions of Aryne-Nickel(0) Complexes with Alkynes: Formation of Naphthalenic Phosphines</i> | L6 Matthias Driess, University of Bochum
<i>Unusual Polyphosphane Ligands Having a Silicon-Phosphorus Backbone</i> |
| 11.05 am | Foyer, Maclaurin Building
MORNING TEA
POSTER SESSION M | |
| 1.00 pm | LUNCH | |

2.00 pm	Lecture Theatre MCLT 103, Maclaurin Building PLENARY LECTURE 3 Edward Baker, University of Auckland <i>The Fight for Iron: New Aspects of Iron Acquisition and Transport Systems in Bacteria and Animals</i> Chairperson: Richard Keene, James Cook University	
3.00 pm	Foyer, Maclaurin Building AFTERNOON TEA	
3.30 pm	CONCURRENT SESSION LECTURES	
	Session B1 Lecture Theatre MCLT 101 Chairperson: James Wright	Session B2 Lecture Theatre MCLT 102 Chairperson: Eric Ainscough
3.30 pm	L7 Anthony Hill, Imperial College <i>New Developments in Ruthenium and Osmium Allenylidene Chemistry</i>	L12 John Ranford, National University of Singapore <i>Metalloprotein Models to Supramolecular Structures from Substituted Amino Acid Antitumour Agents</i>
3.50 pm	L8 Andrew Johnson, University of Durham <i>The Dicarbolide Ligand $[C_2B_9H_{11}]^{2-}$ as a Cyclopentadienyl Analogue: Early Transition Metal Complexes</i>	L13 Ross Edwards, Massey University <i>Distinct Metal Environment in Fe-Substituted Manganese Superoxide Dismutase of E. Coli Provides a Structural Basis of Metal Specificity</i>
4.10 pm	L9 Paul Low, Steacie Institute of Molecular Sciences, Ottawa <i>Electronic Interactions with Metallo-Carbon Clusters – New Components for Multi-Metallic Arrays</i>	L14 Franc Meyer, Universität Heidelberg <i>Cooperative Transformations of Small Molecules at a Dinuclear Nickel(II) Site</i>
4.30 pm	L10 Michael Bruce, University of Adelaide <i>Carbon-Rich Metal Complexes</i>	L15 Hiroshi Tsukube, Osaka City University <i>Aggregation and Chiral Recognition Behaviours of Metallo-Cyclen Receptor</i>
4.50 pm	L11 Anthony Wright, Massey University <i>High Nuclearity Ruthenium-Sulfur Clusters</i>	L16 Nicola Brasch, Australian National University <i>Mechanistic Investigations on the Reaction of the Vitamin B₁₂ Coenzymes with Cyanide</i>
5.10 pm	DINNER	
7.30 pm	Lecture Theatre MCLT 103, Maclaurin Building CONFERENCE LECTURE 1 Mark Humphrey, Australian National University <i>Nonlinear Optical Properties of Organometallics: From Monometallic Complexes to Polymetallic Materials</i> Chairperson: Allan Canty, University of Tasmania	
8.30 pm	Foyer, Maclaurin Building CONFERENCE SOCIAL	

TUESDAY 2 FEBRUARY 1999

- 9.00 am** **Lecture Theatre MCLT 103, Maclaurin Building**
PLENARY LECTURE 4
Peter Comba, Universität Heidelberg
Enforced Coordination Geometries – Preorganisation, Catalysis and Beyond
 Chairperson: Brian Robinson, University of Otago
- 10.00 am** **Foyer, Maclaurin Building**
MORNING TEA
- 10.30 am** **CONCURRENT SESSION LECTURES**
- | | |
|---|---|
| <p>Session C1
 Lecture Theatre MCLT 101
 Chairperson: Geoff Jameson</p> | <p>Session C2
 Lecture Theatre MCLT 102
 Chairperson: Sally Brooker</p> |
|---|---|
- 10.30 am** **L17** Scott Bohle, University of Wyoming
 β -Hematin: A Coordination Polymer Central to Heme Detoxification in Malaria
- 10.30 am** **L21** Bruce Wild, Australian National University
Self-Assembly of Di- and Tri-Nuclear Metal Helicates Containing Poly(tertiary Phosphines) and Related Compounds
- 10.50 am** **L18** Graeme Hanson, University of Queensland
Spectroscopy and Crystallographic Characterisation of Dimethylsulfoxide Reductase from Rhodobacter capsulatus: Structure and Implications for Electron Transfer
- 10.50 am** **L22** Marcel Maeder, University of Newcastle
Formation Kinetics of Pendant Arm Polyamine Macrocycles with Copper(II)
- 11.10 am** **L19** Kymberley Vickery, Macquarie University
 *Λ and Δ -cis- β -[Ru(R*R*-picchxn)(phen)]²⁺ Metalloprobes Show Differential Binding Geometries with d(CGCGATCGCCG)₂*
- 11.10 am** **L23** Owen Curnow, University of Canterbury
"Hypervalent" Molecules: What if there are no d Orbitals?
- 11.30 am** **L20** George Clark, University of Auckland
The Incredible Shrinking Crystal: Formation of a Three-Dimensional DNA Polymer
- 11.30 am** **L24** Stephen Lincoln, University of Adelaide
Chirality, Superchirality and Molecular Reception in Macrocyclic Metal Complexes
- 12.00 pm** **LUNCH & AFTERNOON FREE FOR EXCURSIONS**

WEDNESDAY 3 FEBRUARY 1999

- 9.00 am** **Lecture Theatre MCLT 103, Maclaurin Building**
PLENARY LECTURE 5
Ian Manners, University of Toronto
Ring-Opening Polymerization (ROP) as a Route to Transition Metal Based Polymers with Controlled Architectures
 Chairperson: Colin Raston, Monash University

10.05 am CONCURRENT SESSION LECTURES

Session D1

Lecture Theatre MCLT 101

Chairperson: Kevin Wainwright

Session D2

Lecture Theatre MCLT 102

Chairperson: Jim Simpson

10.05 am **L25** Gottfried Huttner, Universität Heidelberg
Zintl-Ions: An Organometallic Variation

L28 Tom Baker, Los Alamos National Laboratory
Late Metal Coordination Chemistry of a 'Bulky CO' Analogue $\{P[N(dipp)CH_2CH_2(dipp)N]\}OTf$ (dipp=2,6-diisopropylphenyl; OTf=triflate)

10.25 am **L26** Kathryn Hindmarsh, Murdoch University
Improving the Cyanidation Process Using Colloidal Gold

L29 Matthew Byrnes, Australian University
Reactivity of Cis-Bis(Alkene)-Bis(Acetylacetonato)Ruthenium(II) Complexes with Group 15 Donor Ligands

10.45 am **L27** Peter Nichols, Monash University
Supramolecular Chemistry of Nickel(II) Macrocycles with Fullerenes and other Globular Molecules

L30 Geoffrey Crisp, University of Adelaide
New Protocols for Palladium-Catalysed Coupling of Terminal Alkynes with Aryl Halides

11.05 am Foyer, Maclaurin Building
MORNING TEA
POSTER SESSION W

1.00 pm LUNCH

2.00 pm Lecture Theatre MCLT 103, Maclaurin Building
PLENARY LECTURE 6
Galen Stucky, University of California at Santa Barbara
Using Competing Processes, Spatial Domains and Interfaces in the Assembly of Composite Materials
Chairperson: Ian Dance, University of New South Wales

3.00 pm Foyer, Maclaurin Building
AFTERNOON TEA

3.30 pm CONCURRENT SESSION LECTURES

Session E1

Lecture Theatre MCLT 101

Chairperson: Penny Brothers

Session E2

Lecture Theatre MCLT 102

Chairperson: David Weatherburn

3.30 pm **L31** William Rees, Georgia Institute of Technology
Molecular Design of Group 2 Element Compounds as Precursors for Electronic Materials

L36 Lyall Hanton, University of Otago
Copper(I)-Iodide Cores in Coordination Polymers

3.50 pm **L32** Stuart Batten, Monash University
Structure and Magnetism of Meta-Pseudohalide Coordination Polymers

L37 Werner Thiel, Technische Universität München
Coordination Chemistry of Chiral Ligands with Cycloalkane Backbones

4.10 pm **L33** Jim Johnston, Victoria University of Wellington
Geothermal Silica – Specialist Products from a Waste Resource

L38 Alex McAuley, University of Victoria
Synthesis and Reactions of Macro-Polycyclic Complexes

4.30 pm	L34 Douglas Shephard, University of Cambridge <i>Clusters, Catalysis and Supramolecular Ordering of Nano-composites</i>	L39 Leone Spiccia, Monash University <i>Coordination Chemistry of Poly(macrocyclic) Ligands Derived from 1,4,7-triazacyclononane</i>
4.50 pm	L35 Stephen Bagshaw, Industrial Research Limited <i>Symmetric Mesoporous Metallo-Silicate Catalysts by Low Concentration Non-Ionic Surfactant Templating</i>	L40 Paul Bernhardt, University of Queensland <i>Electrochromic Cyano-Bridged Dinuclear Complexes</i>
5.10 pm	DINNER	
7.30 pm	Lecture Theatre MCLT 103, Maclaurin Building CONFERENCE LECTURE 2 Don House, University of Canterbury <i>Inorganic Reaction Mechanisms – at the Frontiers or Past their Best-Used-By-Date</i> Chairperson: Neil Curtis, Victoria University of Wellington	
8.30 pm	Foyer, Maclaurin Building CONFERENCE SOCIAL	

THURSDAY 4 FEBRUARY 1999

9.00 am	Lecture Theatre MCLT 103, Maclaurin Building PLENARY LECTURE 7 Jonathan Sessler, University of Texas at Austin <i>Lanthanide Texaphyrins: A New Approach to Anticancer Drug Development</i> Chairperson: Warren Roper, University of Auckland	
10.00 am	Foyer, Maclaurin Building MORNING TEA	
10.30 am	CONCURRENT SESSION LECTURES	
	Session F1 Lecture Theatre MCLT 101 Chairperson: Gerry Swiegers	Session F2 Lecture Theatre MCLT 102 Chairperson: Neil Milestone
10.30 am	L41 Anthony Burrell, Massey University <i>Bis(ferrocenyl)porphyrins: Compounds with Strong Long-Range Metal-Metal Coupling</i>	L46 Brian Nicholson, University of Waikato <i>X-Ray Absorption Spectra of Some Aryl-Mercury Compounds</i>
10.50 am	L42 Laurence Kelso, James Cook University <i>Electron and Energy Transfer Within Dyads Involving Organic Quenchers and/or Polypyridyl d⁶ Metal Centres Bridged by Rigid Alicyclic "Molracs"</i>	L47 David McMorron, University of Canterbury <i>Quadruple Helicates as Selective Hosts for Anions</i>
11.10 am	L43 John McAdam, University of Otago <i>Fluorescent Switches from Naphthalimides and Ferrocenylamines</i>	L48 Sonya Scott, Massey University <i>Emission Studies of Porphyrin Arrays</i>

11.30 am	L44 Michael Hardie, Monash University <i>Combining Host-Guest Chemistry and Crystal Engineering: Self-Assembly of Hydrogen-Bonded Arrays Incorporating Receptor Sites</i>	L49 Janice Aldrich-Wright, University of Western Sydney <i>DNA-Binding of Metal Complexes</i>
11.50 am	L45 Peter Boyd, University of Auckland <i>Selective Supramolecular Porphyrin/Fullerene Interactions</i>	L50 Russell Howe, University of New South Wales <i>X-Ray Absorption Spectroscopy of Microporous Materials</i>
12.10 pm	LUNCH	
2.00 pm	CONCURRENT SESSION LECTURES	
	Session G1 Lecture Theatre MCLT 101 Chairperson: Lawrence Gahan	Session G2 Lecture Theatre MCLT 102 Chairperson: Richard Hartshorn
2.00 pm	L51 Leonard Lindoy, University of Sydney <i>Large Cage Molecules for the Selective Binding of Metal Ions and Small Molecules</i>	L54 Magnus Sandström, Royal Institution, Stockholm <i>Crystal and Liquid Structures of NN-Dimethylthioformamide (DMTF)) and N,N-Dimethylformamide (DMF) Showing Stronger Effect of C-H...S than of C-H...O Hydrogen Bonding</i>
2.20 pm	L52 Shane Telfar, University of Canterbury <i>The Photochemistry of Cobalt(III)-Amino Acid Complexes</i>	L55 Murray Davies, University of Sydney <i>Ligand Mediated Oxidation of Pt(II) and Stabilization of Pt(IV)</i>
2.40 pm	L53 Peter Lay, University of Sydney <i>Chromium(V) Peptide and Amino Acid Complexes. Possible Intermediates in Chromium-Induced Carcinogenesis</i>	L56 Anthony Baker, University of New South Wales <i>Dwyer and Lions Revisited: Complexes of Sexadentate Ligands</i>
3.00 pm	Foyer, Maclaurin Building AFTERNOON TEA	
3.30 pm	Lecture Theatre MCLT 103, Maclaurin Building BURROWS LECTURE David Buckingham, University of Otago <i>The Timing of Chemical Change</i> Chairpersons: Andrew Brodie, Massey University & John Spencer, Victoria University of Wellington	
4.30 pm	Lecture Theatre MCLT 103, Maclaurin Building RACI INORGANIC DIVISION AGM	
8.00 pm	Rangimarie Suite, Te Papa CONFERENCE DINNER	

BURROWS LECTURE

BURROWS LECTURE: THE TIMING OF CHEMICAL CHANGE

Professor David Buckingham
186 Warren Street
Wanaka, New Zealand

Abstract

For many years I have been concerned at the teaching of reaction mechanism to undergraduates. It has worried me that not enough attention has been placed on how the speed (rate) of a chemical process is interpreted in microscopic terms, and how this is taught to students. To me the timing, and time taken, for a chemical reaction is fundamental; and this is how a beginning undergraduate also sees a reaction (when they think about it). But this is not how it is taught.

A few years ago a IUPAC Commission recognised such difficulties, and suggested fundamental changes to the way a reaction mechanism is described. Such changes are not observationally based; they are based on the timing of separate steps, and the time interval between them.

This lecture will review, with examples, the background to such ideas as they relate to inorganic systems.

PLENARY LECTURES

INSIGHTS INTO THE CHEMISTRY OF COPPER PROTEIN ACTIVE SITES FROM STUDIES OF SYNTHETIC COMPLEXES

William B. Tolman

*Department of Chemistry and Center for Metals in Biocatalysis, University of Minnesota,
207 Pleasant Street SE, Minneapolis, MN 55455 (USA)*

Small molecule activation, hydrocarbon oxidation, and electron transfer are fundamentally important chemical processes performed within the confines of copper protein active sites that are characterized by widely varying geometric and electronic structures. Although there exists much information on the topologies of many of these copper protein active sites, a largely unfulfilled research objective is to understand, in detail, structure/function relationships and mechanisms of enzyme action. In an approach toward this goal, we attempt to reveal fundamental principles that underly the chemistry of the biological systems through the synthesis, characterization, and examination of the reactivity of model complexes. We have focused specifically on understanding the active sites of enzymes that reduce nitrogen oxides during the biological nitrogen cycle (nitrite and nitrous oxide reductase), that bind or reduce dioxygen during respiration (hemocyanin, cytochrome *c* oxidase), and that oxidatively functionalize organic substrates to provide important metabolites (tyrosinase, catechol oxidase, galactose oxidase). A survey will be presented of the chemistry of complexes supported by a range of multidentate, predominantly N-donor ligands that:

- Bind NO and NO₂⁻ to give adducts of unusual structure that react to yield reduced products (N₂O or NO, respectively); thus providing insights into biological NO_x reduction,
- Model the delocalized mixed-valent (Cu^{1.5}Cu^{1.5}), thiolate-bridged “Cu_A” electron-transfer site recently identified in a number of proteins and constructs, thus yielding important knowledge of the novel electronic structure of this motif,
- Contain Cu^{II}-phenolate, Cu^I-phenolate, and Cu^{II}-phenoxyl radical units implicated in galactose oxidase function, thus enhancing our understanding of the chemistry of the growing class of proteins that contain metal-radical arrays, and
- Bind O₂ to yield isomeric (μ-η²:η²-peroxo)- and bis(μ-oxo)dicopper complexes that can interconvert, illustrating reversible O-O bond breaking and making within a dimetal system that is relevant to such processes in a range of metalloproteins. Studies of the oxidative reactivity of these species also has provided new insights into C-H bond activation mechanisms by metalloenzymes.

Hydrocarbon Hydroxylation with Electrophilic Platinum Complexes

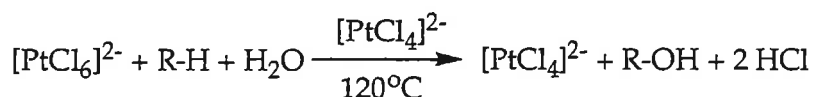
John E. Bercaw

Arnold and Mabel Beckman Laboratories of Chemical Synthesis

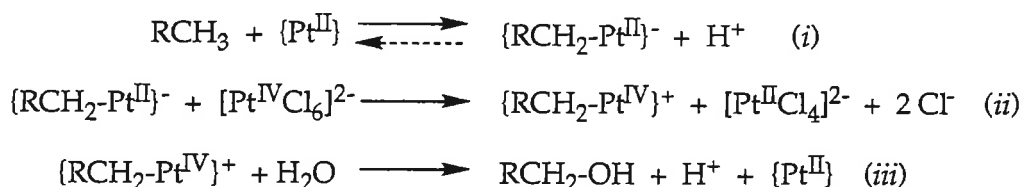
California Institute of Technology

Pasadena, CA 91125

Among organometallic reagents that activate carbon-hydrogen bonds, the "Shilov system" (equation 1)¹ exhibits unusual selectivity² and better compatibility with oxidants and protic reagents.



Using a variety of kinetics, isotopic labeling and stereochemical studies, we have established that alkane oxidation takes place by three distinct steps.³



While direct access to the mechanism of step (i) is difficult, examination of the microscopic reverse - protonolysis of model alkyl platinum(II) complexes - suggests that it too proceeds in several stages, comprising interaction of the alkane with Pt(II) to form a so-called σ complex, oxidative addition of the coordinated C-H bond to give a platinum(IV) alkyl-hydride species, and deprotonation of the latter to afford platinum(II) alkyl.⁴

These studies will be summarized,⁵ along with recent results that encourage us that a truly catalytic variant based on O_2 as the ultimate oxidant might be forthcoming.

References Cited

1. Kushch, L. A.; Lavrushko, V. V.; Misharin, Y. S.; Moravsky, A. P.; Shilov, A. E. *Nouv. J. Chim.* **1983**, 7, 729.
2. (a) Labinger, J. A.; Herring, A. M.; Lyon, D. K.; Luinstra, G. A.; Bercaw, J. E.; Horvath, I. T.; Eller, K. *Organometallics* **1993**, 12, 895.
(b) Sen, A.; Benvenuto, M. A.; Lin, M. R.; Hutson, A. C.; Basicckes, N.; *J. Am. Chem. Soc.* **1994**, 116, 998, and references cited therein.
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5. Stahl, S. S.; Labinger, J. A.; Bercaw, J. E. *Angew. Chem. Int. Ed. Engl.* **1998**, 37, 2181.

THE FIGHT FOR IRON: NEW ASPECTS OF IRON ACQUISITION AND TRANSPORT SYSTEMS IN BACTERIA AND ANIMALS

Edward N. Baker

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Iron is an essential element for almost all living systems, yet it poses severe biochemical problems of solubility and toxicity. For this reasons specialised molecules, both large and small, have been adopted to scavenge iron, transport it to sites of utilisation, deliver it and store it. Part of the fight for survival between pathogenic bacteria and their human (or animal) hosts is indeed a fight for iron, using competing batteries of molecules. In humans, proteins of two types, the transferrins and hemopexin, are used for iron acquisition and transport. Our research on the three-dimensional structures of these proteins has shown that although they have totally different structures their design principles are based on common mechanisms of binding and release. These involve highly specific binding sites between protein domains that can undergo flexible movements. The same design is even used by some of the iron transport proteins of certain pathogenic bacteria, suggesting common evolutionary precursors. In other bacteria, small-molecule chelators are used, but even these bear some relation to their protein cousins. Finally, a full molecular understanding of these systems requires knowledge of the receptors that discriminate between different transport molecules and progress in this area will also be indicated.

Enforced Coordination Geometries - Preorganisation, Catalysis and Beyond

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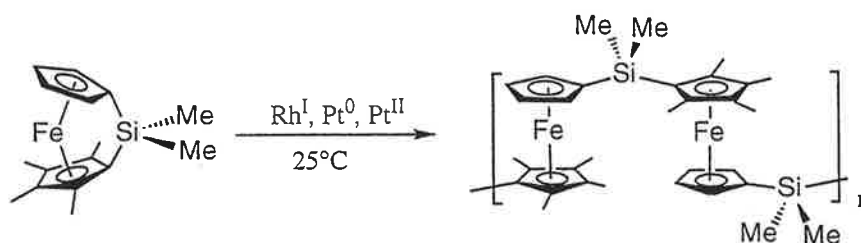
Stabilities, reactivities and electronic properties of transition metal coordination compounds are related to the number and type of donor groups and to their geometric arrangement. Carefully designed rigid ligands may be used to enforce specific coordination geometries that lead to the discrimination between metal ions in specific oxidation and electronic states. The shape and flexibility of the ligands and their cavity is important for the selective stabilization of specific metal ions, for the discrimination between substrates captured by metal complex fragments and for the selective activation of these substrates. There are simple and efficient methods to predict shapes and flexibilities of metal-free and coordinated ligands, and these are used to design transition metal compounds with specific stabilities, reactivities, electrochemical and electronic properties. Applications range from metal ion discrimination and stereoselective coordination of substrates to low molecular weight structural and spectroscopic models of metalloproteins and to catalytically active coordination compounds.

Ring-Opening Polymerization (ROP) as a Route to Transition Metal Based Polymers with Controlled Architectures

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Polymers which possess skeletal transition metal atoms in close proximity to one another are of considerable interest due to their potentially unusual electrical and magnetic properties and other physical and chemical characteristics. However, synthetic routes to well-defined, soluble, and high molecular weight examples of these materials are rare. This presentation will focus on research in our group aimed at developing ring-opening polymerization (ROP) as a route to transition metal-based macromolecules. In particular, the ROP of strained ring-tilted metallocenophanes such as silicon-bridged [1]ferrocenophanes to yield high molecular weight ($M_w = 500,000 - 3,000,000$) poly(ferrocenylsilanes) will be discussed (see reaction below).¹ Current knowledge of the properties and applications of the latter materials and related polymers will also be outlined. The synthesis of polymers with controlled architectures such as block copolymers via anionic and transition metal catalyzed ROP will also be discussed.² Poly(ferrocene) diblock copolymer materials self-assemble in the solid state and solution to yield, for example, stable cylindrical “nanowire” structures with potentially semiconducting organometallic cores and insulating sheaths and these will also be discussed.³



1. Foucher, Tang, Manners, *J. Am. Chem. Soc.*, **1992**, *114*, 6246.
2. Gómez-Elipe, Resendes, Macdonald, Manners, *ibid* **1998**, *120*, 8348.
3. Massey, Power, Manners, Winnik. *ibid* **1998**, *120*, 9533.

USING COMPETING PROCESSES, SPATIAL DOMAINS, AND INTERFACES IN THE ASSEMBLY OF COMPOSITE MATERIALS

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D. Zhao, P. Yang, W. Lukens, Department of Chemistry
N. Melosh, S. Christiansen, B. F. Chmelka, Department of Chemical Engineering
University of California, Santa Barbara, California 93106 U.S.A.

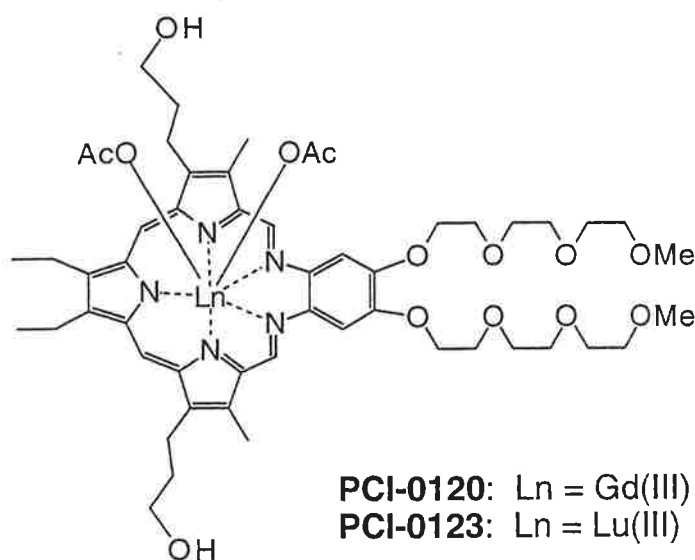
The biogenesis of materials evolves in a single system through a fascinating combination of the space/time definition of structure, function, and morphology at multiple length scales from complex mixtures of reactants and accessible processes. Although we can only model biogenesis at a very elementary level, the general principles have proven to be valuable in developing a strategy for complex-materials synthesis. This talk will present an overview of the use of these concepts to synthesize composite and porous materials that have 3-d patterned structural and physical properties from the nanometer to macroscale length scales. At the microscale level, weak organic-organic interactions, strong inorganic-organic charge matching, and domain separation of the charged wall from the cage and pore contents through templating with organic molecules that have spatially competing hydrophilic-hydrophobic regions have been used to create crystalline transition-metal-rich and main-group zeolite-like structures with intersecting 12-ring cage structures, a crystalline bicontinuous gyroid surface, and a mesoscale (20 Å) cage. The introduction of stronger organic-organic interactions, weaker interactions at the organic-inorganic interface through hydrogen bonding using cationic silica species, and the appropriate organic domain definition gives honeycomb, orthorhombic, rhombohedral, 3-d hexagonal, and several different cubic periodic silica structural phases with unit cells that have volumes of up to 3,000,000 Å³ and unit cell dimensions approaching 200 Å. Hierarchically structured materials with periodic mesopores (~10 nm), patterned submicron-scale pores (~100 nm), and macroscale motifs (~1000 nm) are accessible by multiprocesses using appropriate organized organic domains and kinetic control. The processing and use of these phases as membranes, films, and spheres will be described.

LANTHANIDE TEXAPHYRINS: A NEW APPROACH TO ANTICANCER DRUG DEVELOPMENT

Jonathan L. Sessler,^a Tarak D. Mody,^b Gregory Hemmi,^b Nicolai Tvermoes,^a Pavel Anzenbacher, Jr.,^a and Richard A. Miller^b

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The syntheses and characterization of a range of lanthanide texaphyrins will be presented. The use of certain water-soluble gadolinium(III) and lutetium(III) derivatives (e.g., PCI-0120 and PCI-0123) as sensitizers for, respectively, the X-ray radiation-based (XRT) and photodynamic therapeutic (PDT) treatment of cancer will be summarized. An update of ongoing clinical studies will be provided and the results of ongoing mechanistic investigations will be detailed.



CONFERENCE LECTURES

NONLINEAR OPTICAL PROPERTIES OF ORGANOMETALLICS:
FROM MONOMETALLIC COMPLEXES TO POLYMETALLIC MATERIALS

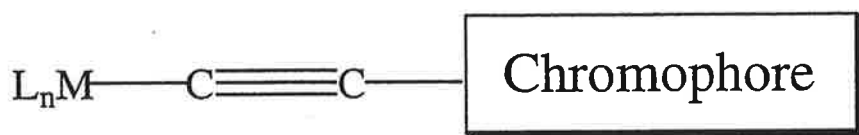
Mark G. Humphrey

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Organic molecules have attracted a great deal of interest as potential new materials for nonlinear optics. They enjoy several advantages over existing inorganic materials, including the possibility of a purely electronic response, ease of modification of the molecular architecture, and ease of processing. Organometallics may have the advantages of organic molecules, and in addition possess greater molecular design flexibility including, *inter alia*, the possibility of varying metal, co-ligands, coordination geometry and oxidation state, all of which may impact favourably on nonlinear optical (NLO) merit.^{1,2} As a consequence, the NLO properties of organometallics have been the subject of an increasing number of studies over the last ten years, with the most intense interest being shown in ferrocene, other cyclic polyene complexes, and their derivatives. The MLCT axis in ferrocene is perpendicular to that of an attached organic π -system, which may not be the most favourable orientation for optimal NLO responses. We have focussed our attention on alkynylmetal complexes, in which the metal is in the plane of the organic π -system; these complexes can be engineered with environmental (oxidative, thermal) stability, and appropriate functionality for incorporation into processable materials (thin films).



In the last three years, we have investigated molecular structure / NLO activity relationships for a range of structural components of alkynylmetal complexes, and have reported the significance of varying metal, valence electron count, ease of oxidation, co-ligands, acceptor group, chain-lengthening at the alkynyl ligand by a variety of bridging groups, and chain-lengthening through the metal; in the process we have prepared the organometallics with the largest quadratic and cubic NLO responses. We have recently extended our studies from monometallic complexes to polymetallic systems. This talk will summarize the results of these studies.

1. I.R. Whittall, A.M. McDonagh, M.G. Humphrey and M. Samoc, *Adv. Organomet. Chem.*, 1998, **42**, 291-362.
2. I.R. Whittall, A.M. McDonagh, M.G. Humphrey and M. Samoc, *Adv. Organomet. Chem.*, 1998, **43**, 349-405.

INORGANIC REACTION MECHANISMS —
AT THE FRONTIERS OR PAST THEIR BEST-USED-BY DATE

D.A. House
Chemistry Department
University of Canterbury
Christchurch, New Zealand

A brief history of Inorganic Reactions Mechanisms will be presented as well as some crystal ball gazing as to possible future developments in the subject.

SESSION LECTURES

ACTIVATION OF H₂ AND OTHER SMALL MOLECULES ON CATIONIC PLATINUM AND RHENIUM COMPLEXES

Gregory J. Kubas, Wayde V. Konze, Jean Vincent, Brian L. Scott; Chemical Sciences and Technology Division, Los Alamos National Laboratory, MS-J514, Los Alamos, NM 87545

We have concentrated recent efforts on developing unsaturated, highly electrophilic, cationic fragments such as $[\text{Re}(\text{CO})_4\text{P}]^+$ and $[\text{PtXP}_2]^+$ (P = phosphine donor; X = H, Me) for binding of H₂ and other nonclassical ligands, where the non-interacting BAr_f anion (B[3,5-C₆H₃(CF₃)₂]₄) stabilizes the cations. The positive charge favors σ -coordination over oxidative addition, and the binding strength of H₂ to cationic complexes is remarkably similar to that in neutral analogues. Increased electrophilicity at the metal increases sigma-donation from H₂ to offset reduced backbonding, and H₂ can adapt to virtually any electronic situation and bind to a great variety of transition metal fragments. The charge and electrophilicity of the metal favors heterolytic cleavage of H-H and Si-H bonds which readily occurs on the Re system. The platinum system, $[\text{PtXP}_2(\text{Sol})][\text{BAr}_f]$ (X = H, Me; P₂ = PR₃ or R₂P(CH₂)₂PR₂; Sol = OEt₂, CH₂Cl₂, NC₅F₅), binds H₂ with loss of Sol and gives novel activation of other molecules. For example, *trans*- $[\text{PtMe}(\text{PPh}_3)_2(\text{OEt}_2)][\text{BAr}_f]$ undergoes B-C bond cleavage of BAr_f under mild conditions to form the neutral, diarylated complex *trans*-Pt(Ar_f)₂(PPh₃)₂ in good yield. This is the first transition metal-mediated reaction of the "non-interacting" BAr_f anion. The diphosphine complexes with X = Me activate benzene by C-H cleavage (with CH₄ elimination) and C-C bond coupling to form a biphenyl molecule with two $[\text{PtP}_2]^+$ fragments coordinated to one ring.

OBSERVATION AND CHARACTERISATION OF ALKANE COMPLEXES USING NMR SPECTROSCOPY

Spili Geftakis and Graham E. Ball

School of Chemistry and NMR Facility, The University of New South Wales, Sydney 2052, Australia

On account of their involvement in the C-H bond activation process and general interest as coordination compounds, the characterisation and ultimately synthesis of complexes of simple alkanes is a continuing goal of organometallic chemistry. Owing to the very poor nature of alkanes as ligands, these complexes are generally very short lived at ambient temperatures.¹

We have just reported the first direct observation of an alkane complex, $\text{CpRe}(\text{CO})_2(\text{cyclopentane})$ (1), using NMR spectroscopy.² *In situ* photolysis of a sample of $\text{CpRe}(\text{CO})_3$ in 95:5 cyclopentane: cyclopentane- d_{10} whilst located within an NMR spectrometer at 180 K leads to the formation of 1. This is observed as two new peaks that grow in at δ 4.92 due to the Cp protons and an upfield shifted quintet at δ -2.32 ($^3J_{\text{HH}} = 6.6$ Hz) due to two protons in a bound methylene unit (Figure 1).

In this presentation, the use of isotopic labelling and heteronuclear 2D NMR experiments to confirm the presence of a bound alkane moiety and to locate the other resonances in the cyclopentane ring will be described. The ^{13}C resonance of the bound moiety is also highly shielded (δ -31.2) and the $^1J_{\text{CH}}$ value (112.9 Hz) is significantly reduced compared to free alkane. Isotopic perturbation of resonance data indicate that the bonding mode is likely *via* a single C-H bond σ interaction and that C-H bonds bind more strongly than C-D bonds.

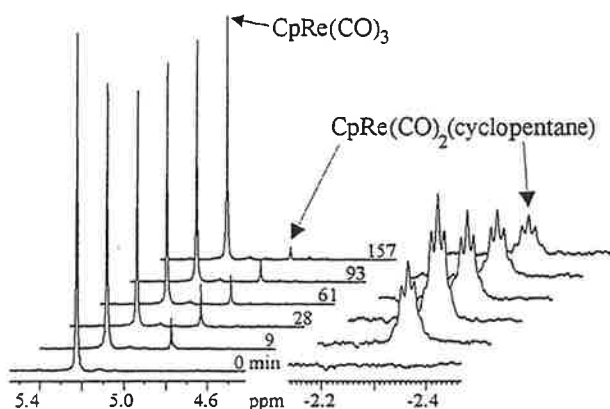


Figure 1. Monitoring the the photolysis of $\text{CpRe}(\text{CO})_3$ in cyclopentane at 180 K vs. time. Irradiation was ceased after 28 minutes in this example.

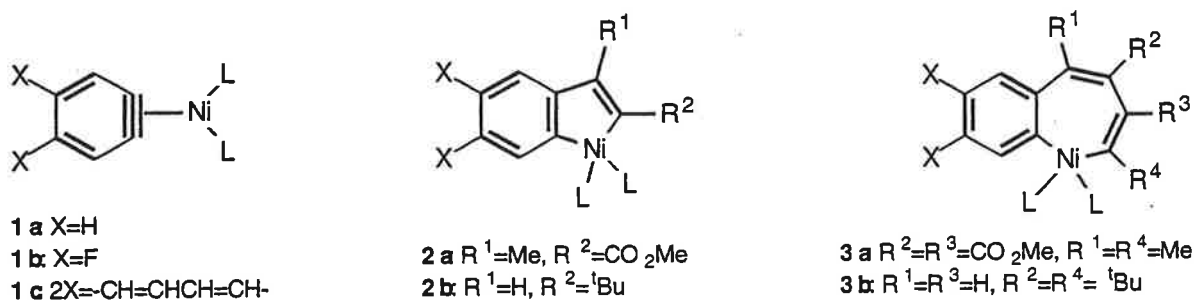
- (1) Hall, C.; Perutz, R.N. *Chem. Rev.*, **1996**, *96*, 3125.
- (2) Geftakis, S.; Ball, G.E. *J. Am. Chem. Soc.*, **1998**, *120*, 9953.

INSERTION REACTIONS OF ARYNE-NICKEL(0) COMPLEXES WITH ALKYNES: FORMATION OF NAPHTHALENIC PHOSPHINES

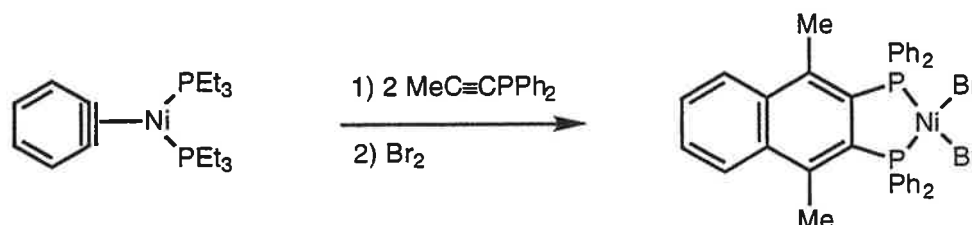
Martin A. Bennett, Christopher J. Cobley and Eric Wenger

Research School of Chemistry, The Australian National University, Canberra, A.C.T. 0200 (Australia)

The highly sensitive η^2 -benzyne- and 2,3 η -naphthalynes-nickel(0) complexes $\text{Ni}(\eta^2\text{-aryne})\text{L}_2$ [aryne = C_6H_4 , 4,5- $\text{F}_2\text{C}_6\text{H}_2$, C_{10}H_6 ; $\text{L}_2 = 2\text{PEt}_3$, dcpe] (**1**) react with a variety of unsaturated molecules such as alkynes, alkenes, CO_2 , and CO. Several examples for the formation of nickelacycles, dihydronaphthalenes and indanones will be presented.¹⁻⁴ With unsymmetrical alkynes, the benzyne complexes undergo successive double insertion and reductive elimination to yield substituted naphthalenes with good regioselectivities. For example, $^t\text{BuC}\equiv\text{CH}$ gives 1,3-disubstituted naphthalenes, whereas $\text{MeC}\equiv\text{CCO}_2\text{Me}$ forms exclusively the 2,3-bis(carbomethoxy)naphthalene. A mechanism for these insertions, probably involving the 5- and a 7-membered nickelacycles **2** and **3**, will be proposed.



This methodology has been applied for the synthesis of several new compounds containing naphthalenic 2,3-diphosphines,⁵ using the alkynylphosphines $\text{RC}\equiv\text{CPh}_2$ ($\text{R} = \text{Ph}$, Me , H , CO_2Me , PPh_2), as illustrated in the example below:



This chemistry, leading to novel chelating phosphines, will be detailed.

- (1) Bennett, M. A.; Hambley, T. W.; Roberts, N. K.; Robertson, G. B. *Organometallics* **1985**, *4*, 1992.
- (2) Bennett, M. A.; Wenger, E. *Organometallics* **1995**, *14*, 1267.
- (3) Bennett, M. A.; Hockless, D. C. R.; Wenger, E. *Organometallics* **1995**, *14*, 2091.
- (4) Bennett, M. A.; Hockless, D. C. R.; Humphrey, M. G.; Schultz, M.; Wenger, E. *Organometallics* **1996**, *15*, 928.
- (5) Bennett, M. A.; Cobley, C. J.; Wenger, E.; Willis, A. C. *Chem. Commun.* **1998**, 1307.

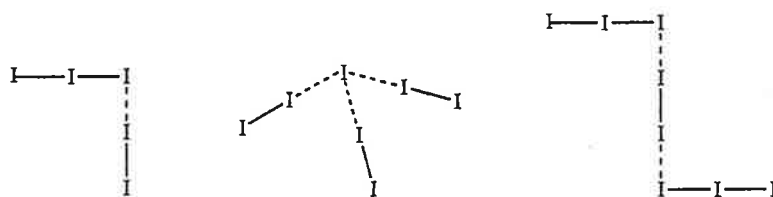
LEGO CHEMISTRY PRACTISED: POLYIODIDES IN THE LIQUID AND SOLID STATE

L. Kloo, J. Rosdahl and P.H. Svensson

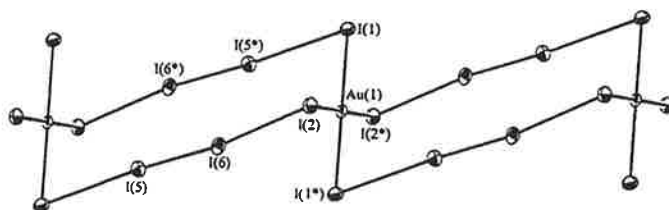
Inorganic Chemistry, Royal Institute of Technology, S-100 44 Stockholm, Sweden

Solid polyiodides have earned much attention since they often display polymeric, low-dimensional structures with an electric conduction ranging from that of insulators to that of metals depending on the actual structure and composition. Such properties obviously implicate technical applications in electronic and electrochemical devices.

Polyiodides have been extensively studied in the solid and liquid state and are characterised by the strong tendency to concatenation. The solid structures may contain small, discrete or large, extended anionic networks of interconnected units. Today, repeating units containing up to about 30 atoms are known. Almost all structures can be described as constructed from only three fundamental building blocks: I^- , I_2 and I_3^- ; where the anions can be regarded as "solvated" by the neutral solvent molecules, I_2 .



By the use of new reaction media based on liquid trialkylsulfonium, crown-ether and hmt polyiodide systems also new materials have been synthesised and characterised. The addition of iodide acceptors, *viz.* metal iodides, exposes iodine to a competition for the iodide ions. This enables the insertion of complex metal iodides into polyiodide networks; thus, new LEGO building blocks can be introduced affecting both physical and chemical properties as well as offering sites for further modification. Examples of such compounds are $(Et_3S)[AuI_4]2I_2$, $(Me_3S)_2[Cd_2I_6]6I_2$ and $(hmtH_2)_2[Hg_2I_6][HgI_3]_2I_2$.



Recently, also metal redox couples have been used in order to make pure polyiodides of high I_2 content, *e.g.* $(Me_3S)_3I_{26}$, with a complicated three-dimensional structure.

PHOSPHINIC AND PHOSPHINOUS ACIDS AND THEIR THIO ANALOGUES AS
LIGANDS IN GOLD CHEMISTRY

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and Annette Schier

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Phosphinous acids R_2POH are hard/soft ambidentate ligands. The free acids or their anions are attached to gold(I) through the phosphorus donor centres leaving hard oxide and/or hydroxide functions available for the building of supramolecular structures. A series of compounds including cations $[(R_2POH)_2Au]^+$, molecules $[(R_2POH)Au(R_2PO)]$, and anions $[(R_2PO)_2Au]^-$ has been prepared and their structure, solution dynamics and reactivity examined. Novel oligomeric, chain and cage structures, some with synergistic aurophilic and hydrogen bonding, have been discovered where these homo- and heteroleptic complexes are part of an extended framework. Phosphinic and thiophosphinic/ous acids can also function as O and S donors for a large variety of mono- and polynuclear complexes of gold(I) with fluxional structures in solution as shown by temperature-dependent NMR spectroscopy.

UNUSUAL POLYPHOSPHANE LIGANDS HAVING A SILICON-PHOSPHORUS BACKBONE

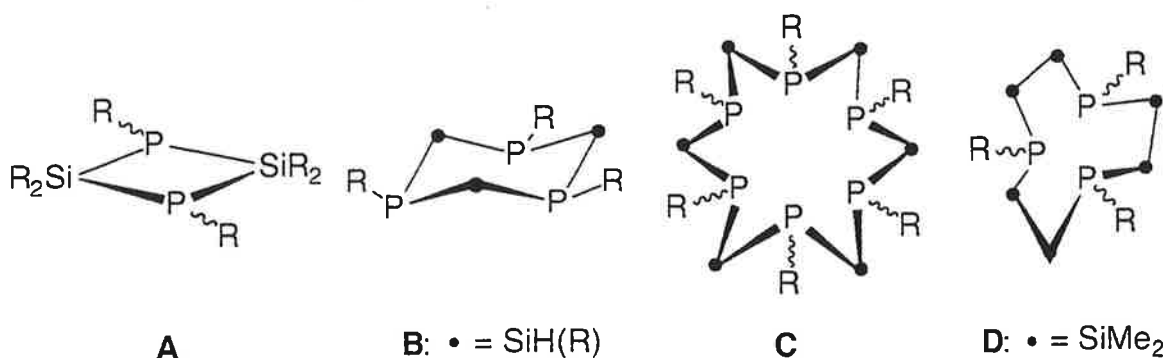
Matthias Driess, Markus Faulhaber, Klaus Merz, and Hans Pritzkow

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Multidentate, cyclic ligands containing N-, O-, S- and P donor atoms are paramount of importance in the coordination chemistry of transition metals. They are more suitable than acyclic chelating ligands for the synthesis of complexes with a rigid stereochemistry and with defined redox and magnetic properties. Since a huge number of macrocycles with nitrogen and sulfur atoms as hard and soft donor centers, respectively, are known, only a few phosphorus macrocyclic ("phosphacrown") ligands can be prepared to date. The need for such ligands is great, since they are "stereochemically superior" to the analogous acyclic phosphane ligands. We found that the ease of the buildup of phosphorus-silicon skeletons can offer some tremendous advantages in the synthesis of novel types of multidentate polyphosphanes. Concomitantly, the high polarity of the Si-P bond rises the phosphorus donor ability and a coordinatively unsaturated metal center can induce unusual modes of Si-E bonding ($E = H, C, Si$) activation, leading to novel catalysts. Thus we succeeded in the synthesis of the novel cyclosilaphosphanes **A-D** and investigated their coordination behavior.¹ The cycle **C** was prepared in an surprising template reaction with M^+ ions ($M = Cu, Ag$) deriving from the six-membered Si_3P_3 cycles **B**.



Major aspects concerning the synthesis of the new ligands, mechanistic features and catalytic properties of the complexes will be presented.

1. M. Driess, M. Reisgys, H. Pritzkow, *Angew. Chem. Int. Ed. Engl.* **1992**, *31*, 1510; *Chem. Ber.* **1996**, *129*, 247; M. Driess, M. Faulhaber, H. Pritzkow, *Angew. Chem. Int. Ed. Engl.* **1997**, *36*, 1892; M. Driess, M. Faulhaber, K. Merz, *Chem. Commun.* **1998**, 1887.

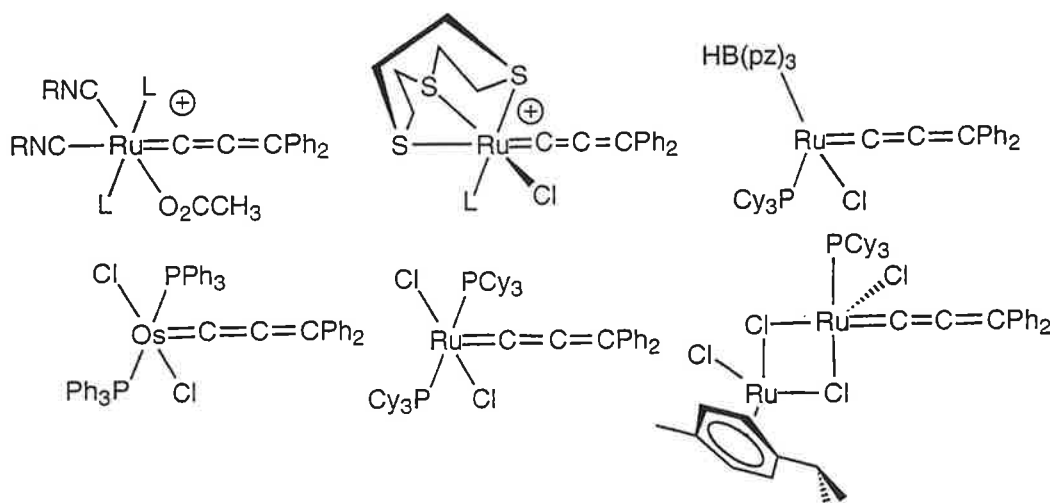
NEW DEVELOPMENTS IN RUTHENIUM AND OSMIUM ALLENYLIDENE CHEMISTRY

Karsten J. Harlow, Anthony F. Hill and James D. E. T. Wilton-Ely

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Although one of the earliest examples of a transition metal allenylidene complex was prepared many years ago by the spontaneous dehydration of diphenylpropynol,¹ it is only recently that such complexes based on ruthenium have begun to attract attention.² Very recently, Dixneuf and Fürstner showed that such complexes could be employed as pro-catalysts for the ring closure metathesis of α,ω -diolefins, in particular with respect to natural product synthesis.³

We have investigated the reactions of a range of ruthenium and osmium complexes with propynols leading to alkynyl, alkenyl, propenylidene (vinyl carbene) and allenylidene ligands. These include the first examples of mono and binuclear allenylidene complexes wherein the ruthenium or osmium centres are coordinatively unsaturated providing a link between the Dixneuf-Fürstner catalyst and Grubbs' olefin metathesis catalysts:⁴



¹ J. P. Selegue, *Organometallics*, 1982, 1, 217.

² Review: A. F. Hill in *Comprehensive Organometallic Chemistry*, II, Vol 7, pp 348 - 356. Eds. E. W. Abel, F. G. A. Stone, G. Wilkinson, Pergamon, Oxford 1995.

³ A. Fürstner, M. Picquet, C. Bruneau, P. H. Dixneuf, *Chem. Commun.*, 1998, 1315.

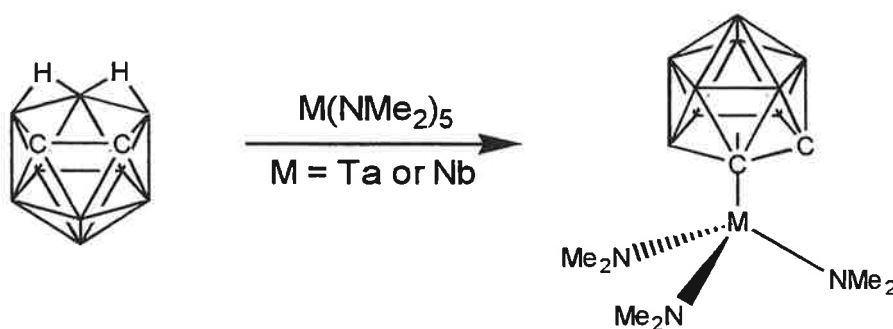
⁴ K. J. Harlow, A. F. Hill, J. D. E. T. Wilton-Ely, *in press*.

The Dicarbolide Ligand $[C_2B_9H_{11}]^{2-}$ As A Cyclopentadienyl Analogue : Early Transition Metal Complexes

A L. Johnson, A K. Hughes and K Wade.

Department of Chemistry, University of Durham, Durham, DH1 3LE, U.K.

The nido-carborane $C_2B_9H_{13}$ reacts with early transition metal homoleptic amides [1],[2], bonding to the metal via the open " B_3C_2 " face in an η^5 fashion and is sterically and electronically comparable to ($\eta^5-C_5Me_5$) [3]. We have also been exploring reactions of $C_2B_9H_{13}$ Group 5 metal homoleptic amides, to give piano stool complexes, and their subsequent reaction with cyclopentadienes.



The replacement of ($\eta^5-C_5R_5$) ligands by $C_2B_9H_{11}^{2-}$ in metallocene complexes provide interesting new opportunities in the design of complexes with new metal/charge combinations [4].

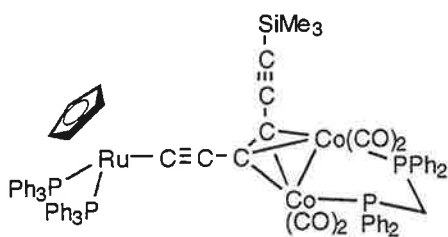
- [1] D. E. Bowen, R. F. Jordan and R. D. Roger, *Organometallics*, **1995**, *14*, 3630.
- [2] A. K. Hughes, A. Meetsma and J. H. Teuben, *Organometallics*, **1993**, *12*, 1936
- [3] G. C. Bazan, W. P. Schaefer and J. E. Bercaw, *Organometallics*, **1993**, *12*, 2126.
- [4] C. Kreuder, R. F. Jordan and H. Zhang, *Organometallics*, **1995**, *14*, 2993.

ELECTRONIC INTERACTIONS WITH METALLO-CARBON CLUSTERS - NEW COMPONENTS FOR MULTI-METALLIC ARRAYS

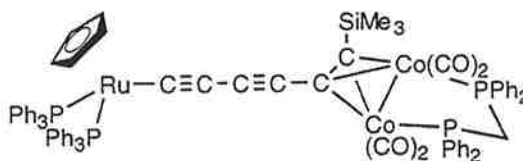
P.J. Low, R. Rousseau, P.Lam, K.A. Udachin, G.D. Enright and A.J. Carty

*Steacie Institute for Molecular Sciences, 100 Sussex Drive, Ottawa, Ontario, K1A
0R6 Canada*

Compounds containing metallo-carbon clusters linked to other clusters and transition metal fragments via poly-carbon bridges have been prepared and structurally characterised. The electronic interactions between the metallic centres have been studied using UV-Vis spectroscopy and cyclic voltammetry. A detailed theoretical study of complexes **1** and **2** has been undertaken using DFT and ZINDO techniques and the results indicate that in each case the HOMO contains appreciable Ru and Co character. The implications of these results on the electronic interaction between the organometallic moieties will be discussed.



1



2

CARBON-RICH METAL COMPLEXES

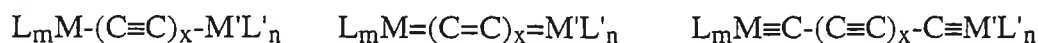
Michael I. Bruce, Ben C. Hall, Brian D. Kelly, Paul J. Low, Mark E. Smith,
Natasha N. Zaitseva

Department of Chemistry, University of Adelaide, Adelaide, South Australia 5005

Brain W. Skelton, Allan H. White

*Department of Chemistry, University of Western Australia, Nedlands,
Western Australia 6907*

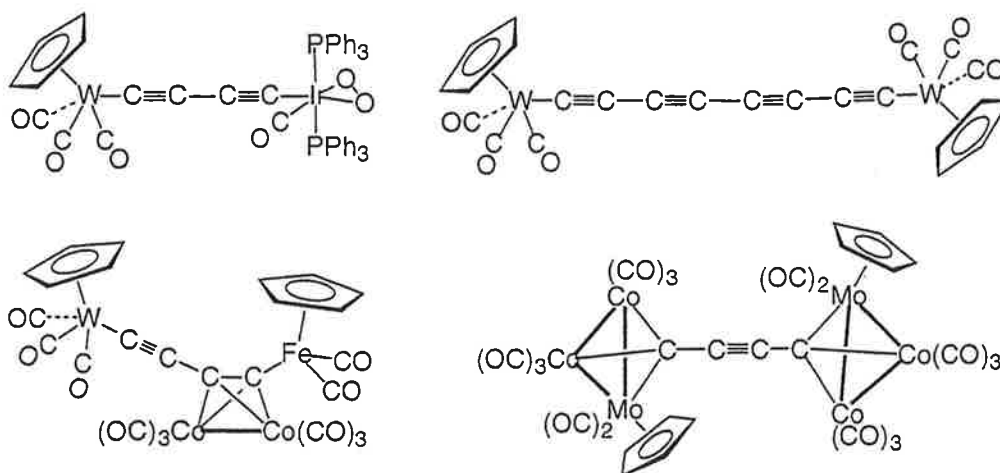
There is increasing interest in the discovery of new forms of familiar materials. Over the last few years, the intensive development of the chemistry of fullerenes has provided many new molecules with novel physical and chemical properties. Smaller but much more reactive carbon molecules can be stabilised by coordination to metals. The electronic structures of the resulting complexes are of interest. With even-numbered carbon chains, three configurations can be written:



With an odd-numbered chain, at least one of the metal centres must be involved in an M-C multiple bond:



We shall describe the synthesis, characterisation and reactions of novel examples of homo- and heterometallic complexes containing chains with up to eight carbon atoms, some examples of which are shown below.



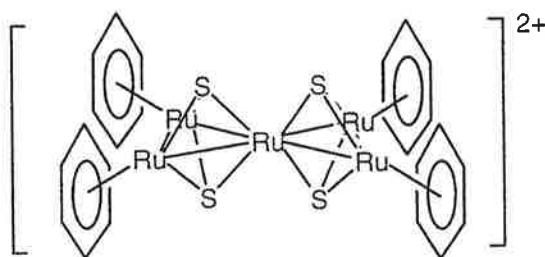
High Nuclearity Ruthenium-Sulfur Clusters

Libei Guo and Tony Wright

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Transition metal clusters provide a link between the well defined chemistry of the single metal centre and the industrially important world of the metal surface. Group VIII metal-sulfur clusters are of note both for their catalytic potential and as models for the biologically important iron-sulfur clusters.

This poster will describe reactions that have lead to the discovery of new high nuclearity ruthenium-sulfur clusters such as the bow-tie cluster $[(\text{cymene})_4\text{Ru}_5\text{S}_4](\text{PF}_6)_2$:



These clusters can be thought of as intermediates in the formation of ruthenium sulfide from monometallic precursors.

Electrochemical studies have shown that these clusters have well defined reduction chemistry. These results will be analysed together with the results of complimentary chemical calculations.

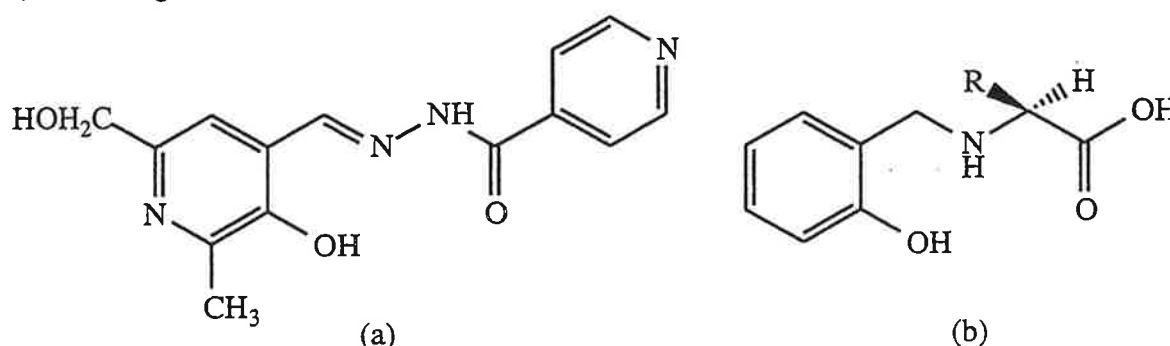
METALLOPROTEIN MODELS TO SUPRAMOLECULAR STRUCTURES FROM SUBSTITUTED AMINO ACID ANTITUMOUR AGENTS

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In the search for orally active iron chelating drugs, one compound with promise is PIH. This, and analogues, have also been shown to be antitumour active with the Cu(II) complexes being up to 100 x more active than the free organic. We prepared a series N-2-hydroxybenzyl substituted L-amino acids (SAA) containing the essential structural features of PIH, initially to investigate their bioactivities.



Structures of (a) Pyridoxal Isonicotinoyl Hydrazone (PIH). (b) N-2-hydroxybenzyl substituted L-amino acids (SAA) where R is amino acid side-chain.

The transition metal chemistry of the SAA complexes has proved rich and unusual. With glycine (R = H), alanine (R = CH₃) or tyrosine (R = 4-OH-C₆H₄) and Cu(II), single-stranded helices are formed. The ligand acts as a chiral, tridentate chelator with the carboxylate bridging Cu(II) centres and the metals magnetically interacting along the chain.

For Zn(II) with alanine, two supramolecular complexes have been characterized¹. In one, a water molecule is bound to Zn and participates in a H-bonding network, forming a 3D honeycomb lattice. On heating all waters are lost and a covalent network with essentially the same structure is formed.

Changing the amino acid to histidine adds a potential fourth coordination site. With Cu(II) this ligand displays three different coordination modes. Changing the metal to Fe(III) gives two complexes, depending on conditions. The predominant species is a 1:2 Fe:ligand complex. However, a Fe₇, OH bridged aggregate can be isolated and this appears to be a good model for the Fe storage protein ferritin.

1 Topochemical Conversion of Hydrogen Bonding to Covalent Three Dimensional Network.

J. D. Ranford, J. J. Vittal and D. Wu, *Angew. Chem. Int. Ed. Engl.*, **1998**, 37, 1114-1116.

DISTINCT METAL ENVIRONMENT IN FE-SUBSTITUTED MANGANESE SUPEROXIDE DISMUTASE OF *E. COLI* PROVIDES A STRUCTURAL BASIS OF METAL SPECIFICITY

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and Geoffrey B. Jameson

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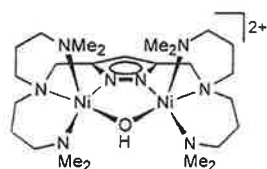
Manganese and iron superoxide dismutases (MnSOD and FeSOD) from *Escherichia coli* share ~50% sequence identity and catalyse the dismutation of O_2^- to H_2O_2 and O_2 . FeSOD is constitutive; MnSOD is expressed under oxidative stress. Substitution of the “wrong” metal ion leads to loss of activity in Fe-MnSOD (and also Mn-FeSOD). Remarkably, MnSOD and FeSOD, which have only 50% sequence identity, share identical active-site structures; whereas MnSOD and Fe-MnSOD, proteins of 100% sequence identity, have different active-site structures, trigonal bipyramidal for Mn and square pyramidal for Fe, thereby stabilising the Fe(III) state sufficiently to prevent reduction to Fe(II) by O_2^- . The surface properties also differ leading to association of MnSOD with DNA. Structures of several mutants, intended to probe hydrogen bonding near the active site (Q146H, Q146A, Y34F) and in the substrate channel (H30A and Y174F) have been determined. For the Y174F we have a 1.1 Å resolution data set, permitting atomic-level resolution of the active site.

Cooperative transformations of small molecules at a dinuclear nickel(II) site

*Franz Meyer**, Elisabeth Kaifer, Peter Kircher, Hans Pritzkow

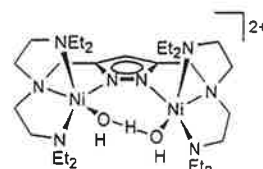
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Numerous enzymes that perform the hydrolysis of biologically relevant substrates like phosphate esters or amides (peptides or urea) are known to employ two divalent metal ions in close proximity within their active site.^[1] Reminiscent of the active site of *urease*, which catalyzes the hydrolysis of urea to ammonia and carbamate,^[2] we have designed and studied a series of pyrazolate-based dinickel(II) complexes where the metal-metal separation can be effectively tuned by the length of chelating side arms attached to the 3- and 5-positions of the heterocycle.^[3] If short side arms pull the two metal centers back and apart, small secondary anions like hydroxide are prevented from spanning both metal centers in a bridging mode (**1** versus **2**).^[4]



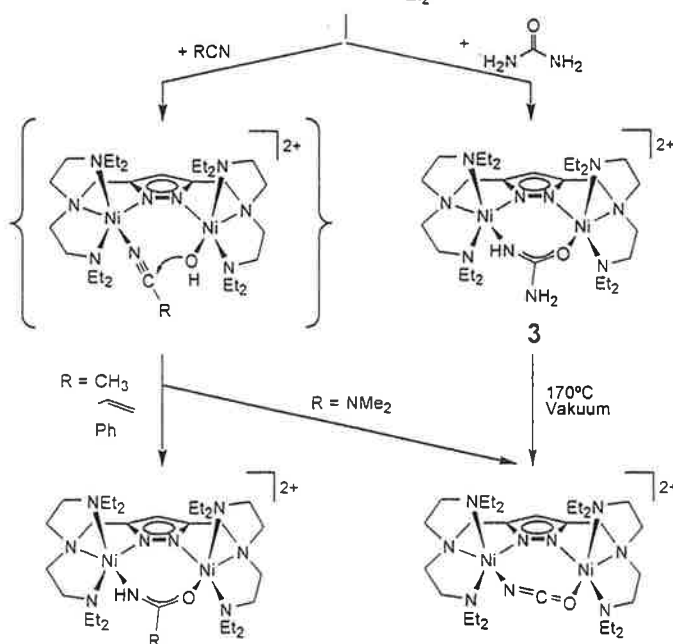
1

2



The intramolecular H_3O_2 bridge in **2** acts as the resting form of an active metal-bound hydroxide in proximity to a second nickel(II) ion and enables various transformations of small substrate molecules within the bimetallic coordination pocket.^[5-7]

Hydrolytic reactions induced by **2**, like the hydration of nitriles and the cleavage of unactivated esters,^[5] as well as a bridging coordination mode of urea^[6] (**3**) and an intriguing cooperative binding of a nitrile moiety at the bimetallic site^[7] will be described.



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³ F. Meyer, K. Heinze, B. Nuber, L. Zsolnai, *J. Chem. Soc., Dalton Trans.* **1998**, 207; F. Meyer, A. Jacobi, B. Nuber, P. Rutsch, L. Zsolnai, *Inorg. Chem.* **1998**, 37, 1213.

⁴ F. Meyer, P. Rutsch, *Chem. Commun.* **1998**, 1037.

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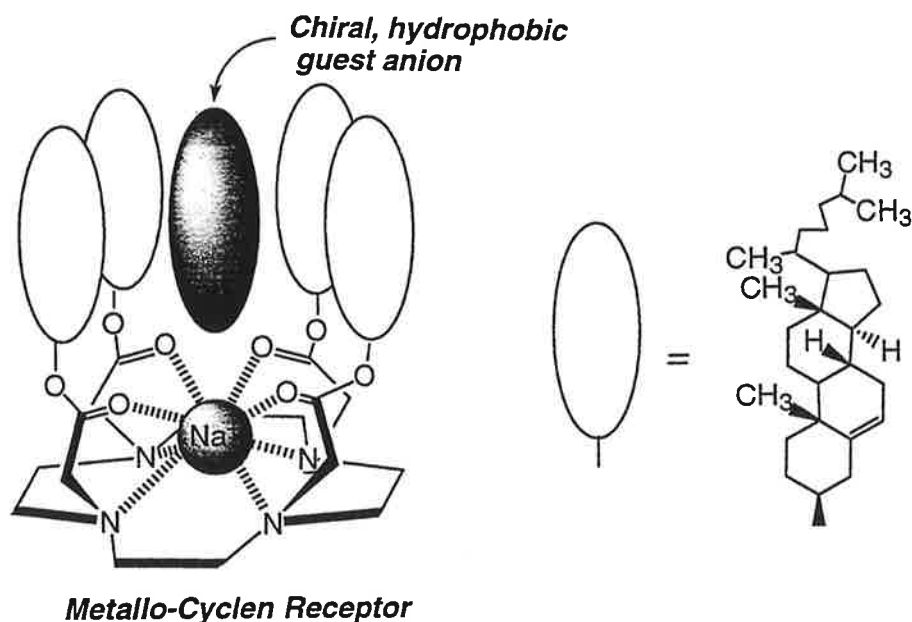
⁶ F. Meyer, H. Pritzkow, *Chem. Commun.* **1998**, 1555.

⁷ F. Meyer, E. Kaifer, submitted.

AGGREGATION AND CHIRAL RECOGNITION BEHAVIORS OF METALLO-CYCLEN RECEPTOR

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Department of Chemistry, Graduate School of Science, Osaka City University,
Osaka 558-8585, Japan

Although the molecular recognition in molecular assembly is one of the most interesting processes,¹⁾ there are only limited numbers of synthetic molecular assemblies in the literature, which recognize the chirality of the specific guests in the aqueous media. Here we report remarkable aggregation and chiral recognition abilities of new "metallo-cyclen receptor". This complex is constituted in combination with three functional components: ester-armed cyclen ligand as a strong octadentate template,²⁾ four cholesterol-functionalized sidearms as chiral, hydrophobic walls, and the bound Na^+ ion as positively charged group of the amphiphile. This metallo-cyclen spontaneously aggregated in an aqueous ethanol solution and provided steroidal domain suitable for chiral recognition of N-dansyl-amino acid carboxylates.



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- 2) H. Tsukube, *et al. Tetrahedron Lett.* **38**, 5021 (1997);
Inorg. Chem., in press.

MECHANISTIC INVESTIGATIONS ON THE REACTION OF THE VITAMIN B₁₂ COENZYMES WITH CYANIDE

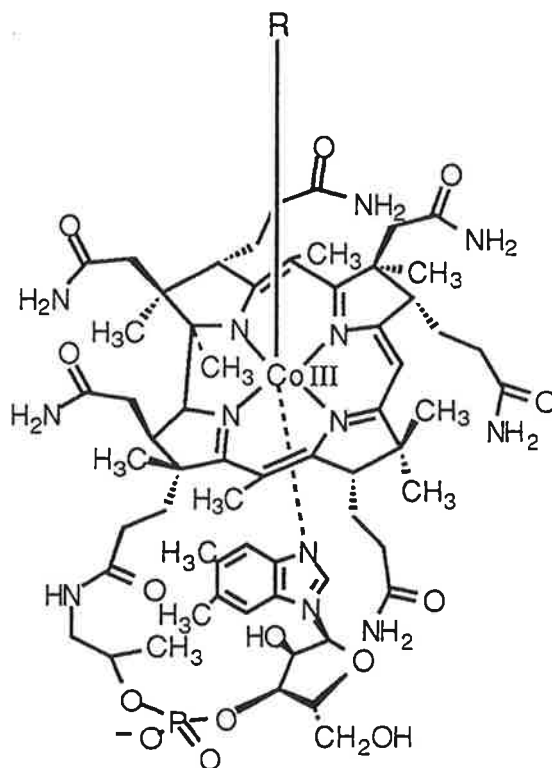
Nicola E. Brasch,¹ Rudi van Eldik,² Mohamad S. A. Hamza,² Frank Müller² and Achim Zahl²

(1) Research School of Chemistry, The Australian National University, Canberra, ACT 0200

(2) University of Erlangen-Nuremberg, Egerlandstrasse 1, 91058 Erlangen, Germany

Vitamin B₁₂ is the most biologically important Co(III) compound known, and is essential in the nutrition of animals and humans. The equatorial sites of vitamin B₁₂ are occupied by a structurally unique corrin ring, while the α axial site is occupied by an intramolecularly - bound 5,6-dimethylbenzimidazole. The β site can be occupied by a number of ligands, including a 5'-deoxyadenosyl (adenosylcobalamin, AdoCbl = 'coenzyme B₁₂') or a methyl group (methylcobalamin, MeCbl). A key step towards understanding the AdoCbl or MeCbl - dependent enzyme reactions is the initial cleavage of the β Co-C bond; this occurs homolytically for AdoCbl - dependent isomerases and heterolytically for MeCbl - dependent transferases. Of considerable interest and poorly understood is the rate enhancement of this bond cleavage in the presence of the enzyme. Homolytic cleavage of the Co-C bond of AdoCbl is enhanced by a factor of ca. 10^{12} , while heterolytic cleavage of the Co-C bond of MeCbl is enhanced by ca. 10^5 .

We have re-examined the reaction of AdoCbl and MeCbl with cyanide, in the absence of an enzyme. In addition to being a model reaction for heterolytic cleavage of the Co-C bond of MeCbl, this reaction is of particular interest as, apart from thiols, there are no other nucleophiles known capable of cleanly heterolytically cleaving the Co-C bond.



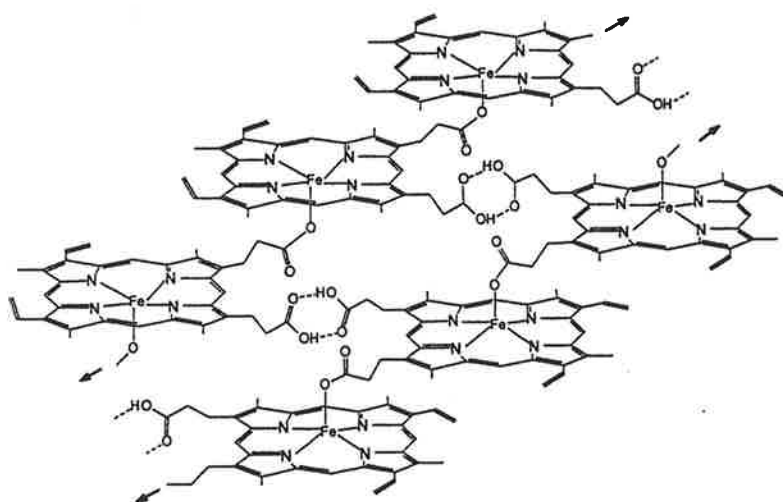
β -HEMATIN: A COORDINATION POLYMER CENTRAL TO HEME DETOXIFICATION IN MALARIA

D. Scott Bohle, Andrew Kosar, Peter A. Jordan, and Sara K. Madsen

Department of Chemistry, University of Wyoming, Laramie, WY 82071-3838 USA.

With the spread of chloroquine resistant strains of *P. falciparum*, and the absence of a suitable replacement for this once very effective antimalarial, there is increasing urgency to understand the biochemistry behind its drug action. The most recent hypothesis, that chloroquine inhibits heme aggregation activity in ring stage, or early, malaria trophozoites, has sustained considerable scrutiny.

We have recently shown that the heme aggregated by-product of malarial trophozoites, termed malarial pigment or hemozoin, is identical by X-ray diffraction to the synthetic phase β -hematin.¹ The proposed structure for this unusual coordination polymer is shown to the right.² This presentation will concern the synthetic and spectroscopic



characterization of this unique 'biomineralization' by-product, and rationalize its formation in terms of its post-parasite biochemistry.

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Spectroscopic and Crystallographic Characterisation of Dimethylsulfoxide Reductase from *Rhodobacter capsulatus*: Structure and Implications for Electron Transfer

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^cDaresbury Laboratory, Warrington WA4 4AD, United Kingdom

Dimethylsulfoxide reductase catalyses oxygen atom transfer from DMSO to DMS with an accompanying two electron transfer. The enzyme contains a pterin molybdenum cofactor (MPT) as its only prosthetic group making it an excellent system for investigating the mechanism of catalysis and the pathway of electron transfer between the native electron donor, cytochrome c_{dms} and the molybdenum centre. Recently, three X-ray crystallographic studies of DMSOR from *R. capsulatus* and *R. sphaeroides* have been published.¹⁻³ All three crystal structures are very similar in terms of protein structure and each contains two molecules of the guanine dinucleotide form of MPT (P-MGD and Q-MGD) which are antiparallel.¹ In contrast, the molybdenum ion's coordination sphere in the three crystal structures are significantly different, varying in the coordination number (5, 6 and 7), the number of oxo groups present and the Mo-S bond distances for the dithiolene sulfur atoms. In all three structures O γ of Ser147 provides the only ligand from an amino acid side chain.

EPR spectroscopy in conjunction with isotope enrichment (⁹⁵Mo, ²H and ¹⁷O) has been used to probe the structure of the Mo(V) intermediates during catalysis. Specifically we have examined the high g-split and -unsplit species⁴ and identified a new orthorhombic spectrum with resonances ($g_1=2.054$, $g_2=2.018$, $g_3=2.000$) which has been attributed to a persulfide radical on the basis of the anisotropic g-matrix, the long spin lattice relaxation time, the absence of ⁹⁵Mo hyperfine coupling in spectra from ⁹⁵Mo enriched samples and its similarity to persulfide radicals.⁵ We propose on the basis of our X-ray crystallographic data³ that the persulfide radical is centered on the Q pterin which is no longer coordinated to the Mo ion in the reduced structure. The ability to add one or more electrons to the Mo ion or the pterin suggests that the Q-pterin is involved in electron transfer between the native electron donor, cytochrome c_{dms} and MoCo in DMSOR. This hypothesis is strengthened by our observation of different redox states (fully oxidized and reduced) for the two pterins.⁶

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Λ and Δ -*cis*- β -[Ru(*R*R**-picchxn)(phen)]²⁺ METALLOPROBES SHOW DIFFERENTIAL BINDING GEOMETRIES with d(CGCGATCGCCG)₂**

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The rigid and stereochemically well-defined framework of octahedral transition metal complexes make them attractive as candidates for sequence selective DNA-binding agents as well as for probes of local DNA structure¹. For some time, the capabilities of ternary cations of the general form [Ru(tetradentate)(bidentate)]²⁺ to function as stereo- and enantiodiscriminatory intercalating probes of DNA structures have been investigated². Here we employ NMR techniques to investigate the interactions between d(CGCGATCGCCG)₂ and the Λ and Δ forms of *cis*- β -[Ru(*R***R**-picchxn)(phen)]²⁺ [where *R***R**-picchxn is *N,N'*-di(2-picolyl)-1,2-diaminocyclohexane] and specifically, examine phenanthroline's capacity to partially intercalate. In these complexes, the tetradentate is chosen to have characteristics which allow it to govern binding selectivity through helical groove interactions, and specifically whether the *cis*- β geometry allows the possibility of selective secondary intermolecular H-bonding with a host DNA molecule.

1D NMR titrations and 2D NOESY and WATERGATE experiments of the enantiomeric probes with the nucleic acid were conducted and chemical shifts of proton resonances of both nucleobase and interacting probe monitored. The major findings of the data can be summarised as follows: (i) both chelate forms bind in the kinetically fast exchange regime and in the minor groove (ii) the binding geometry of the enantiomers were found significantly different, where the major targetted sites for Δ isomer were the terminal base pairs, even at the higher temperatures (38 °C)³. The Λ complex showed significantly increased NOE intensities to the AT sites, and disruption to the amino nucleobase protons, thus indicating a separation of the base pairing to accommodate a partial or 'quasi-intercalator'. Complimentary linear dichroism spectroscopic studies⁴ support this observed differential binding geometry, where the Λ isomer (solely) demonstrates a 'quasi-intercalation' mode.

References

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THE INCREDIBLE SHRINKING CRYSTAL: FORMATION OF A THREE-DIMENSIONAL DNA POLYMER

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³ Chemistry Department, University of Melbourne, Melbourne, Australia.

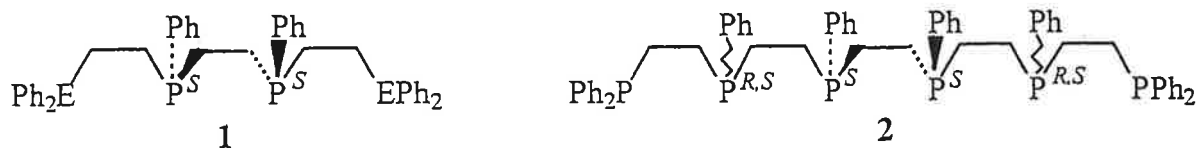
On controlled dehydration, crystals of the complex between the minor groove binding ligand *meta*-iodo *para*-methoxy Hoechst 33258 and the DNA dodecamer d(CGCGAATTCGCG)₂ shrink to approximately 75% of their initial volume, with a dramatic improvement in the resolution of the X-ray diffraction data (from 2.4 to 1.6 Å). Crystal structures have been determined for the “normal” and “fully shrunken” crystals, and for a number of intermediate “partially shrunken” states. The Hoechst ligand is located in two orientations and binding sites in the minor groove of the “normal” structure, but detaches from the DNA and re-locates into just one site in a single orientation as the crystal shrinks. The “fully shrunken” crystal exists as an infinite polymeric network, in which the dodecamer duplexes are crosslinked by covalent bonds through magnesium cations. We have deduced the mechanism for the structural and conformational changes that occur as the crystal dehydrates and the network polymer forms. The covalent Mg-DNA network provides a model for Mg-facilitated DNA-DNA tertiary interactions and Mg-activation of enzymes involved in nucleic acid biochemistry.

**SELF-ASSEMBLY OF DI- AND TRI-NUCLEAR METAL HELICATES
CONTAINING POLY(TERTIARY PHOSPHINES)
AND RELATED COMPOUNDS**

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The homochiral tetra(tertiary phosphine) (*S,S*)-1 ($E = P$) spontaneously self-assembles double-stranded disilver(I) and digold(I) helicates of the type $[M_2(\text{tetraphos})_2]X_2$ upon reaction with appropriate silver(I) and gold(I) salts.¹ The silver complex crystallizes with one molecule each of the left-handed D_2 -double helix and C_2 -side-by-side helix conformers of the cation and associated anions in each unit cell; crystals of the gold complex contain only the C_2 -side-by-side helix. Whereas (*S,S*)-1 ($E = P$) forms a mononuclear copper(I) complex, (*S,S*)-1 ($E = As$) self-assembles a C_2 -side-by-side dicopper(I) helicate. The tetraphos (*S,S*)-1 ($E = P$) has been converted in high yield into the optically active diastereomers of the homologous hexa(tertiary phosphine) 2, which have been separated and used for the preparation of homochiral trinuclear metal helicates of univalent Group 11 metals.



¹ A. L. Airey, G. F. Swiegers, A. C. Willis, and S. B. Wild, *Inorg. Chem.*, 1997, **36**, 1588–1597

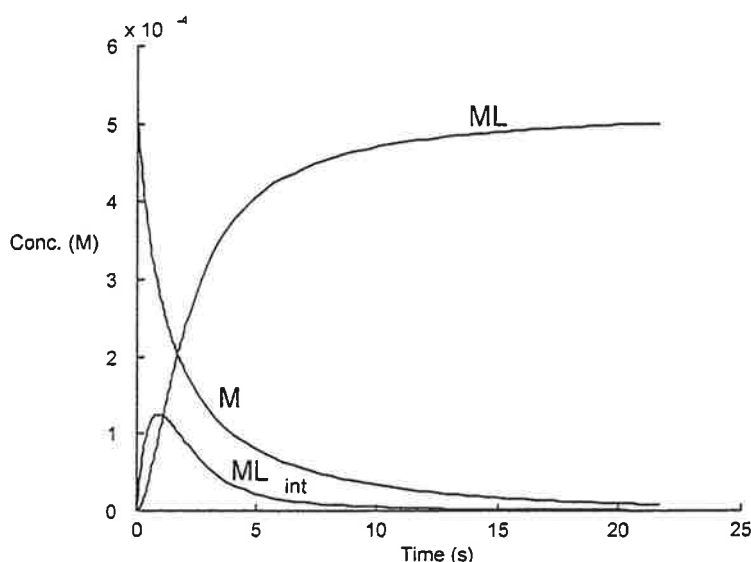
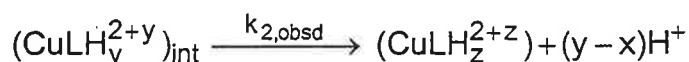
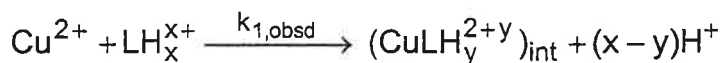
FORMATION KINETICS OF PENDANT ARM POLYAMINE MACROCYCLES WITH COPPER(II)

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2308, Australia

There is a wealth of information on the equilibria between ligands and metal ions. The kinetics of the complex formation reaction has been investigated in much fewer cases. In this contribution we present the results of an investigation of the kinetics of the interaction of cyclam based pendant arm macrocycles with Cu(II) in acidic aqueous solution.

Extensive pH-dependences of multi-wavelength stopped flow measurements allowed a detailed analysis of the formation reactions: there is a first 2nd order reaction between the metal and the ligand (partially protonated) to form an intermediate complex (again partially protonated) which reacts in a 1st order reaction to the final product.

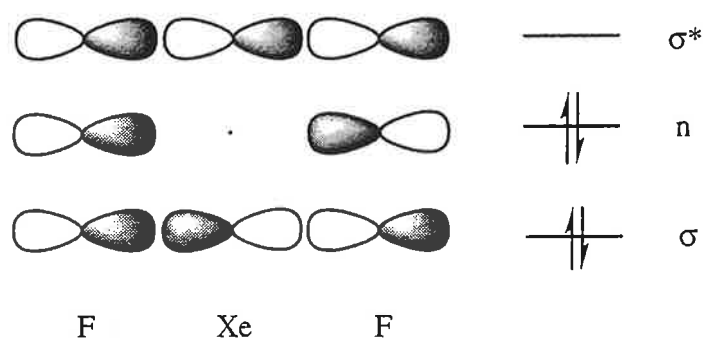


"HYPERVALENT" MOLECULES: WHAT IF THERE ARE NO d ORBITALS?

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The role of d orbitals in the bonding of hypervalent molecules such as PF_5 and SF_6 has been hotly debated for a number of years. However, most researchers now recognise that the role of d orbitals is essentially mathematical in origin and is involved in the polarisation of the p orbitals. Nonetheless, many texts continue to use s/p/d hybridisation schemes to describe the bonding in these molecules because of its pedagogical simplicity. This paper will present an alternative description of the bonding that extends the 3-centre 4-electron bonding description of Rundle [1] and Pimentel [2], shown below, that was originally devised for XeF_2 . Extension to include bonding descriptions for molecules like IF_7 and $[\text{XeOF}_5]^-$ will also be made. The ramifications of this description to the octet rule will be discussed.



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[2] G. C. Pimentel, *J. Chem. Phys.* 19 (1951) 446.

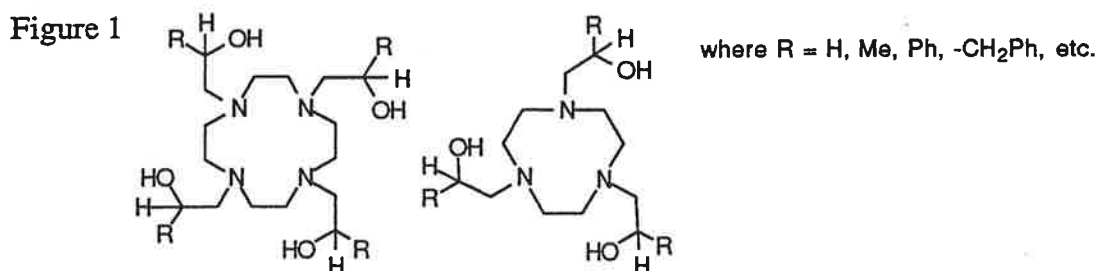
Chirality, Superchirality and Molecular Reception in Macrocyclic Metal Complexes

Stephen F. Lincoln^a, Mark A. Buntine^a, Kevin P. Wainwright^b, Ashley K. W. Stephens^b, Jennifer M. Weeks^a, Sonya L. Whitbread^a and Oska Wyness^a

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The attachment of identical donor pendant arms to each nitrogen of 1,4,7,10-tetraazacyclododecane and 1,4,7-triazacyclononane produce eight- and six-coordinating ligands, respectively, as exemplified by those in Figure 1.^{1,2} When the pendant arms are achiral chirality is induced into the ligand conformation upon metal ion complexation to produce Λ and Δ enantiomers. When the pendant arm incorporates a (*R*)- or (*S*)- stereocentre metal ion complexation produces Λ and Δ diastereomers (superchirality) of which one is dominantly the more stable. A similar situation prevails in the free ligand.



In solution, the rates of interchange between the Λ and Δ enantiomers of the alkali and alkaline earth complex ions are within the NMR timescale while those of the analogous complex ions with other metal centres are not. Exchange between equivalent forms of a single diastereomer of the alkali complex ions, which may be either Λ or Δ , is observed within the NMR timescale (as is also the case for the free ligand), but such exchange is slower for the alkaline earths and other metal ions. In the case of Mg²⁺, the complex ions formed with the 1,4,7,10-tetraazacyclododecane based ligands are seven-coordinate instead of eight-coordinate as found for other metal ions. These data are discussed together with those obtained from *ab initio* molecular modelling and crystallographic studies.

As the size of the pendant arms increases, so does the size of the cavity formed within the ligand and its complex ions. This cavity has the potential to act as a molecular receptor, and some of the design aspects and initial molecular receptor studies are discussed.

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Zintl-Ions: An Organometallic Variation

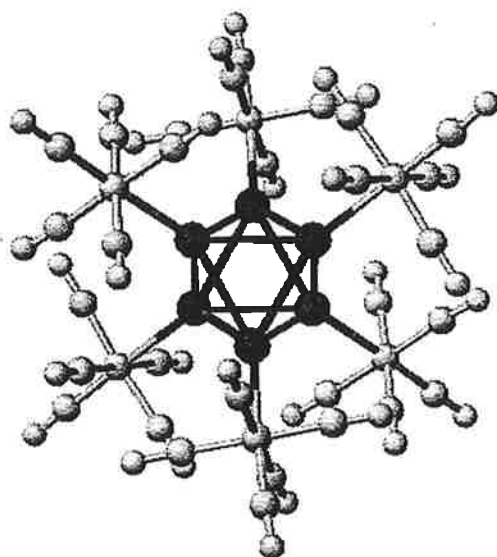
G. Huttner, B. Schiemenz, P. Kircher, G. Renner

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Although it is a long time ago that E.Zintl first systematically analyzed the anionic aggregates E_m^{n-} formed by main group elements under strongly reducing conditions, the structural chemistry of such Zintl ions is still intriguing.

Zintl ions consist of clusters of main group atoms and most of them are electron precise in terms of Wade's rules. In stark contrast, however, to what is known from transition metall chemistry, isolated octahedral aggregates E_6^{n-} are almost never observed in this chemistry.

The structure of $[\text{Ge}_6(\text{Cr}(\text{CO})_5)_6]^{2-}$:



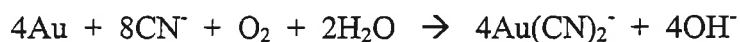
It will be reported that electron precise aggregates E_6^{2-} ($E=\text{Ge}, \text{Sn}$) are formed as discrete anions when the main group centers are protected by organometallic groups. The synthesis and properties of species like $[\text{Ge}_6(\text{Cr}(\text{CO})_5)_6]^{2-}$ will be described.

IMPROVING THE CYANIDATION PROCESS USING COLLOIDAL GOLD

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We are currently developing an on-line method of determining cyanide concentrations in gold mine leach tanks using the reaction between colloidal gold and cyanide. Gold colloids have a characteristic ruby red colour allowing easy measurement using spectrometry. They are easily prepared in a stable form and react with cyanide in a similar way to gold dissolving in its ores during the extraction process.



Preliminary work has involved kinetic studies on the reaction of colloidal gold with cyanide to determine the mechanism of the dissolution process and the effect of other ions such as copper and sulfide. The next stage in the development of the on-line method has been to develop a flow injection analysis system using the colloid/cyanide reaction to determine $[\text{CN}^-]$.

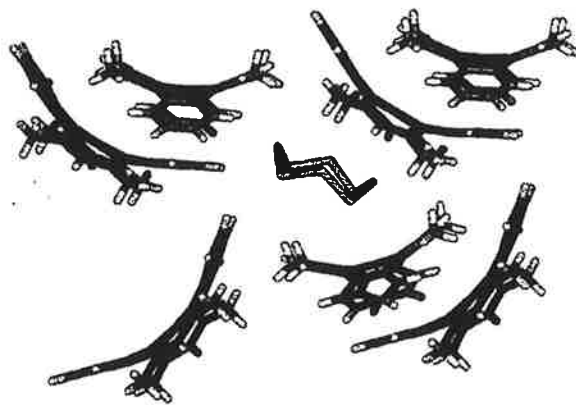
One of the major cost factors in gold mining is the sodium cyanide used in the extraction process. At present there is no simple, robust, continuous method of measuring the actual 'active' cyanide concentration in leach tanks. Developing this new method using colloidal gold will allow better control of cyanide addition to leach tanks, preventing over consumption and thus reducing costs.

SUPRAMOLECULAR CHEMISTRY OF NICKEL(II) MACROCYCLES WITH FULLERENES AND OTHER GLOBULAR MOLECULES

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We have reported the formation of supramolecular complexes of a nickel(II) macrocycle with C_{60} , 1,2-dicarbododecaborane and P_4S_3 .¹ The nickel(II) macrocycle, Ni(TMTAA), [= 5,7,12,14-tetramethyldibenzo[*b,i*][1,4,8,11]tetraaza(1,4)cyclotetradecinenickel(II)], with two concave surfaces acts as a divergent heterotopic receptor or, in its self associated dimeric form, as a divergent homotopic receptor. We have now isolated and structurally characterised complexes containing P_4Se_3 and S_8 (see figure) as 1:2 complexes, $[C\{Ni(TMTAA)\}_2]$, $C = P_4Se_3$ or S_8 . These supramolecular complexes coupled with three crystallographic forms of Ni(TMTAA) as well as a toluene solvate highlight the versatility in incorporating guests into the two shallow concave surfaces. Modification of the nickel(II) macrocycle so as to produce an extended surface (four methyl groups substituted onto the phenyl rings) has resulted in the formation and isolation of the C_{60} and C_{70} complexes of Ni(OMTAA) [= 2,3,6,8,11,12,15,17-octamethyldibenzo[*b,i*][1,4,8,11]tetraaza(1,4)cyclotetradecinenickel(II)], $[C_{60}\{Ni(OMTAA)\}(CS_2)_2]$ and $[C_{70}\{Ni(OMTAA)\}]$.



Environment around S_8 in $[(S_8)\{Ni(TMTAA)\}_2]$

$[(P_4Se_3)\{Ni(TMTAA)\}_2]$ and $[(S_8)\{Ni(TMTAA)\}_2]$ are isostructural with the corresponding P_4S_3 and dicarbaborane complexes indicating the flexibility of this arrangement to incorporation of globular molecules. $[C_{70}\{Ni(OMTAA)\}]$ is isostructural with $[C_{60}\{Ni(TMTAA)\}]$ whereas the incorporation of CS_2 in $[C_{60}\{Ni(OMTAA)\}(CS_2)_2]$ results in a breaking of the C_{60}/C_{70} sheets observed in $[C_{60}\{Ni(TMTAA)\}]$ and $[C_{70}\{Ni(OMTAA)\}]$ respectively and the formation of columns of pairs of C_{60} units instead.

P. C. Andrews, J. L. Atwood, L. J. Barbour , P. J. Nichols and C. L. Raston, *Chem. Eur. J.*, **1998**, 1384.

LATE METAL COORDINATION CHEMISTRY OF A 'BULKY CO' ANALOG,

$\{P[N(dipp)CH_2CH_2(dipp)N]\}OTf$ (dipp = 2, 6-diisopropylphenyl;
OTf = triflate)

Michael B. Abrams, Brian L. Scott, and R. Tom Baker,

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Alamos, NM 87545 USA

The coordination chemistry of the title bulky phosphonium cation is investigated for the Groups 6-10 transition metals. Reactivity with small molecules as a function of transition metal and overall charge will be discussed.

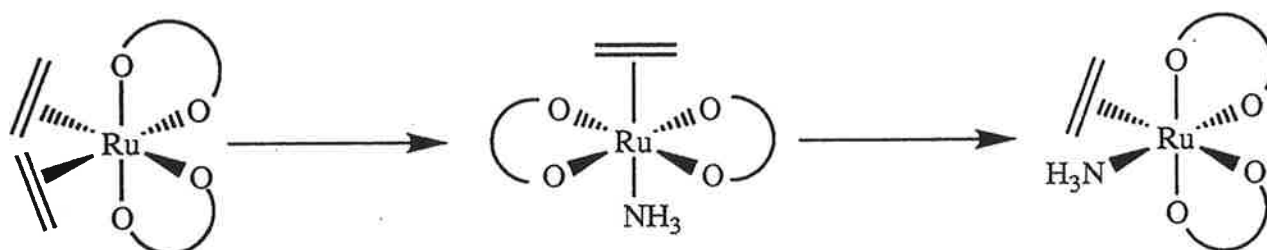
REACTIVITY OF CIS-BIS(ALKENE)- BIS(ACETYLACETONATO)RUTHENIUM(II)
COMPLEXES WITH GROUP 15 DONOR LIGANDS

Martin A. Bennett, Matthew J. Byrnes, Guandolina Chung,
and Horst Neumann

Research School of Chemistry, Australian National University, Canberra ACT 0200
(Australia)

Reduction of $[\text{Ru}(\text{acac})_3]$ with Zn/Hg in aqueous THF in the presence of excess cyclooctene or ethylene gives the labile bis(alkene) complexes $\text{cis}-[\text{Ru}(\text{acac})_2(\text{alkene})_2]$ (alkene = C_8H_{14} , C_2H_4). Both alkenes are readily displaced at room temperature by ligands to give, surprisingly, the *trans*-isomers of $[\text{Ru}(\text{acac})_2\text{L}_2]$ ($\text{L} = \text{NMe}_3$, PPh_3 , PPhMe_2 , $\text{P}(p\text{-tolyl})_3$, $\text{P}(\text{OMe})_3$, AsPh_3 , pyridine and Bu^tNC)¹, which, on heating, give the corresponding, more stable *cis*- isomers (except for $\text{L} = \text{NMe}_3$).

Some ligands, such as CH_3CN and SbPh_3 , react with $\text{cis}-[\text{Ru}(\text{acac})_2(\text{alkene})_2]$ at room temperature to give stable, isolable mono-substitution products $\text{cis}-[\text{Ru}(\text{acac})_2(\text{alkene})\text{L}]$, which react only slowly with more ligand to give $\text{cis}-[\text{Ru}(\text{acac})_2\text{L}_2]$. There was no evidence for the formation of the *trans*- isomer of $[\text{Ru}(\text{acac})_2(\text{alkene})\text{L}]$. Surprisingly, the reaction of $\text{cis}-[\text{Ru}(\text{acac})_2(\text{C}_2\text{H}_4)_2]$ with anhydrous ammonia in a THF solution afforded $\text{trans}-[\text{Ru}(\text{acac})_2(\text{C}_2\text{H}_4)(\text{NH}_3)]$. The properties, reactivities and electrochemistry of these mono-substituted complexes will be discussed.



References:

- (1) M. A. Bennett, H. Neumann, G. Chung; unpublished work.

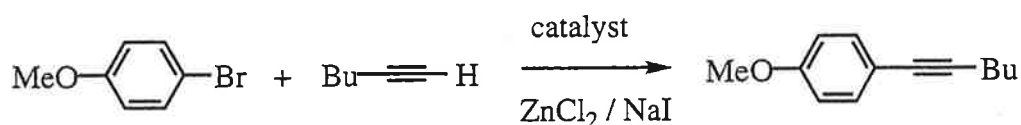
NEW PROTOCOLS FOR PALLADIUM-CATALYSED COUPLING OF TERMINAL ALKYNES WITH ARYL HALIDES

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The ability of terminal alkynes to couple with aryl halides using the traditional methodology of a palladium catalyst (either palladium(0) or (II)), a base (frequently a secondary or tertiary amine) and copper iodide (for the generation of the copper acetylide intermediate), has been known for many years[1]. Several recent alternatives have been reported to this general theme and all proceed well in the absence of a copper co-catalyst but with modified reaction conditions. Examples include coupling in the presence of $\text{Pd}(\text{PPh}_3)_4$ and piperidine or pyrrolidine[2], the use of water soluble phosphine ligands and aqueous solvents[3] and the use of $\text{Pd}(\text{OAc})_2$ in aqueous solvents with quaternary ammonium salts[4].

We were interested in establishing a procedure in which the zinc acetylide (or an equivalent nucleophilic species) could be generated *in situ*, as for the copper acetylides and so provide a more convenient protocol for the use of zinc acetylides in palladium catalysed couplings. In this presentation we report an investigation into the scope and limitations of the use of nucleophilic species generated *in situ* in the presence of zinc. We will also discuss coupling conditions in which a metal co-catalyst is not required and the advantages of these procedures over existing protocols. Some mechanistic speculations will also be presented.



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MOLECULAR DESIGN OF GROUP 2 ELEMENT COMPOUNDS AS PRECURSORS FOR ELECTRONIC MATERIALS

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Several important electronic materials contain Group 2 elements. Among these examples are dielectrics (MgO), ferroelectrics (Ba/SrTiO₃), superconductors (YBa₂Cu₃O₇), and phosphors (SrS:Ce). In general, the demands electronic materials place on purity are exacting, and property degradation below desired limits render them unusable. One technique of choice for the achievement of the demanded purity levels is chemical vapor deposition (CVD). CVD requires volatile, stable source compounds to be conducted in a useable manner. Important considerations in the isolation of volatile, stable compounds include careful design of ligands specifically matched to the coordination environment of a given element. In the specific case of the Group 2 elements, this challenge is defined by the unusually large size/charge ratio exhibited by the heavier members of the group.

This lecture will focus on recent accomplishments in the area of ligand design involving intramolecular coordination for barium. The divalent nature of the element requires two monovalent ligands for achievement of charge neutrality, while the ionic radius prefers to be eight to ten coordinate. Thus, tetradentate and pentadentate monoanionic ligands are demanded. Additionally, for strontium, results relating to use of anhydrous, coordinately saturated β -diketonate compounds in the preparation of electroluminescent flat panel displays will be described. A model relating calculated ligand partial charges and vapor phase stability of intermolecular Lewis base adducts has been developed, and applied to the subsequent design of next generation ligands.

STRUCTURE AND MAGNETISM OF METAL - PSEUDOHALIDE COORDINATION POLYMERS

Stuart R. Batten,^{a,b} Bernard F. Hoskins,^b Paul Jensen,^a Boujemaa Moubaraki,^a Keith S. Murray,^{a,*}

David J. Price,^a and Richard Robson^b

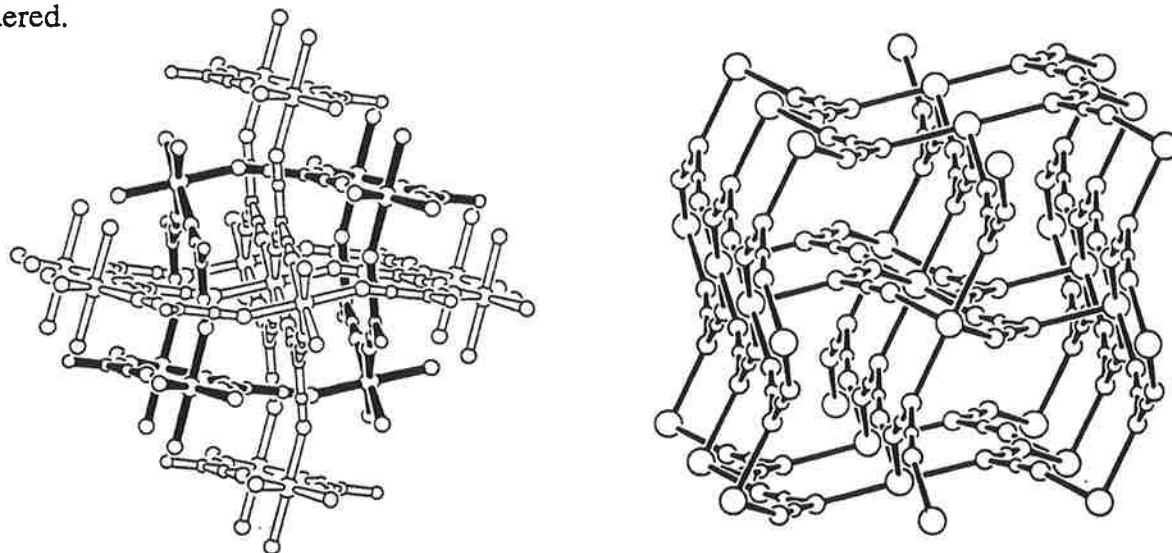
^a Department of Chemistry, Monash University, Clayton 3168, Australia; ^b School of Chemistry, University of Melbourne, Parkville 3052, Australia.

We have recently been studying in detail the synthesis, crystal structures and magnetic properties of the metal complexes of a number of pseudohalide ligands.¹ We shall report selected results of these structures.

The isomorphous $M(\text{tcm})_2$, $\text{tcm} = \text{tricyanomethanide}$, $\text{C}(\text{CN})_3^-$, $M^{\text{II}} = \text{Cr to Zn, Cd, Hg}$ compounds contain two interpenetrating coordination networks. Each identical network has a rutile-like topology, with six-connecting centres (M ions) and three-connecting centres (tcm ligands). Analysis of the magnetic properties indicates weak antiferromagnetic coupling.

The structures of $M(\text{dca})_2$, $\text{dca} = \text{dicyanamide}$, $\text{N}(\text{CN})_2^-$, $M^{\text{II}} = \text{Mn to Cu}$, are also isomorphous, containing rutile-like coordination networks, with octahedral M centres and three-connecting dca ligands (*via* all three N donors). Unlike the tcm compounds, the dca complexes do not interpenetrate. This is due to one in three of the C-CN-M links in the tcm series being replaced by N-M bonds. This greatly reduces the available space within a single framework, which is needed for the formation of a second framework.

Despite having isomorphous crystal structures, the magnetic properties of the dca complexes vary widely, depending on metal ion. $\text{Mn}(\text{dca})_2$ displays weak antiferromagnetic coupling, but has an unusual magnetic phase transition at $T_c = 16\text{K}$. $\text{Co}(\text{dca})_2$ and $\text{Ni}(\text{dca})_2$ are ferromagnets with T_c values of 9K and 20K, respectively. $\text{Cu}(\text{dca})_2$ is very weakly antiferromagnetically coupled and not ordered.



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GEOHERMAL SILICA - SPECIALIST PRODUCTS FROM A WASTE RESOURCE

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In the utilisation of geothermal resources for electricity production, the subsurface water which is usually about 250-320°C and saturated in dissolved silica, is piped to the surface where it is separated by flashing into a steam phase and water at a lower temperature. The steam drives a turbine to produce electricity. The cooler separated water is now supersaturated in dissolved silica which precipitates as a sinter and blocks drains, pipes and reinjection wells. It presents a major operational constraint to geothermal resource utilisation. At the same time the separated water provides a substantial source of silica for potential utilisation (approx 500,000mt.yr⁻¹ worldwide).

By controlling the polymerisation and precipitation chemistry it is possible to produce a range of amorphous silica materials with particular network or microfibrillar structures, and specific light scattering, oil absorption and cation exchange properties. These specialist silica products have particular applications in paper filling and coating where they enhance the print and optical quality of the paper; in paint where they act as opacifiers, flatting and anticorrosion agents; in rubber where they enhance crosslinking and strength properties; and as inert carriers and selective absorbents.

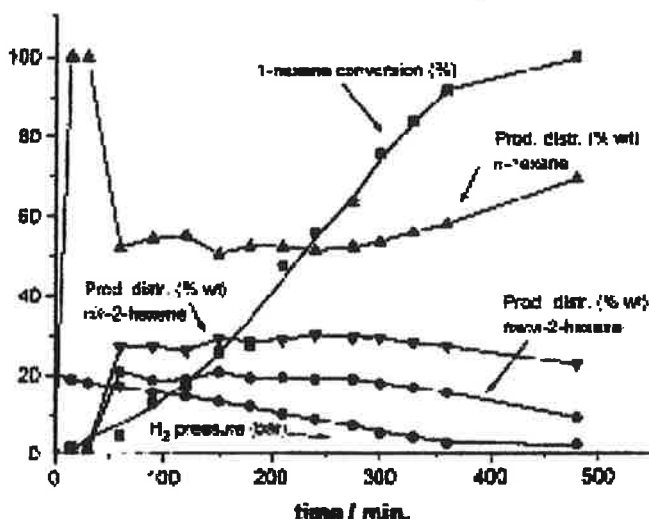
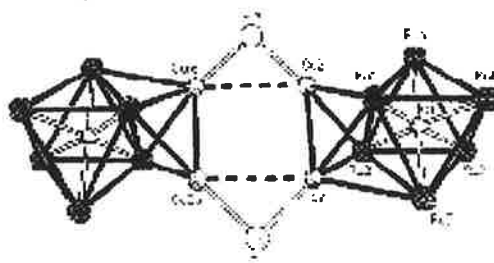
The proprietary chemistry and chemical process technology have been advanced from laboratory to pilot plant scale operation. Full scale paper mill trials have been carried out where one product has been added as a filler to newsprint with excellent results. Other products have also been successfully tested in different applications.

The project represents an excellent example of the development of specialist high value products from a problematic and waste resource. Also, the controlled removal of the silica enhances energy recovery and increases the efficiency of geothermal resource utilisation.

Clusters, Catalysis and Supramolecular Ordering of Nano-composites.

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There has been considerable interest in the formation, structure and further exploitation of the catalytic activity of bimetallic particles ever since Sinfelt *et al.*¹ demonstrated the powerful catalytic reforming properties of alumina-supported Ru-Cu, Pt-Ir and Pt-Re ensembles. With the advent^{2,3} of readily preparable mesoporous solids possessing pore diameters in the range 25 to 100Å and the feasibility^{4,5,6} of inserting 'single site' catalytically active centres in atomically well defined locations inside such mesopores, there is much incentive for extending such strategies to the insertion of bimetallic nanoparticles. As a consequence, one of the key practical aims in this work has been the design and production of discrete supported bimetallic particles of well defined and tuneable atomic composition; another is to so secure the clusters to the support so that they are prevented from sintering.⁷



Also ... "Supramolecular Ordering of Ruthenium Cluster Carbonyls in Mesoporous Silica." W. Zhou, D.S. Shephard, J. M. Thomas, T. Maschmeyer, B. F. G. Johnson, R.G. Bell, *Science*, **1998**, 280, 705.

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⁶ J.M. Thomas, *Faraday Discuss*, **1996**, 105, 1.

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SYMMETRIC MESOPOROUS METALLO-SILICATE CATALYSTS BY LOW CONCENTRATION NON-IONIC SURFACTANT TEMPLATING

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The demand for molecular sieve and heterogeneous catalysts with ever increasing pore dimensions has led to a recent explosion of effort in the development of mesostructured materials. In an extension of hydrothermal crystallisation of zeolite materials, researchers from Japan and the USA simultaneously reported the formation of templated mesoporous silicates exhibiting pores in the range 2.5 to 10.0 nm. In place of single molecule structure directing agents, micellar arrays of alkyl ammonium surfactants were used to template silicate structures. These M41S and FSM-16 materials exhibited crystalline habits mimicking the liquid crystalline phases of the surfactant, but lacked long range order within the solid wall structures. However, alkyl ammonium surfactants are expensive, toxic and environmentally unsound producing NO_x emissions upon calcination.

More recently, the formation of mesoporous silicates was reported using inexpensive, non-toxic and environmentally friendly non-ionic alkyl-polyethylene oxide (PEO) and block co-polymer PPO-PEO based surfactants. These MSU-X materials exhibited three dimensional arrays of "worm-like" pores with no long-range symmetry and were prepared from dilute surfactant solutions at neutral pH and near ambient reaction temperatures. Materials with hexagonally symmetric pore structures have been reported using concentrated liquid-crystal phase alkyl-PEO non-ionic surfactants under very low pH and sophisticated atmosphere control conditions.

Here we describe two new developments in the synthesis of non-ionically templated mesoporous [M]-MSU-X materials that afford hexagonally symmetrical metallo-silicate catalysts from dilute non-ionic alkyl-PEO surfactant solutions. Two new assembly routes are proposed ($\text{N}^\circ, \text{N}^+$) $\text{X}^- \text{I}^+$ and $\text{N}^\circ \text{M}^+ \text{I}^-$ which exploit the acid and base catalysed hydrolysis and simultaneous condensation of metal oxo-salts and silicon tetraethoxide. This very simple chemistry produces the incorporation of catalytically interesting metal atoms (Al, Ti, Zr, V) into the silicate network without the use of expensive and temperamental metal alkoxide reagents. The use of the commercially available Brij® range of alkyl-PEO surfactants produces highly ordered structures with thick pore walls and hence very high thermal and hydrothermal stabilities. Post synthesis hydrothermal treatment causes structural re-ordering of worm-like pores producing structures with well ordered hexagonal and cubic pore symmetries in the 1.8 to 6.0 nm range and high pore volumes.

COPPER(I)-IODIDE CORES IN COORDINATION POLYMERS

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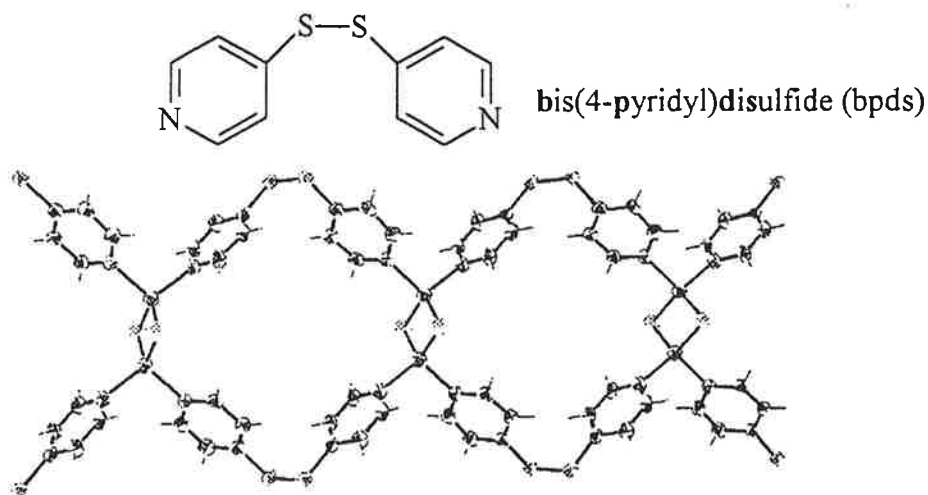
^a*Department of Chemistry, University of Nottingham, University Park, Nottingham, NG7 2RD, England.*

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^c*Department of Chemistry, University of Otago, PO Box 56, Dunedin, New Zealand.*

The development of inorganic coordination polymers has received much attention. The synthesis of uncharged inorganic arrays has the potential to provide zeolite analogues or porous arrays with a variety of physical properties. Using copper halides as the metal source allows for the incorporation of the anion within the polymeric array leaving cavities or channels anion free. To probe the utility of the copper halide motifs as junctions in coordination polymers we are studying the molecular architecture of copper(I) halides with connecting ligands containing the pyridine moiety.

Copper(I) cores are able to provide a variety of junctions for the formation of coordination polymers. Reacting CuI with bis(4-pyridyl)disulfide (bpds) in different stoichiometric ratios in acetonitrile afforded a 1:1 ribbon, $\{\text{CuI}(\text{bpds})\}_\infty$, or a 2:1 tubular polymer $\{(\text{CuI})_2(\text{bpds})\}_\infty$. The CuI motif observed in the 1:1 ribbon $\{\text{CuI}(\text{bpds})\}_\infty$ was a Cu_2I_2 planar bridged dimer whereas in the 2:1 tubular polymer $\{(\text{CuI})_2(\text{bpds})\}_\infty$ it was a Cu_4I_4 cubane tetramer. The nature of the polymers is affected by solvent and a third 1:1 daisy chain polymer $\{\text{CuI}(\text{bpds})\}_\infty$ with Cu_2I_2 dimer was isolated from benzonitrile solutions. All the polymers possess channels which contain solvent molecules. The structures of these coordination polymers will be presented. Powder X-ray data of solvated and desolvated bulk material and the consequences of loss of solvent will be discussed.



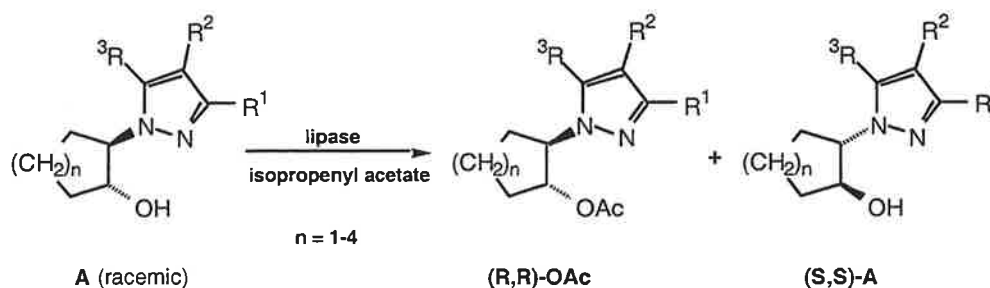
Coordination Chemistry of Chiral Ligands with Cycloalkane Backbones

Werner R. Thiel^{*}, M. Barz, H. Glas,

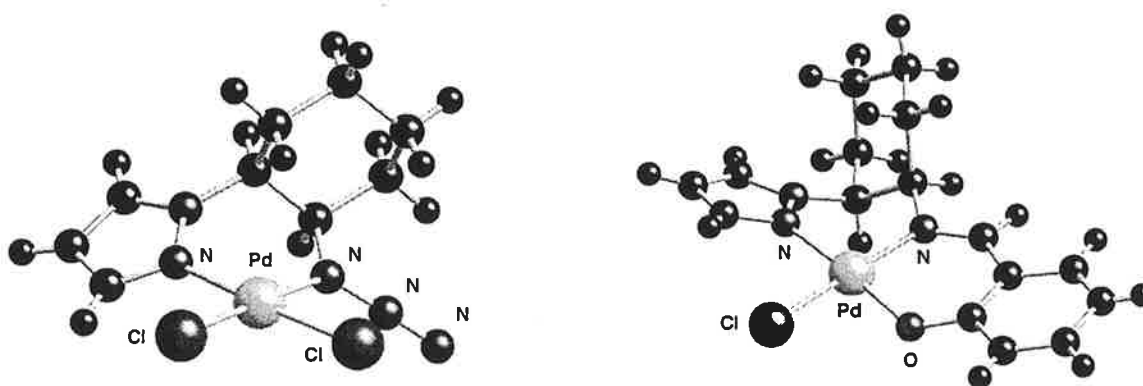
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trans-1,2-Substituted pyrazolyl cycloalkanol ligands **A** are accessible by reacting epoxycycloalkanes with pyrazole derivatives. The enantiomerically pure alcohols can be obtained by kinetic resolution with lipase B from *candida antarctica*.^[1] Following this procedure, a series of pyrazolyl cycloalkanols were synthesized, which have been applied successfully for the enantioselective alkylation of aromatic aldehydes with ZnR_2 reagents, which will be discussed.



During the last two years, we not just investigated the coordination chemistry of these chiral alcohols,^[2,3] but also used them as starting materials for the synthesis of new chiral ligands. Chelating diamines, aminoazides, *P,N*-ligands, or di- and tridentate imines can be obtained stereoselectively starting from the pyrazolyl cycloalkanols **A**.^[4] In addition to catalytic results, the coordination chemistry of such ligands will be presented (see examples below), focussing specially on the first transition metal complexes bearing chelating organo azide ligands.^[5]



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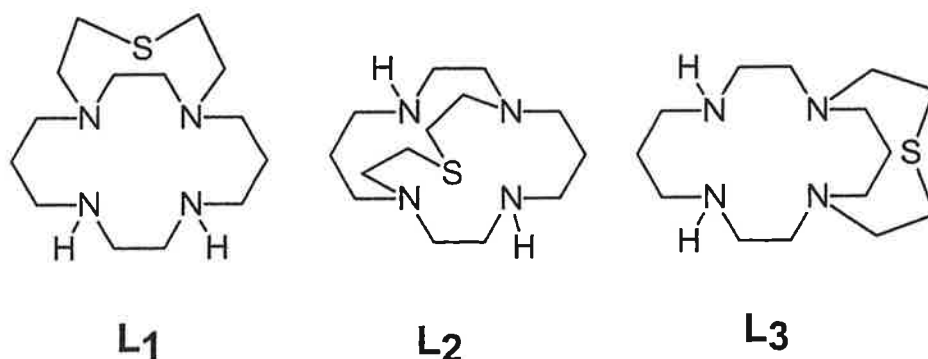
SYNTHESIS AND REACTIONS OF MACRO-POLYCYCLIC COMPLEXES

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Canada V8W 3V6.

Studies currently underway, focus on extending investigations into the formation of bicyclic macrocyclic ligands based upon cyclam ([14]aneN₄). Reactions of the nine- and ten-membered rings ([9]aneN₂X and [10]aneN₂X) with suitable pendant arms, and subsequent ring



closure, results in fused bi- and tri-cyclic ligands.¹⁻³ This presentation reports on extrapolations of the cyclam ligand to yield initially the third isomeric form of the bicycle, L₂.

Reaction of L₂ with Ni(II), Pd(II), Cu(II) and Co(II) results in the formation of a five- or six- coordinate complexes which exhibit redox behaviour. In the case of Ni(II), both Ni(I) and Ni(III) oxidation states are observed. Similar redox behaviour is exhibited by the other metal ions. The results of substitution kinetics at the higher oxidation state centres will be reported.

Further reaction of L₂ to a tricyclic ligand, can be accomplished by ring closure with an appropriate bifunctional reagent. Complexes formed by this system are currently under study by electrochemical, spectroscopic and stopped-flow kinetic methods.

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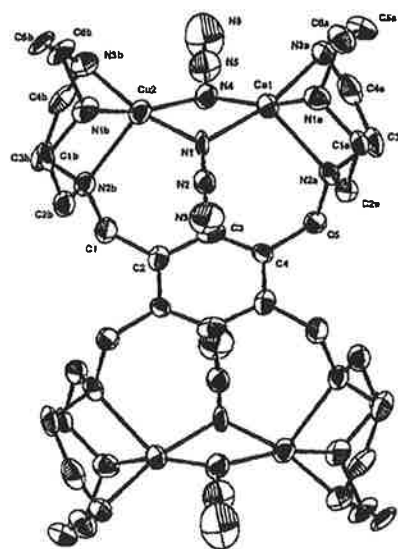
Coordination Chemistry of Poly(macrocyclic) Ligands Derived from 1,4,7-triazacyclononane.

Bim Graham, Milton T. W. Hearn and Leone Spiccia

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The coordination chemistry of macrocyclic ligands capable of binding two or more metal centres is an area which is currently attracting considerable attention. This is due to continuing interest in, for example, the modelling of polynuclear bio-sites, the understanding of magnetic interactions in polynuclear complexes and the ability of such complexes to catalyse hydrolytic and redox processes. We have been investigating the complexation of poly(macrocyclic) ligands based on tacn (1,4,7-triazacyclononane), a facially coordinating, tridentate macrocyclic ligand, from a fundamental and bio-inorganic point of view¹⁻³ but also with a view to applying the resultant complexes in the purification of protein by immobilised metal affinity chromatography (IMAC).⁴ A range of poly(macrocyclic) ligands consisting of two to four tacn rings have been developed and in some cases these have been further elaborated through the attachment of 2-pyridylmethyl and 2-carboxymethyl pendant coordinating groups. Series of metal complexes incorporating Mn(II), Fe(II), Fe(III), Co(III), Ni(II), Cu(II) and Zn(II) have been prepared and characterised.

Our recent studies have focussed on the use of tris(tacn) and tetrakis(tacn) macrocyclic ligands in the synthesis of supported and unsupported Cu(II) and Ni(II) complexes, which range in nuclearity from binuclear to extended polymers. The figure shows an azido-bridged tetranuclear Cu(II) complex, constructed around a durene-linked tetrakis(tacn) ligand, which exhibits moderately strong ferromagnetic coupling.



References:

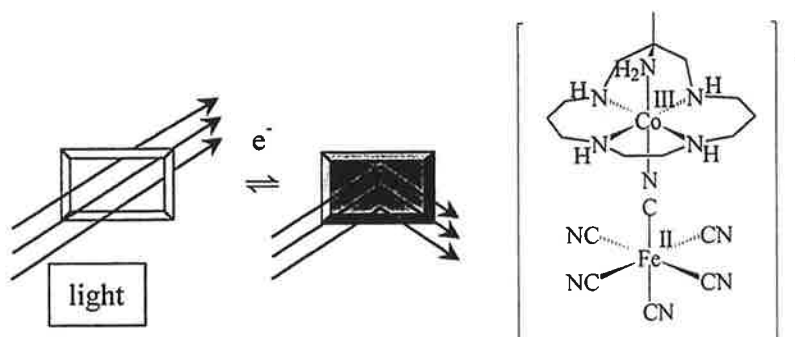
- 1) B. Graham, G. D. Fallon, M. T. W. Hearn, D. C. R. Hockless, G. Lazarev, L. Spiccia, *Inorg. Chem.*, 1997, 36, 6366.
- 2) S. J. Brudenell, A. M. Bond, L. Spiccia, P. Comba, D. C. R. Hockless, *Inorg. Chem.*, 1998, 37, 3705.
- 3) L. Spiccia, B. Graham, M. T. W. Hearn, G. Lazarev, B. Moubaraki, K. S. Murray, E. R. T. Tiekink, *J. Chem. Soc., Dalton Trans* 1997, 4089.
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ELECTROCHROMIC CYANO-BRIDGED DINUCLEAR COMPLEXES

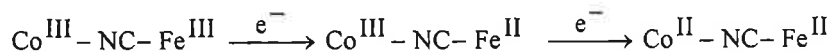
Paul V. Bernhardt

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Molecules that can be switched between two contrasting coloured forms by a reversible chemical reaction have potential applications in light transmissive/reflective devices (windows, protective eyewear) and information storage. One of the simplest chemical reactions is a single-electron oxidation or reduction.



We have recently identified a system that fulfils the above requirements of chemical reversibility and high contrast ratio between the oxidised and reduced form. The bridged dinuclear $\text{Co}^{\text{III}}\text{-Fe}^{\text{II}}$ complex shown above exhibits a prominent metal-to-metal charge transfer (MMCT) transition (Fe^{II} to Co^{III}) at 530 nm, giving the complex an intense maroon colour. One-electron oxidation of this compound generates the bright yellow $\text{Fe}^{\text{III}}\text{-Co}^{\text{III}}$ analogue, with loss of the MMCT transition. This process can be cycled back and forth indefinitely. We are currently pursuing other oxidation states of this system and close relatives. For example, a dinuclear Co/Fe complex might be stable in three different oxidation states (and colours).

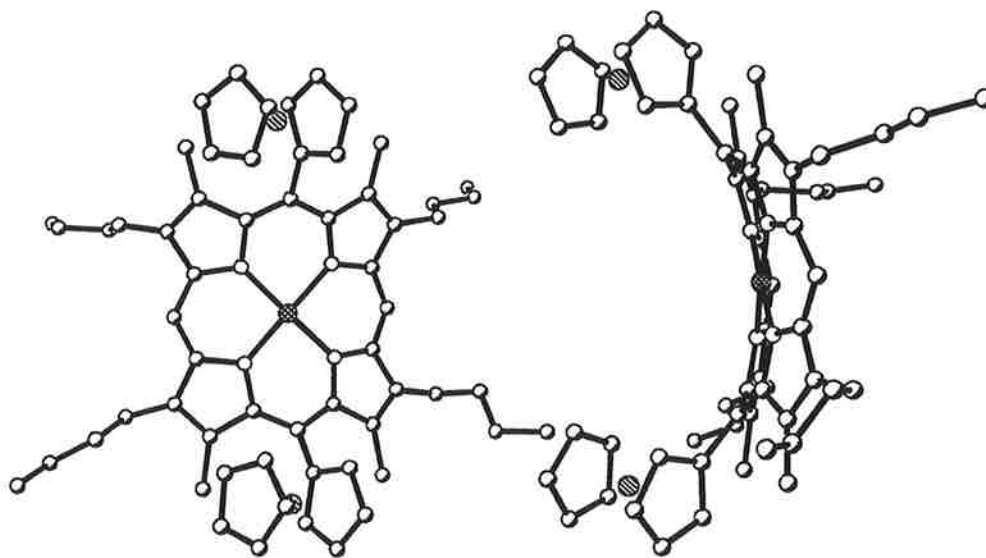


This will require that the ligand systems of the two metal ions are appropriate in order that we can characterise these species over a range of oxidised or reduced forms.

Bis(ferrocenyl)porphyrins. Compounds with Strong Long-Range Metal-Metal Coupling.

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The reaction of ferrocene aldehyde and bis(3-butyl-4-methyl-2-pyrryl)methane results in the formation of α,α -5,15-bis(ferrocenyl)-2,8,12,18-tetrabutyl-3,7,13,17-tetramethylporphyrin (**1**). The single crystal X-ray structures of **1** and its nickel(II) complex (Ni-**1**) were obtained confirming the α,α geometry. The separation between the two ferrocenyl iron centres is 11.21 Å in **1** and 10.30 Å in Ni-**1**. The electrochemistry of **1** and Ni-**1** reveals two consecutive ferrocene-based one-electron oxidation waves, which are separated by 0.19 and 0.41 V, respectively. This large splitting appears to be the result of extensive mixing of both ferrocenyl molecular orbital systems with that of the porphyrin connector π system.



ELECTRON AND ENERGY TRANSFER WITHIN DYADS INVOLVING ORGANIC QUENCHERS AND/OR POLYPYRIDYL d^6 METAL CENTRES BRIDGED BY RIGID ALICYCLIC "MOLRACS"

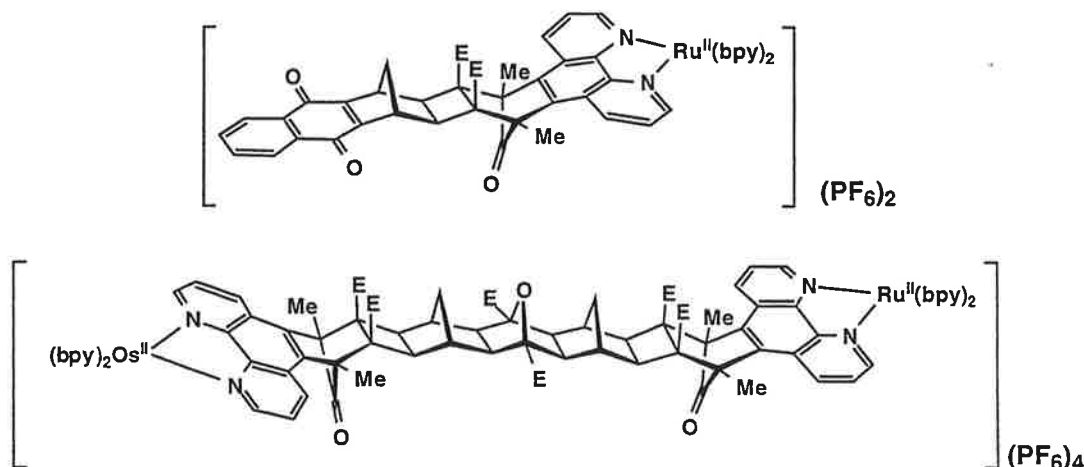
Laurence S. Kelso,¹ Trevor A. Smith,² Austin C. Schultz,³
 Ronald N. Warrener,³ Kenneth P. Ghiggino,² and F. Richard Keene¹

¹ *School of Biomedical & Molecular Sciences, James Cook University, Townsville, Queensland 4811, Australia.*

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We have previously utilised norbornane-modified phenanthroline ligands in the synthesis of mono- and di-nuclear complexes containing ruthenium(II), osmium(II) and platinum(II). Similar scaffold-like structures have also been used in the design of organic molecules containing electron-donor and -acceptor functionalities. The non-conjugated alicyclic nature of the polynorbornane framework has allowed us to design molecules with a fixed distance and known orientation between the two interacting components of the dyad. These conformationally-rigid systems provide a unique opportunity to further our understanding of the factors which control intramolecular electron and energy transfer processes.



In the present study we have extended the work done on rigid space-separated organic systems, by interposing a rigid saturated framework between two d^6 polypyridyl metal-based complex chromophores or alternatively between a metal complex chromophore and an organic quencher (two examples as shown above). We report the effectiveness of polynorbornane ("molrac") structures in mediating electron and energy transfer processes within such inorganic systems. Significantly, electron transfer was observed to be a short range phenomenon while energy transfer occurred over much larger distances.

FLUORESCENT SWITCHES FROM NAPHTHALIMIDES AND FERROCENYLAMINES

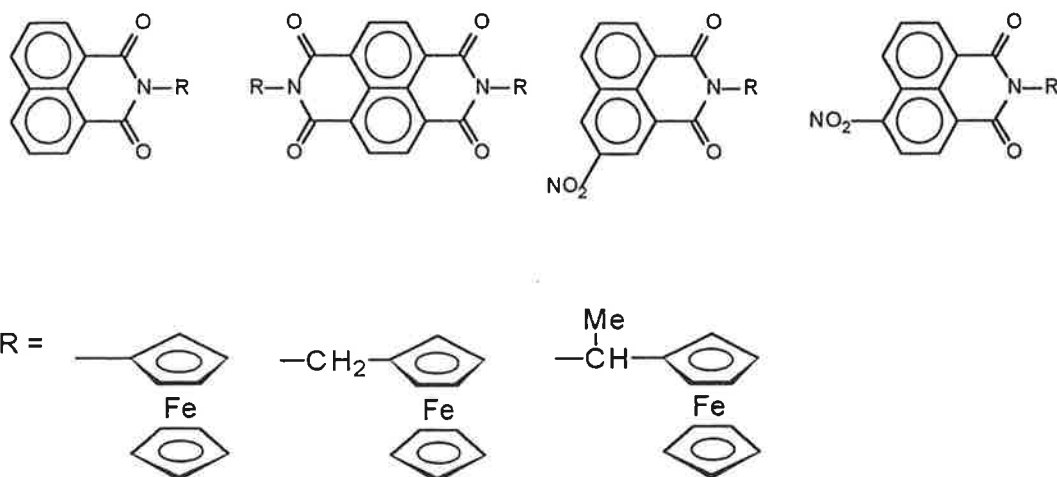
C. John McAdam, Brian H. Robinson and Jim Simpson

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Coupling of fluorescent and electroactive centres in principle leads to one- or two-dimensional molecular switches and sensors. Our strategy is to use low-valent clusters and ferrocenyl derivatives as the electrophores and polyaromatic moieties with long-lived excited states as the chromophore. Aryl naphthalimides are particularly interesting chromophores as their photophysics is dependent on the orientation of the phenyl ring relative to the planar naphthyl moiety; this gives stereochemical control of the fluorescence.

We have coupled naphthylanhydrides with ferrocenylamines to give novel naphthylimides which give us the opportunity to investigate the photophysics as a function of redox potential and stereochemistry, and to determine the influence of cyclopentadienyl / naphthyl ring coplanarity. The compounds shown below have been fully characterised and this data with attendant electrochemistry and spectroscopy will be presented. Quenching of polyaromatic fluorescence by the ferrocenyl moiety is the 'norm' and the possibility of switching off the quench will be discussed.



COMBINING HOST-GUEST CHEMISTRY AND CRYSTAL ENGINEERING:
SELF-ASSEMBLY OF HYDROGEN-BONDED ARRAYS INCORPORATING RECEPTOR
SITES.

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Bowl-shaped container molecules such as calixarenes and cyclotrimeratrylene (= CTV) can bind globular molecules including C_{60} , C_{70} , and 1,2-dicarbododecaborane(12) ($C_2H_{12}B_{10}$ = *o*-carborane) resulting in ball-and-socket complexes held together by non-classical hydrogen bonding and π - π interactions with complementarity of curvature between the host and guest moieties. This chemistry shows considerable potential in the field of separation science and indeed the selective complexation of C_{60} by *p*-Bu^t-calix[8]arene is a simple and cost efficient means of C_{60} extraction from a mixture of fullerenes.

The control of hydrogen bonding interactions to create extended networks in the solid state is one of the central premises of crystal engineering. Here we show that self-assembly of *m*- or *o*-carborane and CTV through bifurcated $C-H\cdots(OMe)_2$ hydrogen bonds results in infinite networks with hexagonal grid or helical topologies. The hydrogen bonded networks incorporate bowl-shaped receptor sites which bind two disparate globular molecules, *o*-carborane or C_{70} . This has implications for building up receptor arrays based on other container molecules and the other isomers of carborane. It is noteworthy that in the absence of carborane, C_{70} fails to form a complex with CTV, in contrast to C_{60} which forms two complexes, $(C_{60})(CTV)$ and $(C_{60})_{1.5}(CTV)$, and that C_{60} and CTV in the presence of *m*-, *o*- or *p*-carborane also affords $(C_{60})_{1.5}(CTV)$.

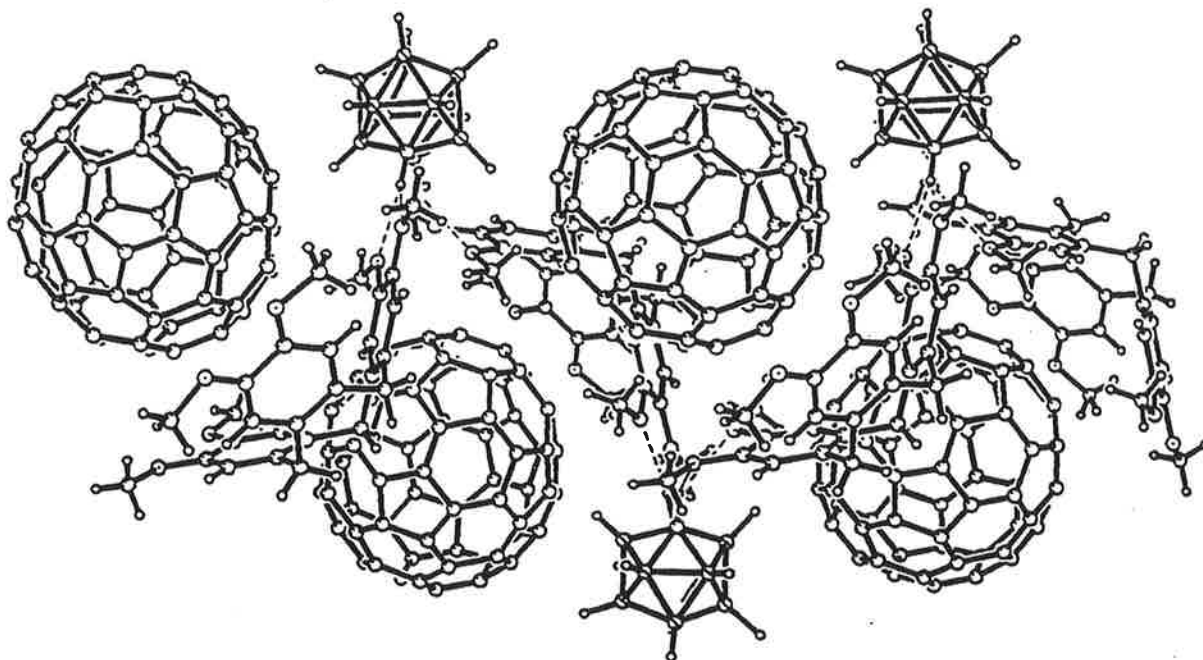


Figure 1: Helical arrangement of (*o*-carborane)(CTV)(C_{70})(1,2-dichlorobenzene).

Selective Supramolecular Porphyrin/Fullerene Interactions

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The recent crystal structure determination of a covalently-linked tetraphenylporphyrin- C_{60} dyad¹ revealed an apparent intermolecular attraction of C_{60} to the center of the porphyrin ring. The porphyrin/fullerene contacts were unusually short (ca. 2.75 Å). Typical fullerene/arene or porphyrin/arene π/π interactions lie in the range 3.0 - 3.5 Å.

We now show that this unique porphyrin-fullerene structural motif is ubiquitous in naturally assembling cocrystallates of untethered tetraphenylporphyrins and metalloporphyrins with C_{60} and C_{70} . Single crystal X-ray structures of many naturally assembling cocrystallates of the fullerenes C_{60} and C_{70} with a variety of tetraphenylporphyrins, from toluene solutions, show unusually short porphyrin/fullerene contacts (2.7 - 2.8 Å). Each fullerene approaches the porphyrin plane in a distinct manner. C_{60} orients the electron rich 6:6 ring juncture over the center of the porphyrin whilst C_{70} lies over the porphyrin plane in a "side on" manner with a carbon atom at the center of three fused six membered rings over the center of the porphyrin.

The porphyrins and fullerenes assemble in the crystal lattice to form either alternating chains with a zig-zag or linear arrangements. These structures provide a basis for the chromatographic separation of fullerenes using zinc tetraphenylporphyrin appended silica stationary phases developed by Meyerhoff². They indicate a new supramolecular recognition element between the curved π surface of a fullerene and a planar porphyrin surface.

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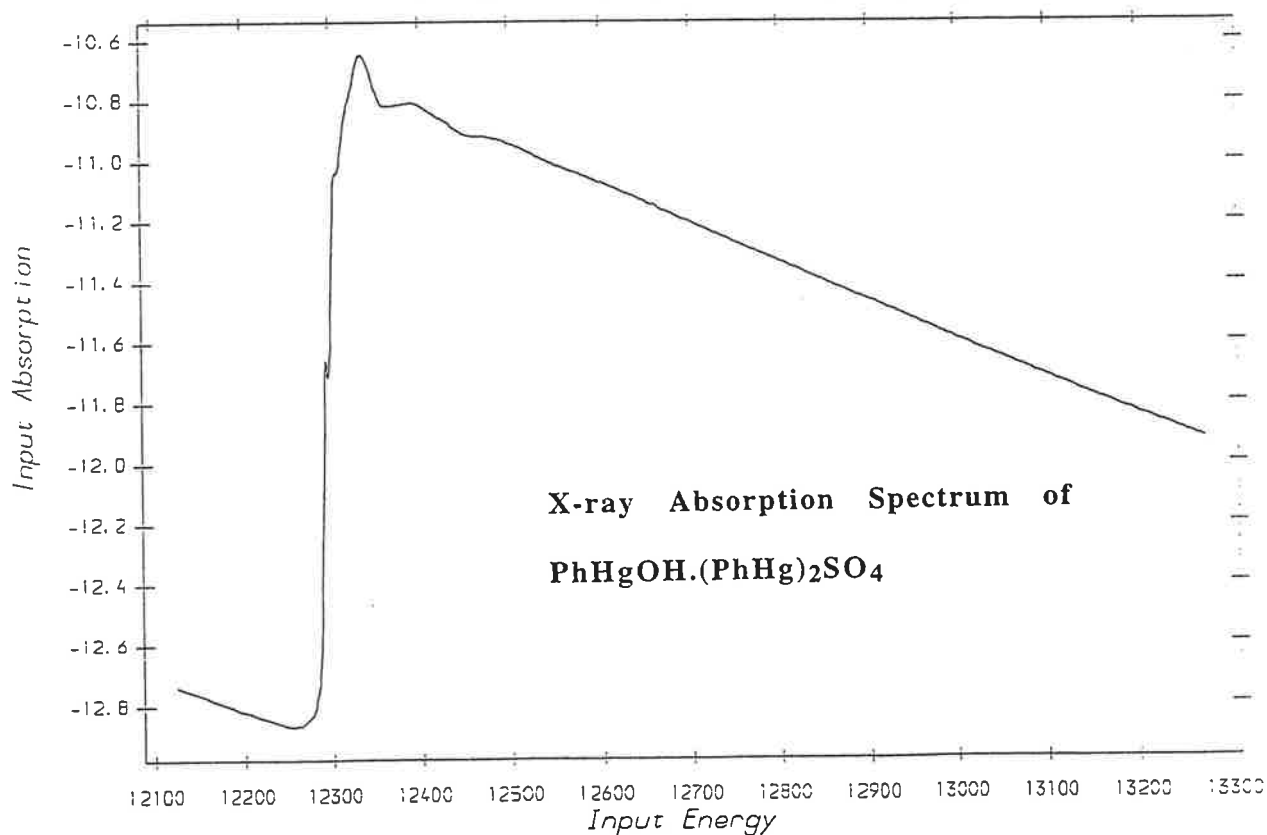
Brian K. Nicholson*, David G. Nicholson** and Wendy J. Jackson*

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** Chemistry Department, Norwegian University of Science and Technology, N-7034, Trondheim, Norway.

Some well-known aryl-mercury compounds have unknown structures, because they do not form single crystals suitable for X-ray crystallography. These include PhHgOH (which may or may not be similar to MeHgOH which is actually $(\text{MeHg})_3\text{O} \cdot \text{OH} \cdot \text{H}_2\text{O}$ [1]), and the "basic salts" $\text{PhHgOH} \cdot \text{PhHgNO}_3$ or $\text{PhHgOH} \cdot (\text{PhHg})_2\text{SO}_4$ (which are possibly related to the basic BF_4^- salt which is $(\text{PhHg})_2\text{OH} \cdot \text{BF}_4 \cdot \text{H}_2\text{O}$ [2]).

There has been little previous X-ray absorption spectroscopy of mercury compounds [3]. We now compare the Hg L_{III} XANES and EXAFS spectra of a number of model compounds of known structure (HgCl_2 , PhHgCl , PhHgOAc , $(\text{PhHg})_2\text{O}$, $(\text{PhHg})_2\text{OH} \cdot \text{BF}_4 \cdot \text{H}_2\text{O}$) with some of unknown structure [PhHgOH , $\text{PhHgOH} \cdot \text{PhHgNO}_3$ and $\text{PhHgOH} \cdot (\text{PhHg})_2\text{SO}_4$].



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QUADRUPLE HELICATES AS SELECTIVE HOSTS FOR ANIONS

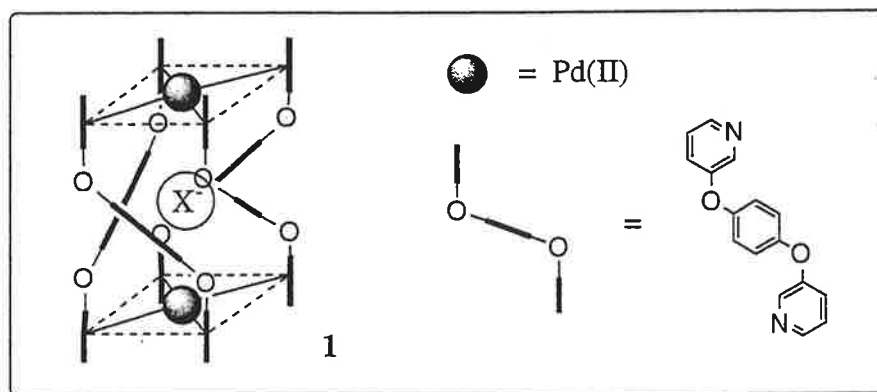
David A McMorran and Peter J Steel

Department of Chemistry

The University of Canterbury

Private Bag 4800, Christchurch, New Zealand

Metallosupramolecular chemistry is becoming recognised as an important new tool in molecular recognition. We have prepared the first coordinatively saturated quadruple helicate, **1**, and have found that it possesses a large internal cavity. ^1H NMR titration studies show that this cavity enables the helicate to selectively recognise anions based on size and shape. X-ray crystal structures of three such host-guest complexes, where the helicate encapsulates PF_6^- , ClO_4^- or I^- , have been determined. These show that the helicate is able to vary the size of the cavity in response to the size of the anion by a twisting action about the helical axis. Thus, addition of anions allows for noncovalent control of the shape and length of the helicate.

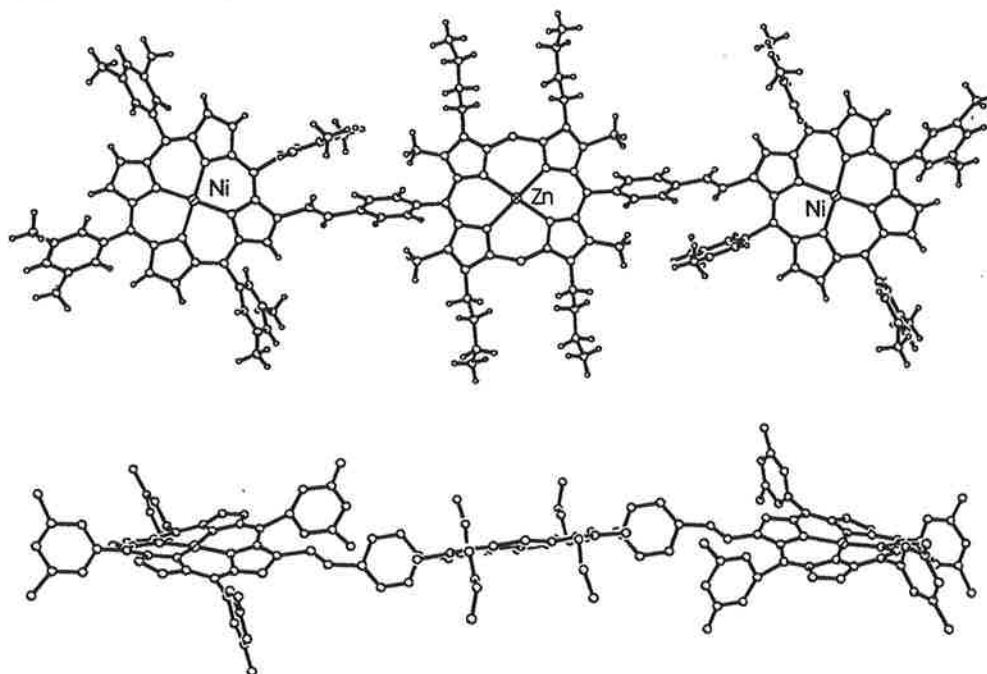


Emission studies of Porphyrin Arrays

Anthony K. Burrell, Wayne M. Campbell, David L. Officer and Sonya M. Scott.

Department of Chemistry, Massey University, Private Bag 11222, Palmerston North, New Zealand

The capture of sunlight by photosynthetic organisms and the ensuing energy transfer to the reaction centre is an important and efficient process.¹ Exploiting photosynthesis as a replacement for traditional chemical processes and energy production methods is a major research target. Many model systems have been designed in an attempt to mimic the function of photosynthetic arrays of chlorophyll. A series of trimeric porphyrin arrays have been synthesised at Massey and studied using emission techniques. These emission studies allow insight into the extent of communication between the chromophores in an array.



¹ (a) C. N. Hunter, R. van Grondelle, J. D. Olsen, *Trends Biochem. Sci.* 1989, **14**, 72.
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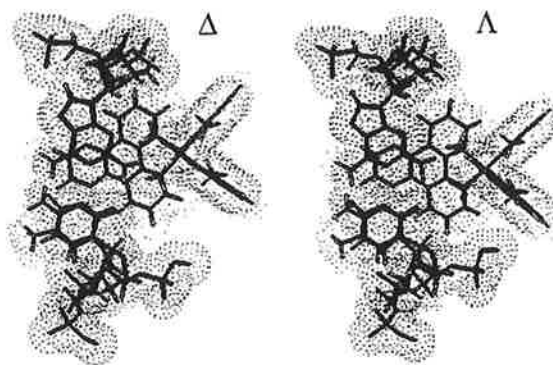
DNA-BINDING OF METAL COMPLEXES

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^bDepartment of Chemistry, University College, (UNSW), Australian Defence Force Academy, Canberra 2600, Australia

There have been extensive efforts to characterise the interactions of simple chiral metal complexes with DNA. This dynamic area of research, at the interface of biology and chemistry, is proving to be a challenge as the fundamental rules, by which the structure of DNA discriminates between different molecules, are far from well understood. Our group has focused on making systematic modifications to $[\text{Pt}(\text{en})(\text{intercalator})]^{2+}$ and $\Delta, \Lambda\text{-}[\text{Ru}(\text{ancillary-ligand})_2(\text{intercalator})]^{2+}$ type complexes, followed by the evaluation of these changes by DNA-binding experiments. Depending on the results obtained, further modifications are then made to improve and clarify these interactions. This style of investigation has been rewarded with the first strong evidence that these compounds bind in the minor groove. Evidence from current investigations suggest that a compromise between intercalator size, shape, functional groups and overall stereochemistry must be reached in order for these complexes to be effective for eliciting the specific structural details required for the exploration of the principles of nucleic acid recognition and site selectivity particularly, by NMR. We report here an examination of the binding modes and the comparative DNA affinity of these compounds by techniques, such as DNA-UV spectroscopy, unwinding of closed circular DNA, viscosity measurements and DNA-paper chromatography, in addition to NMR.



$\Delta, \Lambda\text{-}[\text{Ru}(2,9\text{-dmthethylphen})_2(\text{dpq})]^{2+}$ intercalating into the minor groove of a TC base pair.

X-RAY ABSORPTION SPECTROSCOPY OF MICROPOROUS MATERIALS

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Sydney, NSW 2052, Australia

Zeolites and related micro- and mesoporous materials are attracting wide attention, not only as traditional adsorbents and catalysts, but also as inorganic media for fascinating new host-guest chemistry. These newer applications place particularly stringent demands on characterization techniques. This talk will present some applications of X-ray absorption spectroscopy (EXAFS and XANES) illustrating how these techniques can complement both diffraction methods, sensitive to long range order, and spectroscopic probes such as solid state NMR and EPR which observe local environments.

Three types of experiment will be discussed. X-ray absorption in the hard X-ray region (5 to 30 keV) has been widely used to observe extraframework species: transition metal ions and clusters, for example. Recent work comparing EXAFS data for Pb, Cd and Cu exchanged zeolites with solid state NMR, EPR and diffraction information to determine location of the cations will be presented.

Hard X-ray absorption spectroscopy can also be applied to transition metals substituted into zeolite frameworks. In these systems, the key questions are where does the transition metal locate, and does it remain in the framework under all circumstances? This application of EXAFS and XANES will be illustrated with Co and Fe substituted molecular sieves.

The third experiment, which is very new, is the use of soft X-ray absorption spectroscopy to probe the local structure around light elements (Si, Al, Mg) in micro- and mesoporous materials. The experimental approach will be described, and some recent data indicating the potential utility of the method as a complement to solid state NMR will be described.

LARGE CAGE MOLECULES FOR THE SELECTIVE BINDING OF METAL IONS AND SMALL MOLECULES

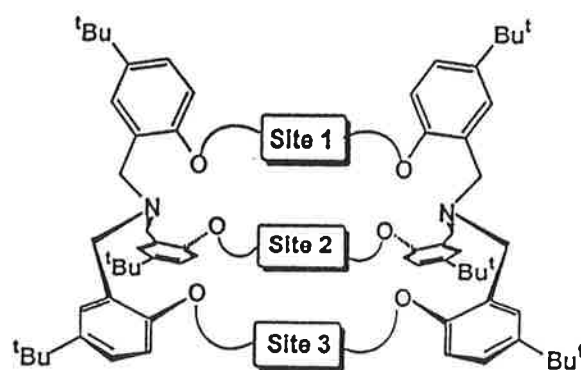
Ian M. Atkinson,* Robert S. A. Gauci,* Jeong Kim,# Leonard F. Lindoy,† George V. Meehan,* Owen A. Matthews,* David F. Perkins,† Fiona Raciti* and Jack Ryan*

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

A series of large cage molecules of general structure **1** have been synthesised using a stepwise 'building block' approach. The procedure enables variation in the nature of the bridging groups designated sites 1 - 3. In addition to simple aromatic moieties such as *m*- and *p*-xylyl, these bridging



(1)

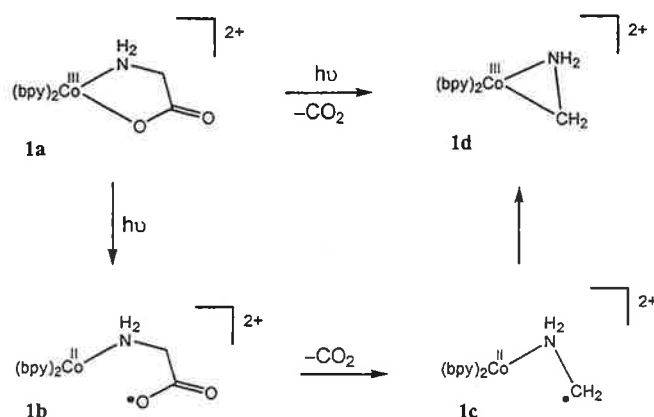
groups include 2,6-lutidyl, the corresponding 4-dimethylamino derivative, N-oxide analogues, together with phenolic derivatives and larger moieties based on 2,2'-bipyridyl. Structure/function relationships underlying the host-guest binding behaviour of these species have been elucidated using a combination of nmr, X-ray, solvent extraction and molecular modelling techniques. For example, the interaction of a series of the smaller cages (incorporating both aromatic and aliphatic 'straps' linking the bridgehead nitrogen atoms) with alkali metal ions has been investigated in some detail while, for example, the tris-2,6-lutidyl cage has been demonstrated to be a selective receptor for phloroglucinol relative to other related polyphenols.

THE PHOTOCHEMISTRY OF COBALT(III)-AMINO ACID COMPLEXES

Shane G. Telfer and Richard M. Hartshorn

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Poznyak's group¹ have shown that irradiation of the bis(2,2'-bipyridine)glycinatocobalt(III) ion ($[\text{Co}(\text{bpy})_2\text{gly}]^{2+}$) **1a** with UV light results in decarboxylation and formation of a complex containing a three-membered Co-C-N metallacycle (**1d**). Natarajan² used flash photolysis to measure the a rate constant of around 10^3 s^{-1} for the formation of the metallacycle.



We have synthesised a cyclopropylglycinato complex and employed it as a radical clock to measure the relative lifetime of the putative aminoalkyl radical intermediate **1c**. We have found that the cyclopropyl group remains intact during the photolysis which implies that any such radical has a sub-microsecond lifetime. This is inconsistent with Natarajan's assignment of the rate determining step in the original kinetic study.

At present we are formulating a new mechanism for this reaction by measuring the kinetics and observing the product distributions for a range of amino acid ligands. Also, we are investigating some novel complexes which contain a Co-C-N metallacycle.

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CHROMIUM(V) PEPTIDE AND AMINO ACID COMPLEXES. POSSIBLE INTERMEDIATES IN CHROMIUM-INDUCED CARCINOGENESIS

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The preparation and characterisation of Cr(V) peptide and amino acid complexes with alanine, glycine and their peptides are described. These complexes can be prepared from both reduction of Cr(VI) in the presence of the ligand, or the oxidation of Cr(III) precursors, and are readily identified by EPR spectroscopy for mononuclear complexes. Dinuclear complexes are EPR silent, but a dimeric complex with alanine has been characterised by multiple-scattering XAFS analyses and electrospray mass spectrometry. These complexes have considerable stabilities under physiological conditions of pH and temperature and are possible intermediates in Cr(VI)-induced genotoxicities.

The Cr(V) amino acid and peptide complexes damage DNA in *in vitro* assays and cause mutations in both bacterial and mammalian lung cells. The permeabilities of the complexes into mammalian lung cells have also been investigated and will be discussed in relation to their genotoxicities.

CRYSTAL AND LIQUID STRUCTURES OF *N,N*-DIMETHYLTHIOFORMAMIDE (DMTF) AND *N,N*-DIMETHYLFORMAMIDE (DMF) SHOWING STRONGER EFFECT OF C-H...S THAN OF C-H...O HYDROGEN BONDING

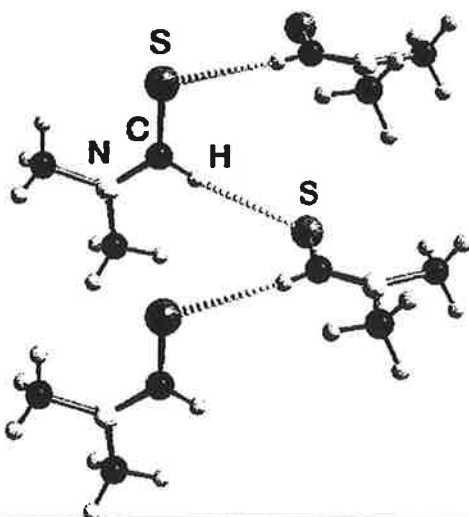
Magnus Sandström,^a Horst Borrmann,^b Ingmar Persson,^c Christina M.V. Stålhandske^c

^a Department of Chemistry, Royal Institute of Technology, S-100 44 Stockholm, Sweden.

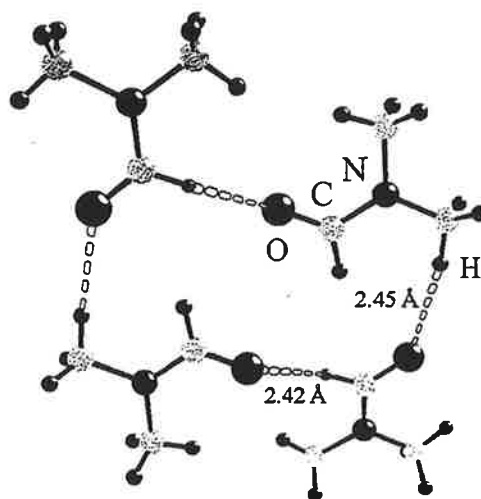
^b Max-Planck-Institut für Festkörperforschung, Postfach 800665, D-70506 Stuttgart, Germany.

^c Department of Chemistry, Swedish University of Agricultural Sciences, P.O. Box 7015, S-750 07 Uppsala, Sweden.

The crystal structures of the useful solvents dmtf and dmf were determined at 90 ± 2 K. The packing of the planar molecules is in both compounds influenced by non-conventional C-H...X hydrogen bonding. In dmtf almost linear C-H...S=C-H...S *cooperative* hydrogen bonding, enhanced by polarisation, connects the thioformyl groups giving rise to helix-shaped chains with an intermolecular C...S distance of 378.1 pm. In dmf four-membered centrosymmetric rings are formed by weak C-H...O intermolecular interactions, two of which *via* the formyl protons (C...O 329.4 pm), and two with methyl protons (C...O 341 pm). X-ray diffraction of liquid dmtf shows bulk order, consistent with a high degree of hydrogen bonding. The liquid structure of dmf can, despite the stronger hydrogen bond *acceptor* properties of the oxygen atom, be described without hydrogen bonding. This apparent anomaly is discussed using results from theoretically estimated charge distributions, which show the formyl hydrogen atom to have a lower charge and thus weaker hydrogen-bond *donor* properties than the thioformyl hydrogen atom.



Cooperative hydrogen bonding between dmtf molecules



Four-membered ring of dmf molecules

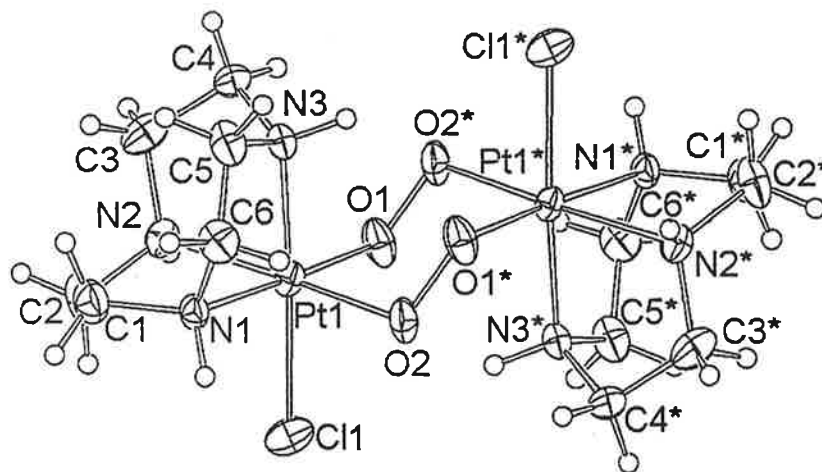
Ligand Mediated Oxidation of Pt(II) and Stabilization of Pt(IV)

Murray S. Davies and Trevor W. Hambley

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There has been much interest in using ligands to stabilize uncommon coordination geometries and oxidation states of transition metals because of the properties that such species exhibit. Our interest comes from examination of Pt...H-C and Pt...H-N “agostic” interactions, and in using tri- and tetradentate ligands to stabilize the Pt(IV) oxidation state in antitumour activity studies.

Described here are the preparation of a number of Pt(II) and Pt(IV) complexes with tri- and tetradentate ligands. Some of these ligands were selected because of their tendency to promote tetrahedral or octahedral geometries, thereby putting the normally square planar Pt(II) into an uncommon geometry. Such complexes have been shown to be susceptible to aerial oxidation by an unknown mechanism. A number of unusual complexes have been isolated that provide some evidence for binding of atmospheric oxygen to Pt(II) species to form bridged peroxo- or superoxo intermediates; $[\text{Pt}_2\text{Cl}_2(\mu_2\text{-O}_2)([\text{9}] \text{aneN}_3)_2]\text{Cl}_2$ shown below is one such species.¹ An oxidative mechanism based on our isolation of this species is proposed.



1 Davies, M. S.; Hambley, T. W. *Inorg.Chem.* 1998, in press.

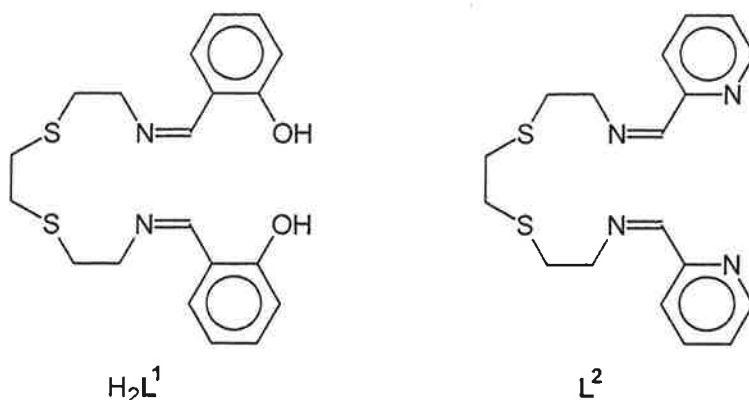
DWYER AND LIONS REVISITED: COMPLEXES OF SEXADENTATE LIGANDS

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Frank Dwyer and Francis Lions successfully collaborated in the 1950s on the synthesis of metal complexes of sexadentate ligands with a view to producing systems with high molecular rotations. As a successful exercise in the design of sexadentate ligands, this body of work represents a high-point for the 'Sydney School' of coordination chemistry. The chemistry deserves further consideration because of recent research indicating that sexadentate ligands can give rise to metal complexes of unusual topologies. Two of the sexadentate ligands (H_2L^1 and L^2) first reported by Dwyer and Lions have been re-prepared and metal complexes isolated. These complexes have been characterised by a number of techniques including x-ray crystallography and electrospray mass spectrometry. The field strength of L^1 , as determined from electronic spectra for the nickel(II) complex, is close to the spin crossover in iron(II). Variable temperature magnetic runs (300-100K) on independently prepared samples of $[FeL^1] \cdot 2H_2O$ indicate some tendency toward spin-pairing. Structures of $[ML^2](ClO_4)_2$, $M = Fe$, Ni and $\{[CuHL^1](ClO_4)\}_2 \cdot CH_3CN \cdot 0.5H_2O$ will be presented.



The work on sexadentate ligands had a contemporary impact on coordination chemistry and has continued to be strongly cited. The current impact of the original work has been determined through the Science Citation Index. The relationship of Dwyer, in particular, to the other members of the 'Sydney School' will also be discussed.

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