

PART 1

Program; Abstracts (oral presentations); Registrants



IC'96

ROYAL AUSTRALIAN CHEMICAL INSTITUTE

INORGANIC CHEMISTRY DIVISION
NATIONAL CONFERENCE

30th JUNE - 4th JULY, 1996

Townsville, Queensland, Australia

PROGRAM
ABSTRACTS
REGISTRANTS



ROYAL AUSTRALIAN CHEMICAL INSTITUTE
INORGANIC DIVISION
IC'96



Townsville, Queensland

PROGRAM AND ABSTRACTS



This publication was edited and compiled by

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Information contained in this publication is correct at the time of the copy deadline of June 4th, 1996. The list of delegates is limited to those persons with valid registrations on that date, and the compilation of Abstracts is restricted to those involving registered authors. A list of subsequent registrants and Abstracts submitted by them will be separately circulated at the Symposium.

ORGANISING COMMITTEE

Organising Committee:

Prof. Len Lindoy (Chairman)
Assoc.-Prof. Richard Keene (Secretary)

Miss Eva King
Mrs Fay Lindoy

The Committee would like to acknowledge the assistance of the collaborators and denizens of the Lindoy and Keene research laboratories for their contributions to the running of the conference - in particular Dr Ken Adam, Dr Ian Atkinson, Professor Grover Everett, Mr Robert Gaudi, Mr Noel Green, Mr Andrew Groth, Mr Mick Henderson, Mr Laurie Kelso, Professor Jinho Kim, Dr Tony Leong, Dr Brian McCool, Ms Myrna Mahinay, Mr David Perkins, Ms Fiona Raciti, Mr David Reitsma, Mr Todd Rutherford, Mr Niels Svenstrup and Mr Michael Thiry. In addition, Mrs Cheryl Keene, Mr Andrew Keene and Mrs Carolyn Everett are thanked for their help.

SPONSORS

The Organising Committee wishes to extend its gratitude to the following for their generous support of IC'96

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CONFERENCE PROGRAM

Venue for all IC'96 activities is the Sheraton Breakwater Casino-Hotel.
Unless otherwise indicated, sessions will be held in Ballroom 1

REGISTRATION: The Registration desk is located in the Lobby Lounge of the Sheraton Breakwater Casino-Hotel, and will operate on Sunday, June 30th from 1400-1700h, and at all times during the Conference.

Sunday, June 30th

1400 - 1700 h	Registration Poster set-up (Group A)	(Lobby Lounge) (Ballrooms 2/3)
1830 - 2200 h	Mixer/buffet meal	(Poolside)

Admission to the Conference Mixer and Barbecue will be by Conference name-tag, which will have been issued to all delegates and accompanying persons. Dress is neat casual.

Monday, July 1st

0830 - 0930 h	Plenary Lecture: Jean-Pierre Sauvage (PL4/M) <i>Rotaxanes and Other Multiporphyrin Assemblies as Models of the Photosynthetic Reaction Centre</i>
0930 - 1030 h	Oral presentations: Introduction to poster papers (1) <u>G. Adefikayo Ayoko</u> , Stephen Balarea, John Arabel, Seni Oroni, and Kirpal Singh (P8/A*) <i>Modelling Multinuclear Redox-Active Manganese Enzymes. Exploratory Kinetic Studies of the Reduction of High-Valent Oxomanganese Complexes</i> <u>Rachel Codd</u> and Peter Lay (P27/A*) <i>The Interaction of Optically-Active Cr(V) Complexes with DNA</i> <u>Rodney M. Cusack</u> , John Abbenante, Lawrence R. Gahan, David P. Fairlie, and Graeme R. Hanson (P30/A*) <i>Cyclic Peptides as Metal Ion Receptors</i> Hugh Harris, <u>Keith Fisher</u> , and Ian Dance (P40/A*) <i>Gas Phase Metal Sulfide Cluster Anions $M_nS_y^-$ of the First Row Transition Elements</i> Xavier B. Delaigue, C. David Gutsche, Jack M. Harrowfield, <u>Mark I. Ogden</u> , and Donald R. Stewart (P53/A*) <i>Calixarenes as Uranophiles</i>

1030 - 1100 h MORNING TEA

(cont.)

1100 - 1230 h

Oral presentations: Introduction to poster papers (2)

Alan Bond, Glen Deacon, Lai Yoong Goh, Susan Jenkins, Douglas McFarlane, Leone Spiccia, Ian Watkins, and Jim Woolfrey (P72/A*)
Electric Windows: A Breakthrough in Voltaics

Michael I. Bruce, Larisa Denisovich, Paul J. Low, Svetlana M. Peregodova, and Nikolai Ustynyuk (P90/B*)
The Redox Chemistry of Two Diruthenium Diacetylides - Towards Molecular Wires?

Graham A. Heath, Stuart A. Macgregor, and Klaus H. Moock (P102/B*)
An Electrochemical and Computational Study of Transition Metal Halides: $[MCl_6]^{n-}$ versus $[MF_6]^{n-}$

Scott C. Courtney, David C.R. Hockless, Boujemaa Moubaraki, and Keith S. Murray (P105/B*)
Homo- and Hetero-Trinuclear Metal Chelate Complexes of the Schiff-Base Type

Roy Doyle, Geoffrey Salem, and Anthony C. Willis (P124/B*)
Stereoselective Synthesis of Chiral Multidentate Ligands with As_2NP or As_4P Donor Atoms

M.J. Lavery, Z. Xiao, M. Ayhan, S.D.B. Scrofani, M. Guss, and A.G. Wedd (P137/B*)
The Rubredoxin from Clostridium Pasteurianum: Mutation of the Four Cysteinyll Ligands of the Iron

S.T. Horner, C.E.F. Rickard, S.J. Webb, and L.J. Wright (P142/B*)
Metal Complexes of New N-Amidate Cleft and Macrocyclic Ligands

1230 - 1400 h

LUNCH

1400 - 1530 h

Oral presentations: "New Researchers"

Lisa Martin (L11/M)
Modelling Metalloenzymes - Structures and Strategies

Paul Bernhardt (L3/M)
Multifunctional Pendant Armed Macrocycles

Lou Rendina (L13/M)
Luminescent Organoplatinum(IV)-Tin Metallacycles by Oxidative Addition

1530 - 1600 h

AFTERNOON TEA

1600 - 1730 h

Oral presentations: "New Researchers"

George Koutsantonis (L9/M)
Recent Advances in Main Group and Transition Metal Organometallic Chemistry. Application to New Materials

Sally Brooker (L5/M)
Advantages of Macrocyclic Thiolates

Janice Aldrich-Wright (L1/M)
Molecular Design: The Systematic Approach

1900 - 2200 h

Informal viewing of Posters (Group A)

Ballrooms 2/3

Tuesday, July 2nd

- 0830 - 0930 h Plenary Lecture (Nyholm Lecture): Tom Meyer (PL3/Tu)
Multiple Electron Oxidations
- 0930 - 1200 h Scientific Poster Session (Group A) (Ballrooms 2/3)
(Incl. morning tea)
- 1200 - 1330 h LUNCH (Student lunch with invited speakers)
- 1330 - 1415 h Conference Lecture: Odile Eisenstein (L7/Tu)
Electron Deficient Complexes. The Importance of Metal-Metal σ and π Bonds
- 1415 - 1515 h Specialist lectures
Leon Kane-Maguire (L8/Tu)
Mechanisms of Nucleophilic Attack by Iodide and Hydroxide Ions on [(Dienyl)Fe(CO)₃]⁺ Cations
Kevin Wainwright (L16/Tu)
Hydroxyalkylation of Macrocyclic Ligands as a Technique for Enhancing Complex Stability
- 1515 - 1545 h AFTERNOON TEA
- 1545 - 1645 h Specialist lectures
Stephen Lincoln (L10/Tu)
Aspects of Molecular Recognition in Macrocyclic Complexes
Bruce Wild (L17/Tu)
Self-Assembly of Optically Active Poly-Tertiary Phosphine Metal Helicates
- 1645 - 1800 h Forum
Teaching experimental inorganic chemistry
(Discussion: Chair - **James Beattie**, with contributions from **Peter Tregloan** and **Ron Dickson**) (L19/Tu)
- 1900 - 2200 pm Informal viewing of Posters (Group B) (Ballrooms 2/3)

Wednesday, July 3rd

- 0830 - 0930 h Plenary Lecture: Peter Tasker (PL5/W)
Ligand Design for New Metal-Recovery Processes: New Highly Selective Zinc Extractants
- 0930 - 1200 h Scientific Poster Session (Group B) (Ballrooms 2/3)
(Incl. morning tea)
- 1200 - 1330 h LUNCH (Inorganic Division - Committee meeting)

(cont.)

1330 - 1530 h	<u>Specialist Lectures: "Applications of Inorganic Chemistry"</u> Pete Williams (L18/W) <i>Coordination Chemistry in the Big Laboratory and the Search for New Ore Deposits</i> James Beattie (L2/W) <i>Electroacoustics</i> Leone Spiccia (L15/W) <i>Applications of the Sol-Gel Process</i> Stuart Carr (L6/W) <i>Science-Led Innovation in an Industrial Environment</i>	
1530 - 1600 h	AFTERNOON TEA	
1600 - 1730 h	<u>Burrows Award</u> - presentation and lecture Ian Dance (PL2/W) <i>Inner and Outer Frontiers in Inorganic Chemistry</i>	
1900 for 1930 h	Conference Banquet	(Ballroom 1)

Admission to the Conference Banquet will be by presentation of the Invitation. Dress is neat casual. The Banquet will take the form of a buffet which features local seafoods and meats - during the meal you are invited to serve yourself to as much (and as often) as you wish. As part of the cost of the Banquet, pre-dinner drinks will include spirits, beer, wine or soft drinks: during the dinner, wine, beer or soft drink will be served by the Hotel staff - should you wish anything different in the range of drinks, full bar service is available but at your own cost.

Thursday, July 4th

0830 - 0930 h	<u>Plenary Lecture: Hans Bock</u> (PL1/Th) <i>Alkali Metal Cations in Molecular Crystals: from Contact Ion Pairs to Polyanion Aggregates</i>	
0930 - 1030 h	<u>Specialist Lectures</u> Richard Robson (L14/Th) <i>Coordination Networks</i> Alan Bond (L4/Th) <i>Electrochemical and Spectroscopic Studies on Redox Active Microcrystalline Inorganic and Organometallic Compounds</i>	
1030 - 1100 h	MORNING TEA	
1100 - 1145 h	<u>Conference Lecture: Dick Puddephatt</u> (L12/Th) <i>Oxidative Addition Reactions: From Mechanisms to Dendrimers</i>	
1145 - 1300 h	Divisional AGM and Closing of Conference	

PLENARY LECTURES

ABSTRACTS

The designation **PL** indicates "Plenary Lecture", and the Abstracts are listed alphabetically according to the surname of the presenting author. The final designation **M**, **Tu**, **W** or **Th** indicates the day of presentation of the paper on the program.

ALKALI METAL CATIONS IN MOLECULAR CRYSTALS: FROM CONTACT ION PAIRS TO POLYION AGGREGATES

Hans Bock, Christian Näther, Zdenek Havlas, Claudia Arad, Camilla Bogdan, Rüdiger Dienelt, Uwe Enduschat, Katayoun Gharagozloo-Hubmann, Tim Hauck, Erik Heigel, Delia Hess, Andreas John, Norbert Nagel, and Klaus Ruppert

Department of Chemistry, University of Frankfurt, Marie Curie Str. 11, D-60439 Frankfurt/Main, Germany

Crystals contain molecules in their ground state close to the global minimum of the total energy with largely "frozen" dynamics, which provides a suitable starting point both for the discussion of essential molecular properties as well as for quantum chemical calculation. Based on preceding investigations,¹ therefore, prototype interactions have been studied in crystals such as Coulomb effects of ions, hydrogen bonding, donor/acceptor complexation or van der Waals attraction.

Cation solvation phenomena, which govern a multitude of reactions including those of geo- or biochemical importance, are exemplified by:

- The selective preparation and crystallization of solvent-shared or solvent-separated contact ion multiples of molecular anions $M^{\ominus n}$, $[M^{\ominus n}(Me^{\oplus}Solv_x)_n]$ or $[M^{\ominus n}][Me^{\oplus}Solv_{x+y}]_n$, including the first "naked" naphthalene radical anion salt, $[C_{10}H_8^{\bullet\ominus}][Na^{\oplus}(diglyme)_2]$, or the first hydrocarbon tetraanion isolated as an ion quintuple [rubrene $^{\ominus\ominus\ominus\ominus}(Na^{\oplus}(THF)_2)_4$].
- The selective sodium metal reduction of large hydrocarbons M to their anion salts with selectively solvated cations e.g. $[Na^{\oplus}(THF)_6]$, $[Na^{\oplus}(DME)_3]$, $[Na^{\oplus}(diglyme)_2]$ or $[Na^{\oplus}(2.2.1.cryptand)_1]$, which allow quantum chemical estimates of the cation solvation enthalpies based on the structures determined.
- Information from series of crystallized solvate ligand complexes on the multidimensional network of electron transfer, contact ion formation as well as solvation and aggregation in solution, activated by redox reactions.
- Information on microscopic reaction pathways as provided by quantumchemical hypersurface calculations based on experimental structures of isolated intermediates.

All of the above single crystal structural data and their evaluation provide hints and clues concerning their lattice packing and thus contribute facets to crystallization as a model for self-organization - verified by the (planned) synthesis of novel lipophilically wrapped polyanion aggregates such as

- $\{[(Ba^{\oplus\oplus})_6(Li^{\oplus})_3(O^{\ominus\ominus})_2]^{\oplus 11}(\ominus O-C_4H_9)_{11}\}$
- $\{[OP-N^{\ominus}-PONa^{\oplus}]_6(C_{144}H_{120}O_{24})\}$
- $\{[(Li^{\oplus})_6(NH_3)_2](C_{44}H_{52}O_4^{\ominus\ominus\ominus})_2\}$

reported in 1995,² and rationalized partly by density functional calculations.

1. "Distorted Molecules: Perturbation Design, Preparation and Structures", *Angew. Chem.* 1992, 104, 564-595; *Int. Ed.* 1992, 31, 550-581.
2. "A Face-Sharing (Octahedral +Prismane) $Ba_6Li_3O_2$ Polyhedron in a Hydrocarbon Ellipsoid", *Angew. Chem.* 1995, 107, 1439; *In. Ed.* 1995, 34, 1353.

INNER AND OUTER FRONTIERS IN INORGANIC CHEMISTRY

Ian Dance

School of Chemistry, University of New South Wales, Sydney 2052.

The progress we make in research depends on the perspectives we take and the questions we ask. The conventional view of an inorganic molecule has a core of metal and donor atoms surrounded by a ligand framework and/or substituents. I will adopt two different perspectives, one focussing inwards on the core, and the other on the supramolecular frontier between an inorganic molecule and its surroundings.

Unexpected and unprecedented molecules M_xE_y ($E = C, O, S, Se, Te, P$) can be synthesized and studied in the gas phase: these are *molecular* forms of binary compounds which are otherwise known only as *non-molecular* solids. I will present experimental and theoretical results for metal-sulfide and metal-carbide molecules.

Those who synthesize new compounds know that ligands like Ph_3P and $Ph_2P(CH_2)_nPPh_2$, and cations like Ph_4P^+ and $Ph_3PNPPh_3^+$, commonly yield nicely crystalline products which are often less soluble and are rarely disordered. These phenomena are due to concerted supramolecular motifs known as multiple phenyl embraces, which are appreciably more attractive than hydrogen bonds. Molecular crystals are supramolecular entities *par excellence*, yielding voluminous geometrical data (but not energy data) on supramolecular interactions. I will describe analyses of multiple phenyl embraces, in the context of supramolecular inorganic chemistry.

Both of these themes, namely bare metal sulfide clusters and through-space interactions with their surroundings, are embodied in the questions about structure and mechanism at the active site of the enzyme nitrogenase. An underligated Fe_7MoS_9 cluster core binds, activates and reduces a small molecule, N_2 , under the control of a protein environment which is mostly not bonded to the core. I will present my mechanism for the binding and activation of N_2 at the active site, and the supporting density functional calculations.

MULTIPLE ELECTRON OXIDATIONS
THOMAS J. MEYER
THE UNIVERSITY OF NORTH CAROLINA AT CHAPEL HILL
CHAPEL HILL, NC 27599-3290

By taking into account the thermodynamic and mechanistic requirements in multiple electron reactions, it is possible to design reagents to carry out difficult chemical transformations. Good examples of this design strategy exist in oxidation chemistry in the utilization of metal oxo complexes of Ru. In these complexes there is access to higher oxidation states based on oxidation and proton loss from bound aqua ligands. In polypyridyl complexes of ruthenium this has led to a versatile family of oxidants with an extensive multiple electron transfer chemistry toward a variety of inorganic and organic reductants. This includes epoxidation of olefins and oxidation of water to dioxygen. In ammine complexes oxidation and proton loss leads to intermediate nitrene or nitrodo species which are stable or can be trapped by added reductants.

ROTAXANES AND OTHER MULTIPORPHYRIN ASSEMBLIES AS MODELS OF THE PHOTOSYNTHETIC REACTION CENTRE

Jean-Pierre SAUVAGE

Laboratoire de Chimie Organo-Minérale, URA 422 CNRS,
Université Louis Pasteur, Faculté de Chimie, 4, rue Blaise Pascal,
67070 Strasbourg (France)

The ability of transition metals to assemble various chemical fragments and thus to allow construction of complex multicomponent molecular systems, has been applied in relation with electron transfer studies and photosynthesis.

Oblique bis-porphyrins containing a 1,10-phenanthroline spacer are interesting structures owing to the coordinating ability of the spacer towards transition metals. Rotaxanes consisting of a coordinating macrocyclic compound threaded by a molecular string bearing two porphyrins as stoppers have been made. The various multi-porphyrins elaborated have been studied (A. Harriman et al.). Ultra-fast intramolecular electron transfer processes have been observed in some instances.

Another interesting example of molecular systems "in action" is that of a multiply functional [2]-catenane (molecule consisting of two interlocking rings). The gliding motion of one ring within the other can be externally controlled at will by redox processes. The concept might be related to molecular hysteresis and bi-stability.

A few recent references related to the work to be discussed :

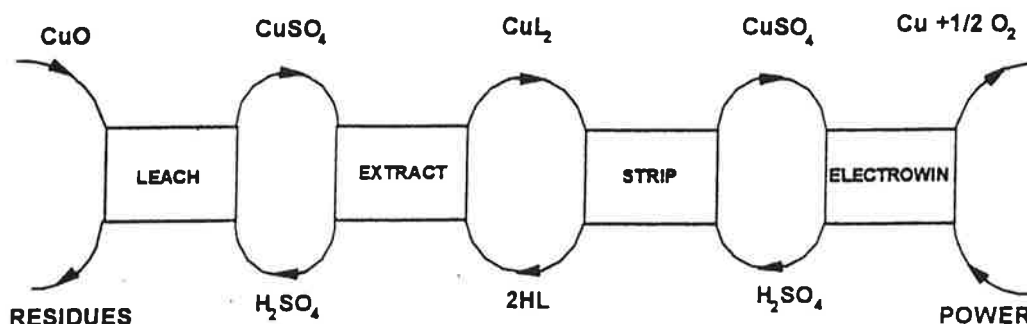
- A. Harriman, F. Odobel, J.-P. Sauvage, *J. Am. Chem. Soc.*, **116**, 5481-5482 (1994).
A. Livoreil, C.O. Dietrich-Buchecker, J.-P. Sauvage, *J. Am. Chem. Soc.*, **116**, 9399-9400 (1994).
J.-C. Chambron, C.O. Dietrich-Buchecker, V. Heitz, J.-F. Nierengarten, J.-P. Sauvage, C. Pascard, J. Guilhem, *Pure and Appl. Chem.*, **67**, 2, 233-240 (1995).

LIGAND DESIGN FOR NEW METAL-RECOVERY PROCESSES: NEW HIGHLY SELECTIVE ZINC EXTRACTANTS

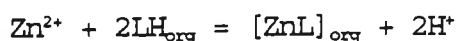
Peter A. Tasker

Department of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ and ZENECA Specialties, Research Centre, Blackley, Manchester M9 8ZS.

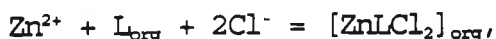
Solvent extraction is being used increasingly in primary metal recovery. The efficiency and robustness of the technology were proven initially in the nuclear industry¹ but more recently have provided the incentive for development of much larger scale operations² for copper based on the flowsheet:



This paper will consider the design of extractants for such leach/solvent extraction/electrowin circuits, focusing on the development of new reagents for zinc. Recovery of zinc from most primary and secondary sources using such a flowsheet requires a "strong" extractant which shows a very high selectivity over iron(III) in a "pH-swing" process:

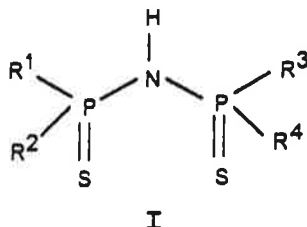


A biomimetic approach has been used to the design of the zinc extractants by incorporating imidazole-nitrogen or anionic sulfur atoms into tetrahedral donor sets. ZENECA's new extractant DS5869, based on the bisdithiophosphoramidate structure I, shows³ remarkably high selectivity for Zn(II) over Fe(III). So too do derivatives of bis-benzimidazoles in both "pH-swing" and "chloride-swing",



equilibria.

Novel approaches to the design of tetrahedral proligands and to the assembly of organised donor sets in hydrocarbon solvents will also be discussed.



1. A Chesne and M Germain, Proceedings of Intern. Solvent Extraction Conference '90, ed. T Sekine (Elsevier, 1992).
2. B Townson and K Severs, *Mining Magazine*, **162**, 26 (1990).
3. D C Cupertino, R F Dalton and B Townson, Proceedings of Intern. Solvent Extraction Conference '96, ed. D. Shallcross et al (University of Melbourne, 1996).

CONFERENCE and SPECIALIST LECTURES

ABSTRACTS

The designation **L** indicates "Lecture", and the Abstracts are listed alphabetically according to the surname of the presenting author. The final designation **M**, **Tu**, **W** or **Th** indicates the day of presentation of the paper on the program.

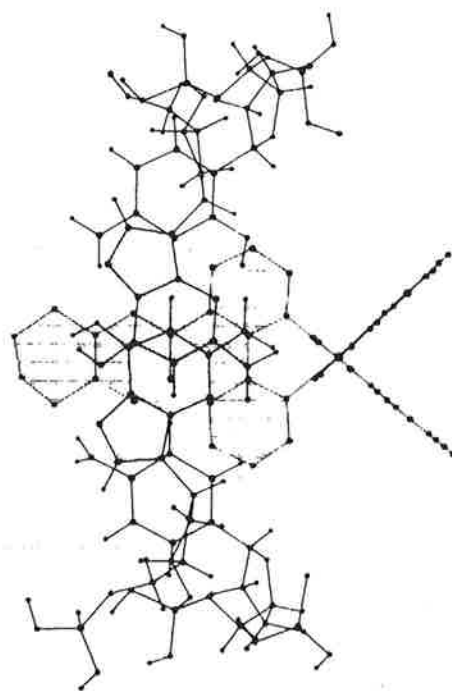
MOLECULAR DESIGN: THE SYSTEMATIC APPROACH

Janice Aldrich-Wright¹

Department of Chemistry, University of Western Sydney, New South Wales 2560, Australia

If metal complexes are intended to be have been used as probes for DNA structure and conformation, then their design and synthesis requires a systematic approach. The effect of each structural change on DNA affinity must be assessed. The interaction of these complexes with DNA can be seen as involving intercalation, overall stereochemistry (achieved by the disposition of the ancillary bidentates or a tetradentate) and site selectivity. The intercalating portion of the molecule (compounds such as dipyrido[3,2-a:2'3'-c]phenazine (*dppz*)², dipyrido[3,2-d:2'3'-f]quinoxaline (*dpq*)³, 7,8-dimethyldipyrido[3,2-a:2'3'-c]phenazine (*dppzMe*)³ and dipyrido[6,7-d:2'3'-f][6,7,8,9-tetrahydro]-phenazine (*dpqc*)⁴) needs to be of an appropriate size and shape. Adjustment of the overall shape will determine the best fit of the molecule whilst the incorporation of a base sequence-selective arm can provide specificity. Optimisation of each factor in turn is preferable as this represents a superior refinement technique. Improved DNA affinity can be then attributed to the particular fragment's function and further refinements can proceed.

We report here the results of experiments along these lines involving DNA and a series of complexes based on $[\text{Ru}(\text{X})_2(\text{L})]^{2+}$ where intercalation and overall shape parameters have been explored.



A view of $[\text{Ru}(\text{phen})_2(\text{dpqc})]^{2+}$ intercalating in the minor groove of a $\text{d}(\text{GC})_2$ DNA sequence.

1. J. Aldrich-Wright@UWS.edu.au
2. A. E. Freidman, J. Chambron, J. Sauvage, N. J. Turro and J. K. Barton., *J. Am. Chem. Soc.*, **1990**, 112, 4960.
3. J. R. Aldrich-Wright, PhD. Thesis, Macquaire University (1993)
4. I. Greguric, Hons. Thesis, UWS (1994)

James K Beattie, Alex Djerdjev, Richard W O'Brien, William N Rowlands and Theresa A Wade
School of Chemistry, University of Sydney, NSW 2006, Australia

Electroacoustics is a new technique which allows the charge and size of colloidal particles to be measured in concentrated, opaque suspensions. Electroacoustic effects arise from the interaction of alternating electric fields or of ultrasound with ions or charged colloidal particles. If a megahertz ac electric field is applied to an electrolyte solution or to a colloidal suspension, ultrasound of the same frequency is generated by the different mobilities of the cations and anions or by the distortion of the double layer around charged colloidal particles. By measurement of the magnitude and phase of the ultrasound over a range of frequencies, a dynamic mobility spectrum is obtained (the ac analogue of the electrophoretic mobility). The technology has been incorporated into a commercial scientific instrument termed the 'AcoustoSizer'.¹

Electrolytes generally give small electroacoustic effects, but a large signal is obtained from millimolar solutions of potassium 12-tungstosilicate due to the very large mass and inertia of the heteropolyanion compared to the potassium cations. All of the quantities which determine this effect can be evaluated independently, so these salt solutions provide a convenient and reliable means of calibrating the AcoustoSizer.

Electroacoustics provides a unique means of measuring the mean size and the charge of colloidal particles in concentrated suspensions of 1-40 vol%. We have been able to observe the change in the zeta potential of alumina suspensions as a polymeric polyelectrolyte is adsorbed onto the alumina particles; the effect of coating titania particles with silica or alumina or both; and the competition between phosphate and humates in adsorption on goethite, a process of environmental interest. Other studies include the effect of pH and of the rennet enzyme on the zeta potential and the average size of casein micelles in skim milk.²

1. R. W. O'Brien, D. W. Cannon and W. N. Rowlands, 'Electroacoustic Determination of Particle Size and Zeta Potential', *J. Colloid Interface Sci.*, **173**, 406 (1995).

2. T. A. Wade, J. K. Beattie, W. N. Rowlands and M. A. Augustin, 'Electroacoustic Determination of the Size and Zeta Potential of Casein Micelles in Skim Milk', *J. Dairy Res.*, in press.

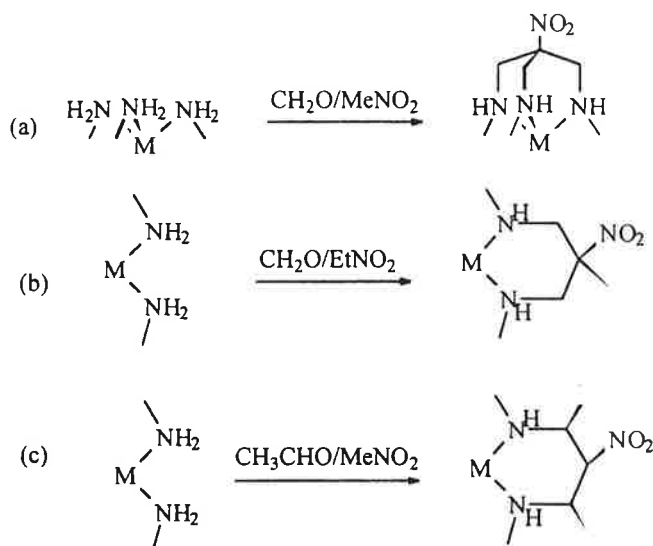
MULTIFUNCTIONAL PENDENT ARMED MACROCYCLES

Paul V. Bernhardt

Department of Chemistry, University of Queensland, Brisbane, 4072.

Metal directed condensations of coordinated primary amines with formaldehyde and nitroalkanes offer versatile and inexpensive routes toward C-functionalised macrocyclic amines. In template reactions of types (a) and (b) illustrated in the Scheme, the number of H-atoms on the 'carbon acid' that may be substituted by the intermediate methylene imine residues is limited by the degree of alkylation of the α -C-atom *i.e.* nitromethane (three) or nitroethane (two), leading to 'capped' or 'linked' nitro-substituted products, respectively.

Scheme



Linking only *two* coordinated imine residues with a *tribasic* acid, such as nitromethane (reaction (c) in the Scheme), offers the opportunity of a potentially nucleophilic centre attached to the macrocyclic ring at which further chemistry may be performed. Recent work in this group^{1,2} has revealed some rather interesting and unexpected coordination chemistry with these systems, some of which will be the subject of this presentation.

¹ P.V. Bernhardt, K.A. Byriel, C.H.L. Kennard and P.C. Sharpe, *J. Chem. Soc., Dalton Trans.*, **1996**, 145.

² P.V. Bernhardt and P.C. Sharpe, *J. Chem. Soc., Chem. Commun.*, **1996**, in press.

**ELECTROCHEMICAL AND SPECTROSCOPIC
STUDIES ON REDOX ACTIVE MICROCRYSTALLINE
INORGANIC AND ORGANOMETALLIC COMPOUNDS**

Professor Alan M Bond
Monash University
Department of Chemistry
Clayton Victoria 3168

Traditionally, voltammetric studies on inorganic compounds are undertaken in the solution phase or in some cases on thin films of material attached to an electrode surface. Recent work has demonstrated that mechanical attachment of arrays of microcrystals to carbon or metal electrodes enables solid state studies to be undertaken on insulating as well as semi-conducting solids. In this paper features related to the size and spacing of the microcrystals as well as the theory describing the solid state electron transfer, charge neutralisation and phase changes that accompany the change in oxidation states will be addressed. Examples considered will be taken from a wide range of compounds and will include cobalt coordination, transition metal carbonyl and organometallic compounds. Methods for in-situ and ex-situ monitoring of the redox state changes and structural changes based on the use of techniques such as infra red spectroscopy, electron spin resonance, the quartz crystal microbalance, electron probe and X-Ray diffraction will also be described. The important conclusion to be reached is that electrochemical studies on insulating solids can now be as routine as are solution phase studies.

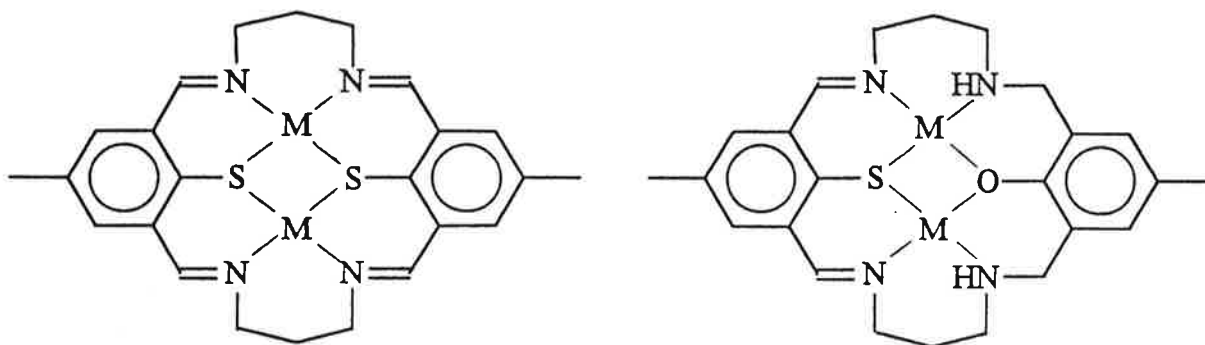
ADVANTAGES OF MACROCYCLIC THIOLATES

Sally Brooker*, Paul D. Croucher, Tony C. Davidson, Geoffrey S. Dunbar, and
Fiona M. Roxburgh

Department of Chemistry, University of Otago, PO Box 56, Dunedin, New Zealand

Research into the synthesis, structure and properties of first row transition metal complexes of thiolate-containing ligands is expected to shed light on the structure and mechanism of action of thiolate-containing metalloproteins such as Fe-S clusters, Ni-Fe hydrogenase and the Cu_A site of cytochrome c oxidase. The use of macrocyclic complexes to model a wide variety of metalloprotein active sites or to mimic their chemistry is well established. Our aim is to incorporate thiolate donors into Schiff-base macrocycles, thus allowing the formation of thiolate-bridged complexes of controlled nuclearity and avoiding the uncontrolled production of disulfides.¹ In addition to acting as model compounds, the properties of the resulting complexes are expected to provide an interesting contrast to those of complexes of the widely used phenol and pyridine "head units" which provide much harder donors.

We have prepared a range of polynucleating ligands from the exciting "head unit" S-(2,6-diformyl-4-methylphenyl)dimethylthiocarbamate (two examples are shown below).¹ The synthesis, structure and properties of a series of dizinc(II) and dinickel(II) complexes of both symmetrical and unsymmetrical Schiff-base macrocycles derived from this "head unit" will be presented. The thiolate-bridged dinickel complexes are first generation model complexes for the dinuclear Ni-Fe hydrogenase active site: until 1995 the active site was thought to be a mononickel centre so previous model complexes were largely mononuclear.



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Science-Led Innovation in an Industrial Environment

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This talk will aim to deal with the trends in the way research is being done in industry and the changes in the process of the use of scientific knowledge to lead to innovation. The first part will focus on the way industrial organisations are changing in the more competitive global markets. The second part of the talk will focus on examples from my experience where new scientific concepts have led to new products.

ELECTRON DEFICIENT COMPLEXES. THE IMPORTANCE OF METAL-L σ AND π BONDS.

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The structure of electron-deficient transition metal complexes is highly metal and ligand dependant and cannot be easily understood using classical ligand field theory. It will be shown using core-potential ab initio calculations that the M-L σ bond is central to the understanding of the structure and that M-L π bonding is of slightly lesser importance. This will be illustrated by discussing the structures of several old and recent d^0 and d^4 ML_6 complexes^{1,2}. The importance of M-L σ bonds will be also discussed in the case of some d^6 ML_5 complexes.³

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2 Gusev, D.G.; Kuhlman, R.; Sini, G.; Eisenstein, O.; Caulton, K.G. *J. Amer. Chem. Soc.* 1994, **116**, 2685. Gusev, D.G.; Kuhlman, R.; Rambo, J.R.; Berke, H; Eisenstein, O; Caulton , K.G. *J. Am. Chem. Soc.* 1995, **117**, 281.

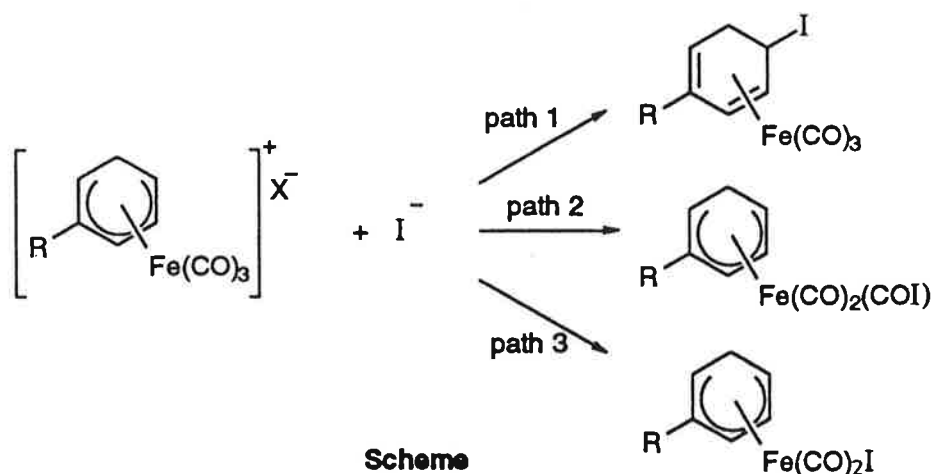
3 Jean, Y; Eisenstein, O. *Polyhedron* 1988, **7**, 405.. Rachidi, I.E.-I.; Eisenstein, O.; Jean, Y. *New J. Chem.* 1990, **14**, 671. Riehl, J.-F.; Jean, Y.; Eisenstein, O.; Pélissier, M. *Organometallics* 1992, **11**, 729 . Heyn, R. Ogazawara, M. MacGregor, S. A.; Streib, W.B. Eisenstein, O. Caulton, K.G. *Inorg. Chim. Act.* submitted.

MECHANISMS OF NUCLEOPHILIC ATTACK BY IODIDE AND HYDROXIDE IONS ON [(DIENYL)Fe(CO)₃]⁺ CATIONS

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Attack by nucleophiles on [π -hydrocarbon) M(CO)₃]⁺ complexes may in principle occur at the coordinated π -hydrocarbon, the metal, or a carbonyl ligand. In the case of the dienyl cations [(η^5 -dienyl)Fe(CO)₃]⁺ **1** (dienyl = C₆H₇, 2-MeOC₆H₆, or C₇H₉) in which the hydrocarbon ligand is relatively electrophilic, the vast majority of nucleophiles (tertiary phosphines and phosphites, amines, aromatic heterocycles, and the anions H⁻, CN⁻, CNS⁻, NCO⁻, etc) have been reported to undertake π -hydrocarbon ring addition only¹⁻³.

In a re-examination of the reaction of iodide ion with type **1** cations we have found that this provides a rare example exhibiting each of these possible pathways for nucleophilic attack, as summarised in the Scheme below. We report here detailed synthetic, spectroscopic and kinetic studies of these reactions. These reveal a strong dependence of the reaction pathway on the nature of the dienyl ligand and the solvent employed, and provide useful insights into the mechanisms involved.



We also report similar studies of the reactions of the hydroxide ion with cations **1** in water, which are also shown to involve rapid initial attack by OH⁻ on a carbonyl ligand to generate a [(η^5 -dienyl)Fe(CO)₂(COOH)] species, followed by a slower addition to the dienyl ring. These results provide the first quantitative data for the nucleophilicity of anions towards type **1** substrates.

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**RECENT ADVANCES IN MAIN GROUP AND TRANSITION METAL
ORGANOMETALLIC CHEMISTRY.
APPLICATION TO NEW MATERIALS**

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Our current research interests are centered on the application of organometallic and inorganic chemistry to the preparation of new materials. Specifically our recent work leading towards the preparation of organometallic polymers of the type known as rigid-rod polymers, illustrated, below will be developed;



In addition our work towards new single source precursors for the deposition of thin films of compound binary semiconductors, insulators and conductors will also be discussed. Initially this has involved the preparation and characterisation of a number of heavy alkali metal phosphides, arsenides and stibides. The formation of group 13-15 materials from these is facile and involves the preparation of new main group compounds whose decomposition characteristics will be investigated for utility in Chemical Vapour Deposition (CVD).

ASPECTS OF MOLECULAR RECOGNITION IN MACROCYCLIC COMPLEXES

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Molecular recognition may be broadly described as a process whereby highly specific intra- and intermolecular interactions occur as a consequence of stereochemical and other molecular compatibilities. Macrocyclic complexes often exhibit intra- and intermolecular recognition as are respectively exemplified by the eight coordinate sodium(I) pendant arm macrocyclic complex¹ in which an achiral ligand assumes a chiral configuration (Fig 1a), and the ternary metallocyclodextrin² in which enantioselective complexation of the tryptophan anion occurs (Fig 1b). These and related systems will be used to illustrate some equilibrium, kinetic and structural aspects of molecular recognition in macrocyclic complexes.

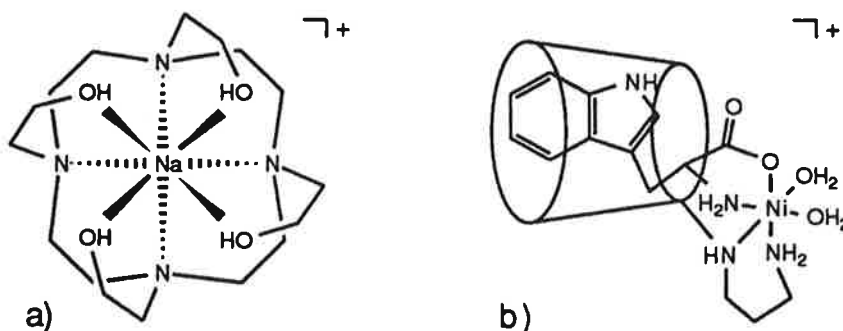


Fig. 1. Stylised representations of a) 1,4,7,10-Tetrakis(2-hydroxyethyl)-1,4,7,10-tetraazacyclododecanesodium(I). b) A ternary complex of 6A-(3-aminopropyl-amino)-6A-deoxy- β -cyclodextrinnickel(II) and a histidine anion. The truncated cone represents the annulus of β -cyclodextrin.

- ¹ R. Dhillon, A.K.W. Stephens, S.L. Whitbread, S.F. Lincoln and K.P. Wainwright, *J. Chem. Soc., Chem. Commun*, 1995, 97-98.
- ² S.E. Brown, J.H. Coates, C.J. Easton and S.F. Lincoln, *J. Chem. Soc., Faraday Trans.*, 1994, 90, 739-743.

Modelling Metalloenzymes - Structures and Strategies

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The relationship between the structural and electronic contributions to metal ion selectivity and specificity of metalloenzymes continues to remain elusive. Metal complexes containing highly symmetrical coordination motifs have been used successfully to model oxygen binding^{1,2} and other small molecule reactions of biochemical interest. However, the corresponding asymmetric model compounds have proven to be synthetically difficult to prepare, even though these structurally asymmetric centres are found to be quite ubiquitous as the active sites of many metalloenzymes.

The focus for this talk is to present our strategies for the design, synthesis, structural and 'sporting method' characterisation of mono-, bi-, and tri- nuclear complexes that contain dissimilar asymmetric coordination sites about the metal ions^{3,4,5}. The structural and electronic features of these new complexes will be discussed and their role as more relevant models for specific metalloenzymes outlined^{6,7}.

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OXIDATIVE ADDITION REACTIONS: FROM MECHANISMS TO DENDRIMERS

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Oxidative addition reactions to organoplatinum(II) complexes are of current interest because a wide range of functional groups can participate and because many of the reactions are suited to mechanistic study.

This paper will present details of recent mechanistic studies on the reversible oxidative addition of protonic acids and of organotin and organosilicon halides to dimethylplatinum(II) complexes and of subsequent reductive elimination reactions. Some of these reactions are easily reversible and some are also extremely fast, thus allowing new ways of studying the mechanisms. The first μ -hydridodiplatinum(IV) complexes, which also contain methylplatinum groups, are shown to be unusually stable with respect to reductive elimination of methane.

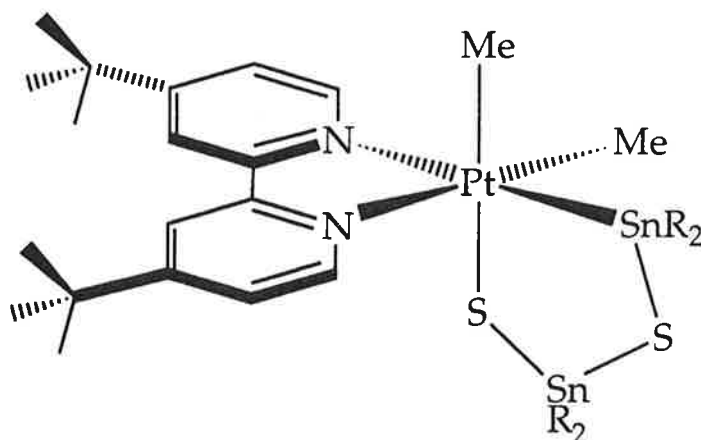
The use of oxidative addition of alkyl halides as a key step in the synthesis of new types of organometallic oligomers, polymers and dendrimers will also be described.

LUMINESCENT ORGANOPLATINUM(IV)-TIN METALLACYCLES BY OXIDATIVE ADDITION

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In the first examples of oxidative addition of Sn-S bonds to a transition metal complex, the trimeric ring compounds $(R_2SnS)_3$ ($R = Me, Ph$) react with the electron-rich organoplatinum(II) precursor $[PtMe_2(^tBu_2bpy)]$ ($^tBu_2bpy = 4,4'$ -di-*tert*-butyl-2,2'-bipyridine) to give new, luminescent organoplatinum(IV)-tin metallacycles. As shown by multinuclear (1H , ^{119}Sn , and ^{195}Pt) NMR spectroscopy and by X-ray crystallography, the products contain the new 5-membered $PtSnSSnS$ ring, thus using only two of the R_2SnS units present in $(R_2SnS)_3$. The complexes show reactivity toward electrophilic reagents and also undergo interesting redistribution reactions.



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COORDINATION NETWORKS

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A number of coordination polymers derived from ligands with a range of connectivities and geometries will be described. In some cases the infinite networks so formed generate solvent-filled cavities and channels of large dimensions whilst in others the channels formed within one network are occupied by one or more independent but interpenetrating networks. In a third structural type two infinite networks interpenetrate to generate completely sealed off chambers of unprecedented size, capable of imprisoning of the order of twenty molecules of solvent.

APPLICATIONS OF THE SOL-GEL PROCESS

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The Sol-Gel Process is an extremely versatile method for preparing metal oxide based materials. The wide applicability of the process arises from the enormous range of inorganic and metal-organic precursors which can be used as well as the ability to incorporate organic, inorganic and biological molecules with specific functions into the products. In addition, sol-gel products can be obtained in the form of powders, as moulded pieces (monoliths), fibres or thin films. The general principles of the sol-gel process will be described concentrating primarily on the "organic route", which uses readily hydrolysable metal alkoxides. Such compounds are formed by all metallic elements thus giving enormous potential for the formation of wide variety of oxide based materials.

The lecture will also describe some of our recent work on: (i) the sol-gel deposition of vanadium and tungsten oxide thin films for application in electrochromic devices; (ii) the development of tinted, transparent solar cells which utilise Ru(II) dye sensitised titania semiconductor layers to convert light into electrical energy; and (iii) the preparation of silicon based aerogels by supercritical drying of gels. Aerogels are very high surface area (250 - 1500 m²/g) ceramic foams which have found application as Cerenkov detectors but have great potential for application in many other areas. Of particular interest is the ability of aerogels to absorb up to 100% by weight of pollutant gases from vehicles, power plants and other industrial processes and the doping of aerogels with suitable transition metal oxides so that they can be used in the catalytic conversion of pollutant gases. Our recent investigations of silica-vanadium oxide aerogels will be described.

HYDROXYALKYLATION OF MACROCYCLIC LIGANDS AS A TECHNIQUE FOR ENHANCING COMPLEX LABILITY

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Observation by Hancock *et al.*,¹ in 1984, of the enhanced rate of metal ion ingress into tetraaza macrocycles that can be induced by pendant 2-hydroxyethyl groups provided evidence, perhaps for the first time, of a useful perturbation to the chemistry of macrocyclic systems that could be made by the addition of pendant donors. Many questions concerning the precise role of the pendant arms in the process of complex formation and stabilisation, however, were left unanswered. This talk will address some of the findings that have been made, in our group, both on free macrocycles and on their complexes, which help to clarify this situation. In particular, considerable circumstantial evidence is now building for pre-coordination of the metal by the pendant donors as the origin of the rate enhancement. The lowering of the formation constants for the complex, in comparison with an equivalent complex lacking the hydroxyl groups, can be explained in terms of preorganisation of the ligand against coordination through internal hydrogen bonding, and the lability of the hydroxyethyl donors can be seen in a variety of dynamic processes which have been observed by variable temperature NMR studies.

1. C.M. Madeyski, J.P. Michael and R.D. Hancock, *Inorg. Chem.*, 1984, **23**, 1487.

SELF-ASSEMBLY OF OPTICALLY ACTIVE POLY-TERTIARY PHOSPHINE METAL HELICATES

S. Bruce Wild

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The enantiomers of the linear C_2 -tetra(tertiary phosphine) (R^*,R^*)-(\pm)-1,1,4,7,10,10-hexaphenyl-1,4,7,10-tetraphosphadecane spontaneously self-assemble into homochiral 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 dinuclear 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, whereas crystals of the analogous gold complex contain only the C_2 -side-by-side helix and associated anions. The enantiomers of the tetra(tertiary phosphine) can be individually converted in high yield with retention of configuration at the inner-phosphorus stereocentres into the diastereomers of the corresponding homologous hexa(tertiary phosphine). The three optically active diastereomers of the hexa(tertiary phosphine) have been quantitatively separated by preparative HPLC as their hexa-borane adducts. Following removal of borane in each case, the homochiral [R -(R^*,R^*,R^*,R^*)] and [S -(R^*,S^*,S^*,R^*)] diastereomers of the hexa(tertiary phosphine) have been used for the synthesis of double-stranded trinuclear metal helicates.

¹ A L. Airey, G F Swiegers, A C Willis and S B Wild, *J. Chem. Soc., Chem. Commun.*, 1995, 693, 695.

**COORDINATION CHEMISTRY IN THE BIG LABORATORY
AND THE SEARCH FOR NEW ORE DEPOSITS**

Peter A Williams

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Exploration geochemistry aims to discover new orebodies by detecting the dispersion of elements from them. In the supergene environment, dispersion of metals from oxidising sulfide orebodies involves the complex coordination chemistry of naturally occurring ligands in groundwaters. The "chemical signature" of an orebody expressed in terms of the distribution of species in solution depends in turn on the kinds of secondary minerals formed in the oxidized zone. A number of studies have explored these relationships, involving base metal ores at Girilambone, NSW, Cloncurry and Chillagoe, Qld. Inorganic solution chemistry can point directly to the phases responsible for controlling dispersion of metals in groundwaters. For copper, these are basic phosphates and carbonates such as malachite, $\text{Cu}_2\text{CO}_3(\text{OH})_2$, azurite, $\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$, libethenite, $\text{Cu}_2\text{PO}_4(\text{OH})$, pseudomalachite, $\text{Cu}_5(\text{PO}_4)_2(\text{OH})_4$, and cornetite, $\text{Cu}_3\text{PO}_4(\text{OH})_3$. For lead, a more complex suite including carbonates, sulfates tungstates and molybdates is involved (cerussite, PbCO_3 , anglesite, PbSO_4 , stolzite, PbWO_4 , and wulfenite, PbMoO_4). Rarer species formed during previous cycles of oxidation exert little influence on metal buffering between solid state and solution.

FORUM:

*Laboratory Courses in Inorganic Chemistry.
Distilling Purer/Better/Louder or Just More Bang for the Buck!*

At IC'94 in Perth, the Division resolved to include some discussion related to the teaching of Inorganic Chemistry in each Conference Program. Following our meeting with the Education Division as part of 10NC, a prototype WWW database on general and inorganic chemistry courses has been set up (<http://www.chemistry.unimelb.edu.au/RACI/InorgCrsProj.html>). Links to and from other campuses are now invited.

At IC'96, the focus will be on laboratory training and practice. There are some tensions we are all having to resolve in providing modern and effective laboratory courses -

- Experiments are the heart of chemistry.
- Laboratories are expensive to run.
- Chemistry is potentially dangerous.
- Students seem to know less than they did.

James Beattie, Ron Dickson and Peter Tregloan have agreed to lead a discussion about directions, changes, innovations and experiences in inorganic laboratory courses.

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