

JOURNAL OF THE CHEMICAL SOCIETY

Dalton Transactions

Inorganic Chemistry

including bioinorganic, organometallic and solid-state chemistry

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Papers

- 3635 **Ramaswamy Murugavel,
Setharampattu S.
Krishnamurthy and
Munirathinam Nethaji**

When does a nitrogen attached to a λ^3 -phosphorus assume a pyramidal geometry? Crystal structures of Group 6 metal carbonyl complexes of isomeric forms of λ^3 -cyclotriphosphazanes

The complexes $[\text{Mo}(\text{CO})_4(\text{L}^1)]$ $\{\text{L}^1 = \text{trans}[\text{EtNP}(\text{OC}_6\text{H}_3\text{Me}_2-2,6)]_3\}$ and $[\{\text{Mo}(\text{CO})_4(\mu\text{-L}^2)\}_2]$ $\{\text{L}^2 = \text{cis}[\text{EtNP}(\text{OCH}_2\text{CF}_3)]_3\}$ represent the first organometallic transition-metal derivatives of λ^3 -cyclotriphosphazanes and reveal the different co-ordination behaviour of the *cis* and *trans* isomeric forms of this type of ligand. A pyramidal geometry is observed around one of the nitrogen atoms of the P_3N_3 ring in the former complex which is unprecedented among λ^3 -phosphazanes.

- 3641 **Richard G. Compton, Roula
Barghout, John C. Eklund,
Adrian C. Fisher, Stephen G.
Davies, Michael R. Metzler,
Alan M. Bond, Ray Colton and
Jacky N. Walter**

Photoelectrochemistry of some organochromium carbonyl compounds

Dual photo- and electro-chemical activation of three different organochromium carbonyl species is reported. In the case of $[\text{Cr}(\text{CO})_6]$ and $[\text{Cr}(\text{CO})_3(\eta^6\text{-C}_6\text{Et}_6)]$ electron transfer to the electrode follows photoactivation; photosubstitution in the former, and photofragmentation in the latter modifies the pathway of the electrode reaction. For *trans*- $[\text{Cr}(\text{CO})_2(\text{dppe})_2]^+$ [*dppe* = 1,2-bis(diphenylphosphino)ethane] photochemical reaction is seen only after electro-oxidation and is demonstrated to lead to a disproportionation reaction.

- 3647 **Koji Araki, Takashi Kuboki,
Makihiro Otohata, Nobuyuki
Kishimoto, Masaki Yamada and
Shinsaku Shiraishi**

Dioxygen adducts of cobalt(II) complexes of 6,6'-bis(*p*-substituted benzoylamino)-2,2'-bipyridines and their catalytic activities in oxygenation of 2,6-di-*tert*-butylphenol

The properties of monomeric $\text{Co}^{\text{III}}(\text{O}_2^-)$ -type oxygen adducts $[\text{CoL}(\text{B})(\text{O}_2)]$ [H_2L = 6,6'-bis(benzoylamino)-2,2'-bipyridine and its 4-methyl-, -*tert*-butyl- or -chloro-benzoylamino analogues; *B* = axial base] are studied, and their catalytic activities in oxygenation of 2,6-di-*tert*-butylphenol to the corresponding quinone are discussed.

- 3653 **Sarath D. Perera, Bernard L.
Shaw and Mark Thornton-Pett**

Reactions of an azine diphosphine with platinum(II) and palladium(II) and the formation of a novel heterocyclic diphosphine ligand. Crystal structure of $[\text{PdI}_2\{\text{PPh}_2\text{CH}=\text{C}(\text{Bu}^t)\text{N}=\text{N}=\text{C}(\text{Bu}^t)\text{CH}_2\text{PPh}_2\}]$

The azine diphosphine $Z,Z\text{-PPh}_2\text{CH}_2\text{C}(\text{Bu}^t)=\text{N}=\text{N}=\text{C}(\text{Bu}^t)\text{CH}_2\text{PPh}_2$ reacts with *trans*- $[\text{PtCl}_2(\text{NCMe})_2]$ to give the hexanuclear species *trans*- $[\{\text{PtCl}_2[\text{PPh}_2\text{CH}_2\text{C}(\text{Bu}^t)=\text{N}=\text{N}=\text{C}(\text{Bu}^t)\text{CH}_2\text{PPh}_2]\}_6]$ with a 54-atom ring or with $[\text{PtX}_2(\text{cod})]$ (*cod* = cycloocta-1,5-diene) to give nine-membered ring chelates (*X* = Me or Cl) involving the *E,Z*-diphosphine. Tridentate salts, $[\text{MCl}\{\text{PPh}_2\text{CH}_2\text{C}(\text{Bu}^t)=\text{N}=\text{N}=\text{C}(\text{Bu}^t)\text{CH}_2\text{PPh}_2\}]^+$ (*M* = Pd or Pt) are also obtained which on heating lose benzene to give novel heterocyclic diphosphine-metal complexes $[\text{MCl}_2\{\text{PPh}_2\text{CH}=\text{C}(\text{Bu}^t)\text{N}=\text{N}=\text{C}(\text{Bu}^t)\text{CH}_2\text{PPh}_2\}]$.

- 3661 **Vincenzo G. Albano, Luigi Busetto, Carlo Castellari, Magda Monari, Antonio Palazzi and Valerio Zanutti**
- Electrophilically promoted cyanide abstraction in diiron cyano(amino)-alkylidene complexes: molecular structure of $[\text{Fe}_2(\text{CO})_2(\eta\text{-C}_5\text{H}_5)_2(\mu\text{-CO})\{\mu\text{-CN}(\text{CH}_2)_4\text{CH}_2\}][(\text{OC})_5\text{WCNW}(\text{CO})_5]$**
- The electrophiles H^+ , Me^+ and $[\text{W}(\text{CO})_5]$ abstract the CN group from $[\text{Fe}_2(\text{CO})_2(\text{cp})_2(\mu\text{-CO})\{\mu\text{-C}(\text{CN})(\text{NR}_2)\}]$ ($\text{cp} = \eta\text{-C}_5\text{H}_5$) with formation of the cation $[\text{Fe}_2(\text{CO})_2(\text{cp})_2(\mu\text{-CO})(\mu\text{-CNR}_2)]^+$. In the case of $[\text{W}(\text{CO})_5]$ the cyanide is trapped in the anion $[(\text{OC})_5\text{WCNW}(\text{CO})_5]^-$. The crystal structure of $[\text{Fe}_2(\text{CO})_2(\text{cp})_2(\mu\text{-CO})\{\mu\text{-CN}(\text{CH}_2)_4\text{CH}_2\}][(\text{OC})_5\text{WCNW}(\text{CO})_5]$ reveals the presence of well defined and ordered cations and anions.
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- 3667 **Yasuo Izumi, Teiji Chihara, Hiroshi Yamazaki and Yasuhiro Iwasawa**
- Selective carbonyl insertion and ethene hydroformylation on a $[\text{Ru}_6\text{C}(\text{CO})_{16}\text{Me}]^- \text{SiO}_2$ catalyst**
- Stoichiometric acetaldehyde formation and catalytic ethene hydroformylation are investigated on the cluster $[\text{Ru}_6\text{C}(\text{CO})_{16}\text{Me}]^-$ supported on SiO_2 . This supported cluster is selective for both stoichiometric and catalytic reactions and its metal framework remains intact. A reaction mechanism for ethene hydroformylation is proposed.
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- 3675 **Michiel Heijden, Paul M. van Vliet, Jaap G. Haasnoot and Jan Reedijk**
- Synthesis and characterization of *cis*-(2,2'-bipyridine)(2,2'-biquinoline)-dichlororuthenium(II) and its co-ordination chemistry with imidazole derivatives**
- The synthesis, characterization and reactions with imidazole derivatives of *cis*- $[\text{Ru}(\text{bipy})(\text{bquin})\text{Cl}_2]$ ($\text{bipy} = 2,2'\text{-bipyridine}$, $\text{bquin} = 2,2'\text{-biquinoline}$) are studied by ^1H NMR spectroscopy and electrochemistry. It is shown that substitution of the first chloride ligand only takes place *trans* to the bquin ligand.
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- 3681 **Manabu Nakahanada, Kazuhito Ino and Sumio Kaizaki**
- Synthesis and characterization of novel binuclear chromium(III) complexes bridged by aromatic heterocyclic compounds**
- Two novel types of binuclear bis(acetylacetonato)chromium(III) complexes bridged by dicarboxylate derivatives of five-membered aromatic nitrogen heterocyclic compounds are prepared and their spectroscopic and magnetic properties studied by means of luminescence, ^2H NMR and magnetic susceptibility measurements.
-
- 3685 **Roberto Cortés, M. Karmele Urtiaga, Luis Lezama, Jose Ignacio R. Larramendi, M. Isabel Arriortua and Teófilo Rojo**
- Synthetic strategy, magnetic and spectroscopic properties of the terpyridine complexes $[\text{Cu}(\text{terpy})\text{X}(\text{H}_2\text{O})_n]\text{Y}$ ($\text{X} = \text{NCO}$, NCS or N_3 ; $n = 0$ or 1 ; $\text{Y} = \text{NO}_3$ or PF_6). Crystal structures of the azidenitrate and azidehexafluorophosphate**
- A synthetic strategy to yield one-dimensional copper(II) systems with pseudohalide ligands, having the formula $[\text{Cu}(\text{terpy})\text{X}(\text{H}_2\text{O})_n]\text{Y}$ ($\text{X} = \text{NCO}$, NCS or N_3 ; $n = 0$ or 1 ; $\text{Y} = \text{NO}_3$ or PF_6 ; $\text{terpy} = 2,2':6',2''\text{-terpyridine}$) is developed. Their spectroscopic and magnetic properties are studied. The extremely weak exchange interactions of the nitrate complexes allow the observation of singlet-to-triplet transitions in the EPR spectra, and the magnetic interaction mechanisms are analysed. Crystal structures of the azidenitrate and azidehexafluorophosphate compounds ($n = 1$) are reported.
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- 3695 **Christopher J. Pickett, Karl S. Ryder and Jean-Claude Moutet**
- Iron-sulfur clusters in ionic polymers on electrodes**
- The methodology for construction of electrodes possessing iron-sulfur clusters confined within cationic polymer films and their characterisation by reflectance FTIR, EPR and electrochemical techniques are described. It is observed that (i) stoichiometries of the cluster-modified polymer electrodes are self regulated; (ii) electrostatic (ion-pairing) effects shift the redox potentials of confined clusters to values positive of those observed in solution; and (iii) charge propagation within the polymer film is enhanced by an electron-hopping mechanism for the $[\text{Fe}_4\text{S}_4(\text{SR})_4]^{2-/-3-}$ couples ($\text{R} = \text{alkyl}$ or aryl) whereas for the $[\text{Fe}_4\text{S}_4(\text{SR})_4]^{3-/-4-}$ system electron self exchange is relatively slow and physical diffusion controls the rate of charge transfer through the film.

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- 3705 **Edwina C. H. Ling, Gregory W. Allen and Trevor W. Hambley**
The preparation and characterisation of some aminesulfoxidedichloro-platinum(II) complexes
 A series of complexes, $[\text{Pt}\{\text{MeS}(\text{O})\text{CH}_2\text{CH}_2\text{NH}_2\}\text{Cl}_2]$ and (2*S*,*SR*)- and (2*S*,*SS*)- $[\text{Pt}\{\text{MeS}(\text{O})\text{CH}_2\text{CH}_2\text{CH}(\text{CO}_2\text{Me})\text{NH}_2\}\text{Cl}_2]$, designed to bind to GpA sequences of DNA are prepared and characterised. The crystal structures of the complexes show that unlike analogous thioether groups the sulfoxide group does not exert any significant *trans* influence. Molecular mechanics modelling of these complexes is carried out in order to develop a force field for aminesulfoxide complexes of Pt^{II} which could be used in the modelling of interactions of such complexes with DNA.
- 3711 **Robert J. Deeth**
The *trans* influence in $[\text{Rh}(\text{PH}_3)_3\text{Cl}]$: a density functional theory study
 Optimised structures for $[\text{Rh}(\text{PH}_3)_3\text{Cl}]$ using density functional theory (DFT) are in better agreement with experiment than those from other *ab initio* studies; DFT continues to demonstrate useful accuracy in a reasonable time for transition-metal species
- 3715 **Kazuaki Yamanari, Yoshinori Kushi, Masahiro Yamamoto, Akira Fuyuhiko, Sumio Kaizaki, Tatsuya Kawamoto and Yoshihiko Kushi**
Photochemical synthesis and crystal structures of tetrakis(ethane-1,2-diamine)dichloro(III) complexes bridged by 1,3,5-triazine-2,4,6-trithionate and 4-oxo-1,3,5-triazine-2,6-dithionate
 Photochemical preparation of $[\{\text{Co}(\text{en})_2\}_2(\mu\text{-ttcy})]^{3+}$ [en = ethane-1,2-diamine, ttcy = 1,3,5-triazine-2,4,6-trithionate(3-)] leads to the formation of two types of dinuclear complexes bridged by either ttcy or 4-oxo-1,3,5-triazine-2,6-dithionate(3-) (dtcy) which is formed *via* desulfurization of ttcy .
- 3723 **Samiran Mahapatra, Ray J. Butcher and Rabindranath Mukherjee**
Observation of the longest Fe–N(pyridine) bond in an $\text{Fe}^{\text{II}}\text{N}_6$ chromophore. Crystal structure and ^1H nuclear magnetic resonance studies of $[\text{FeL}_2][\text{ClO}_4]_2$ [L^2 = 2-(3,5-dimethylpyrazol-1-ylmethyl)-6-(pyrazol-1-ylmethyl)pyridine]
 A unique high-spin ($S = 2$) bis(ligand) iron(II) complex of the tridentate heterocyclic ligand 2-(3,5-dimethylpyrazol-1-ylmethyl)-6-(pyrazol-1-ylmethyl)-pyridine is structurally characterized. A fairly distorted metal co-ordination geometry reveals two very long Fe–N(pyridine) bonds. NMR studies show that the solid-state geometry is retained in CD_3CN solution.
- 3727 **Alexander J. Blake, Paul E. Y. Milne and Richard E. P. Winpenny**
Solvent control of structural type: three different structures from the reaction of a dimeric copper complex with lanthanum nitrate in three different solvents
 The crystallographically characterised product from the reaction of $[\text{Cu}_2\text{L}_4]$ (where HL = 6-chloro-2-pyridone) with hydrated lanthanum nitrate depends on the solvent used. In methanol– CH_2Cl_2 a compound with a Cu_3La core is formed with methoxide and methanol moieties involved in the structure. In contrast in ethanol– CH_2Cl_2 and acetonitrile– CH_2Cl_2 compounds result in which solvent molecules play little part, and which have Cu_3La and Cu_2La_2 cores respectively. The crystal structures of the three compounds $[\text{Cu}_3\text{LaL}_5(\text{NO}_3)_3(\text{OMe})(\text{MeOH})_2] \cdot 1.5\text{MeOH} \cdot 0.5\text{Et}_2\text{O}$, $[\text{Cu}_3\text{LaL}_8(\text{NO}_3)(\text{EtOH})] \cdot 0.5\text{Et}_2\text{O}$ and $[\text{Cu}_2\text{La}_2\text{L}_8(\text{HL})_2(\text{NO}_3)_2] \cdot 2\text{HL} \cdot 2\text{MeCN}$ are determined.
- 3735 **Anthony M. Cartner, John Fawcett, William Henderson, Raymond D. W. Kemmitt, Peter McKenna and David R. Russell**
Syntheses of the cyclic platinum(II) thiolate complexes $[\text{Pt}\{\text{SCH}_2\text{C}(\text{O})\text{CH}_2\}(\text{PPh}_3)_2]$ and $[\{\text{Pt}\{\text{SCH}_2\text{C}(\text{O})\text{CH}_2\}(\text{PPh}_3)_2\}]_2$
 The synthesis of the cyclic platinum(II) thiolate complex $[\text{Pt}\{\text{SCH}_2\text{C}(\text{O})\text{CH}_2\}(\text{PPh}_3)_2]$ is accomplished by oxidative addition of 1,3-dichloroacetone to $[\text{Pt}(\eta^2\text{-RCH=CHR})(\text{PPh}_3)_2]$ ($\text{R} = \text{H}$ or Ph) and treatment of the resulting chloroacetyl complex *cis*- $[\text{PtCl}\{\text{CH}_2\text{C}(\text{O})\text{CH}_2\text{Cl}\}(\text{PPh}_3)_2]$ with sodium sulfide. Ligand displacement reactions of the complex are described. Reaction of $[\text{Pt}\{\text{SCH}_2\text{C}(\text{O})\text{CH}_2\}(\text{PPh}_3)_2]$ with $[\text{Rh}_2(\mu\text{-Cl})_2(\text{CO})_4]$ affords the dimeric complex $[\{\text{Pt}\{\text{SCH}_2\text{C}(\text{O})\text{CH}_2\}(\text{PPh}_3)_2\}]_2$ which is characterised by a single-crystal X-ray diffraction study.

- 3741 **Gion Calzaferri, Roman Imhof and Karl W. Törnroos**
● **Synthesis and crystal structure of $[\text{Co}(\text{CO})_4(\text{H}_7\text{Si}_8\text{O}_{12})]$. A new type of monosubstituted octanuclear silasesquioxane with a silicon–cobalt bond**
- A new octanuclear silasesquioxane of the type $\text{RH}_7\text{Si}_8\text{O}_{12}$ [$\text{R} = \text{Co}(\text{CO})_4$] with a silicon–cobalt bond is prepared and analysed by ^1H , ^{13}C , ^{29}Si NMR and IR spectroscopies, mass spectrometry and microanalysis. The crystal structure is determined and compared with the structures of $\text{H}_8\text{Si}_8\text{O}_{12}$, $[\text{Co}(\text{CO})_4(\text{SiCl}_3)]$ and $[\text{Co}(\text{CO})_4(\text{SiF}_3)]$. The electronic structure is investigated by extended-Hückel molecular orbital calculations.
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- 3749 **John S. Field, Raymond J. Haines, Jörg Sundermeyer and Stephen F. Woollam**
● **Variable co-ordination behaviour of ethyne and other alkynes towards the diruthenium complexes $[\text{Ru}_2(\mu\text{-CO})_4\{(\text{RO})_2\text{PN}(\text{Et})\text{P}(\text{OR})_2\}_2]$ and $[\text{Ru}_2(\mu_{\text{sb}}\text{-CO})_2(\text{CO})_2\{(\text{RO})_2\text{PN}(\text{Et})\text{P}(\text{OR})_2\}_2]$ (sb = semi-bridging, $\text{R} = \text{Me}$ or Pr^i)**
- The reactions of $[\text{Ru}_2(\mu\text{-CO})(\text{CO})_4\{(\text{RO})_2\text{PN}(\text{Et})\text{P}(\text{OR})_2\}_2]$ and $[\text{Ru}_2(\mu_{\text{sb}}\text{-CO})_2(\text{CO})_2\{(\text{RO})_2\text{PN}(\text{Et})\text{P}(\text{OR})_2\}_2]$ ($\text{R} = \text{Me}$ or Pr^i , sb = semi-bridging) with a range of terminal and internal alkynes is investigated and found to afford vinylidene-bridged $[\text{Ru}_2(\mu\text{-}\sigma\text{-C}=\text{CHR}')(\text{CO})_4\{(\text{RO})_2\text{PN}(\text{Et})\text{P}(\text{OR})_2\}_2]$ ($\text{R}' = \text{H}$, Me , Ph or CO_2Me) and/or alkenediyl-bridged products $[\text{Ru}_2(\mu\text{-}\sigma^2\text{-R}'\text{C}=\text{CR}'')(\text{CO})_4\{(\text{RO})_2\text{PN}(\text{Et})\text{P}(\text{OR})_2\}_2]$ ($\text{R}' = \text{H}$, Me or CO_2Me , $\text{R}'' = \text{H}$; $\text{R}' = \text{R}'' = \text{CO}_2\text{Me}$) with the relative yields of the two products in each reaction being dependent on the identity of the alkyne and the diphosphazane ligand employed. Possible mechanisms for the formation of the two types of products are described as is the crystal structure of $[\text{Ru}_2(\mu\text{-}\sigma^2\text{-HC}=\text{CH})(\text{CO})_4\{(\text{MeO})_2\text{PN}(\text{Et})\text{P}(\text{OMe})_2\}_2]$.
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- 3759 **Angela Rosa, Giampaolo Ricciardi, Marzio Rosi, Antonio Sgamellotti and Carlo Floriani**
● **The σ - and π -bonding modes of a tetraanionic porphyrinogen ligand in zirconium(IV) complexes: a theoretical investigation**
- A density-functional study of the bonding modes of the porphyrinogen ligand L^{4-} ($\text{H}_4\text{L} = 5,10,15,20,22,24$ -hexahydroporphyrin), with the metal ion Zr^{4+} in the limiting coordinations $\eta^5, \sigma, \eta^5, \sigma$ and $\sigma, \sigma, \sigma, \sigma$ shows that in both co-ordination modes σ bonding is by far the most dominant. Largely because of the stronger π -bond interaction, the $\eta^5, \sigma, \eta^5, \sigma\text{-}[\text{ZrL}]$ complex is more stable, but only by 2.1 eV, which makes the interconversion between the two configurations a relatively easy process. The most stable co-ordination mode is preserved after interaction of the substrate with the Lewis bases tetrahydrofuran or H^- .
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- 3767 **Richard Busby, Michael B. Hursthouse, Penelope S. Jarrett, Christian W. Lehmann, K. M. Abdul Malik and Coral Phillips**
● **Dimorphs of $[1,2\text{-bis}(\text{diphenylphosphino})\text{ethane}]\text{dichloronickel(II)}$**
- The crystal and molecular structure of form A of $[\text{Ni}(\text{dppe})\text{Cl}_2]$ [$\text{dppe} = 1,2\text{-bis}(\text{diphenylphosphino})\text{ethane}$] is described and compared with that of form B. The two forms have the same chelate-ring conformation but differ in the orientations of the phenyl rings, which is the source of the lower symmetry of form A. Solid-state ^{31}P NMR is better than IR spectroscopy for distinguishing between the forms.
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- 3771 **Athinoula L. Petrou**
● **Kinetics and mechanism of the reaction between chromium(II) and 1,2-bis(2-pyridyl)ethylene in acidic aqueous solutions**
- The reaction between $\text{Cr}^{2+}(\text{aq})$ and 1,2-bis(2-pyridyl)ethylene in acidic aqueous solutions leads to $\text{Cr}^{3+}(\text{aq})$ and 1,2-bis(2-pyridyl)ethane through the formation of a σ -bonded organochromium complex. The results are discussed in terms of the nature of the substrate's lowest unoccupied molecular orbital which is ethylenic.
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- 3777 **Kiyoshi Sawada, Toshihiko Miyagawa, Tomoko Sakaguchi and Kunio Doi**
● **Structure and thermodynamic properties of aminopolyposphonate complexes of the alkaline-earth metal ions**
- Thermodynamic parameters of formation and protonation of nitrilotris-(methylenephosphonato) and ethylenediaminetetrakis(methylenephosphonato) complexes of alkaline-earth metal ions are determined by means of potentiometry and calorimetry. The structures of the complexes in aqueous solution are discussed with the help of ^{31}P NMR data.

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- 3785 **Stephen A. Benyunes, Lutz Brandt, Arno Fries, Michael Green, Mary F. Mahon and Trevor M. T. Papworth**
Reactions of co-ordinated ligands. Part 57. Synthesis, structure and interrelationship of 2- σ -butadienyl and cationic (1,2,3- η)-*trans*-butadienyl-platinum and -palladium complexes; crystal structures of *cis*-[PtCl(σ -C(CH₃)C(Et)=CH₂)(dppf)] and [Pt{(1,2,3- η)-*trans*-CH₂C(Et)C=CH₂)-(PPh₃)₂][PF₆][dppf = 1,1'-bis(diphenylphosphino)ferrocene]
 The synthesis of a range of new 2- σ -butadienyl-platinum(II) and -palladium(II) complexes is described including their transformation, on halide abstraction with Ti[PF₆], into cationic complexes carrying (1,2,3- η)-*trans*-CH₂C(R)C=CH₂ (R = Et, Me or H) ligands.
- 3795 **Edward W. Abel, Peter J. Heard, Keith G. Orrell, Michael B. Hursthouse and Mohammed A. Mazid**
Halogenotrimethylplatinum(IV) complexes of 2,6-bis(*p*-tolylthiomethyl)-pyridine (L¹): nuclear magnetic resonance studies of their solution state stereodynamics and the crystal structure of *fac*-[PtBrMe₃L¹]
 The complexes *fac*-[PtXMe₃L¹] [L¹ = 2,6-bis(*p*-tolylthiomethyl)pyridine, X = Cl or Br] involving bidentate S/N co-ordination of L¹ display three fluxional processes in solution, pyramidal S inversion, and S-S switching both with and without correlated S inversion. The crystal structure of *fac*-[PtBrMe₃L¹] is reported.
- 3803 **G. J. Anthony A. Koolhaas, Willem L. Driessen, Petra J. van Koningsbruggen, Jan Reedijk and Anthony L. Spek**
Synthesis, crystal structure and magnetic properties of [Cu₆(tidah)₂Cl₁₀(H₂O)₄].6H₂O [Htidah = 1,1,6,6-tetrakis(imidazol-2-yl)-2,5-diazahehexane], a unique imidazolato- and chloro-bridged hexanuclear copper(II) compound
 The hexanuclear copper(II) compound [Cu₆(tidah)₂Cl₁₀(H₂O)₄].6H₂O is obtained by the reaction of copper(II) chloride with the polyimidazole 1,1,6,6-tetrakis(imidazol-2-yl)-2,5-diazahehexane (Htidah). One of the four imidazole groups of Htidah is spontaneously dehydronated during the complexation reaction. The analysis of the temperature-dependent magnetic susceptibility data reveals an antiferromagnetic interaction of $-2J = 90 \text{ cm}^{-1}$ between the imidazolato-coupled copper(II) ions.
- 3809 **Jan Janczak and Ryszard Kubiak**
Crystal and molecular structure of diindium triphthalocyaninate at 300 K
 The synthesis of a new type of indium phthalocyanine is described. A double-sandwich type structure is revealed by X-ray crystallography which is compared with other phthalocyanines.
- 3813 **Catherine F. Edwards, William P. Griffith, Andrew J. P. White and David J. Williams**
Salicylato (sal) complexes of second- and third-row transition elements, and the crystal structure of [NMe₄]₂[MoO₂(sal)₂].2H₂O
 New salicylato (sal) complexes of molybdenum, tungsten and osmium are prepared and their vibrational, ¹H and ¹³C NMR spectra measured to ascertain their structures in solution as have known salicylato complexes of rhodium and palladium. The crystal structure of [NMe₄]₂[MoO₂(sal)₂].2H₂O is also determined.

Dalton Communications

- 3821 **James H. Cameron and Elinor L. Scott**
Unusual specificity in alkylation reactions of a nickel(II) cyclidene macrocyclic complex
 Kinetic control of alkylation of a macrocyclic complex allows selective preparation of species with desired structural features.
- 3823 **Hiroshi Sakiyama, Hisashi Ōkawa and Masatatsu Suzuki**
Geometrical significance of a μ -phenoxo-bis(μ -carboxylato)dimanganese core as an active-site model of manganese catalase
 μ -Phenoxo-bis(μ -carboxylato)dimanganese(II) complexes of C_s symmetry show a high catalase-like activity to disproportionate hydrogen peroxide whereas those of C₂ symmetry show only a low activity.

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- 3827 **Tsuyoshi Kijima, Yoshinori Kawagoe, Kenji Mihara and Masato Machida**
- A simple route to amide-functionalized tetravalent metal phosphonates. Interlayer amidation of an ethylenediammonium exchanged form of zirconium carboxyethylphosphonate**
- Layered zirconium carboxyethylphosphonate intercalates ethylenediamine by a mode in which the protons of the interlayer CO_2H groups are replaced by the terminal NH_3^+ cations. Heating the ion-exchanged solid to *ca.* 200 °C results in the conversion of the ionic-bonded $-\text{CO}_2^-\text{NH}_3^+$ group into a covalently bonded $-\text{CONH}-$ form in the interlayer space. This model reaction demonstrates a simple route from the acid-modified form of layered tetravalent metal phosphonates to their amide derivatives.
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- 3829 **S. W. Annie Bligh, Nick Choi, W. Jon Cummins, Evagoras G. Evagorou, J. Duncan Kelly and Mary McPartlin**
- Synthesis and crystal structure of a novel hexaaza macrocyclic ligand with 2-hydroxy-3,5-dimethylbenzyl pendant arms and its gadolinium(III) complex**
- Two new hexaaza macrocycles substituted with 2-hydroxy-3,5-dimethylbenzyl groups on the secondary amine nitrogens are synthesized; the crystal structure of one shows that the six nitrogen donor atoms adopt a chair conformation in the solid state. The gadolinium(III) complex of the monodeprotonated form of the other macrocycle has a nine-co-ordinated gadolinium(III) ion bound to the phenolic oxygen atom of one pendant arm, six nitrogen donors of the macrocyclic ligand and two oxygen atoms of a nitrate.
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