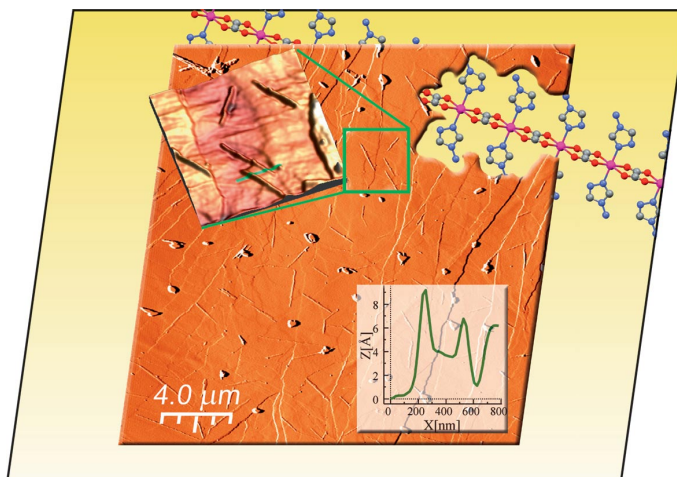


A union formed by chemical societies in Europe (ChemPubSoc Europe) has taken the significant step into the future by merging their traditional journals, to form two leading chemistry journals, the *European Journal of Inorganic Chemistry* and the *European Journal of Organic Chemistry*. Three further members of ChemPubSoc Europe (Austria, Czech Republic and Sweden) are Associates of the two journals.

## COVER PICTURE

The cover picture shows an Atomic Force Microscopy image of single chains based on a one-dimensional oxalato-bridged manganese(II) complex with 4-aminotriazole isolated on a graphite surface. The inset shows the height profile of two of these chains. This is an example of the results obtained in the adsorption of coordination polymers on surfaces. The Microreview by F. Zamora et al. on p. 2885ff focuses on the state-of-the-art experimental procedures for the isolation of single chains of these supramolecules and on different pathways to obtain molecular assemblies. Potential applications of these compounds as molecular wires are also presented.



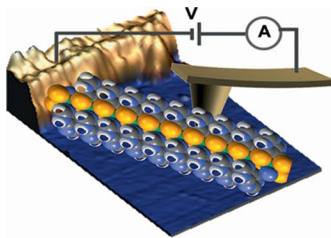
## MICROREVIEW

### Nanocircuits

R. Mas-Ballesté, O. Castillo,  
P. J. Sanz Miguel, D. Olea,  
J. Gómez-Herrero,  
F. Zamora\* ..... 2885–2896

Towards Molecular Wires Based on Metal-Organic Frameworks

**Keywords:** Nanotechnology / Molecular electronics / Single-molecule studies / Nanostructures / Scanning probe microscopy



The emergent area of nanotechnology requires suitable procedures to organize materials on nanometer scale. In molecular electronics, molecular wires are essential building blocks for the construction of nanocircuits. A young area of research centered on the initial studies of the organization of coordination polymers on surfaces towards conductive molecular wires is presented.

## SHORT COMMUNICATIONS

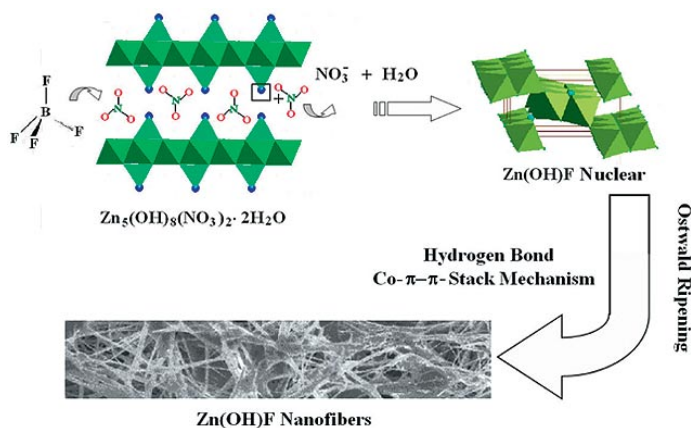
### Zinc Nanofibers

L. Wu, J. Lian, G. Sun, X. Kong,  
W. Zheng\* ..... 2897–2900



Synthesis of Zinc Hydroxyfluoride Nanofibers through an Ionic Liquid Assisted Microwave Irradiation Method

**Keywords:** Zinc / Fluorine / Microwave chemistry / Ionic liquids / Nanostructures



Zn(OH)F nanofibers were prepared from  $\text{Zn}_5(\text{OH})_8(\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$  by microwave irradiation in the presence of the ionic liquid [Tmim][BF<sub>4</sub>] (1,2,3-trimethylimidazolium tetrafluoroborate). The fibers are 80–

200 nm in diameter and several micrometers in length. A hydrogen bonding  $\pi$ – $\pi$  stacking mechanism is responsible for the 1D feature of the Zn(OH)F nanofibers.

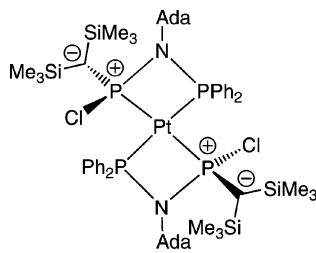
### P Atom Insertion into Metal–Cl Bonds

D. Lungu, C. Daniliuc, P. G. Jones,  
L. Nyulászi, Z. Benkő, R. Bartsch,  
W.-W. du Mont\* ..... 2901–2905



Exceptional Coordination Mode of Unsaturated PNP Ligands  $(\text{Me}_3\text{Si})_2\text{C}=\text{PN}(\text{R})\text{-PPh}_2$  with Palladium and Platinum Dichlorides: Insertion of Phosphaalkene Phosphorus Atoms into Metal–Chlorine Bonds

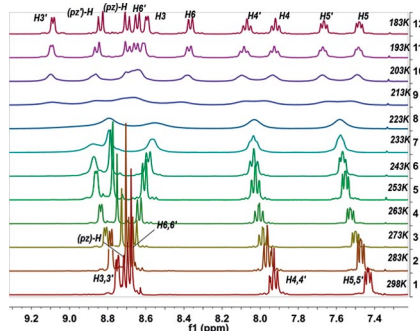
**Keywords:** Palladium / Platinum / Insertion / *P*-Chloroylides / Phosphaalkenes / Density functional calculations



Coordination of two bidentate phosphanyl-amino phosphaalkene ligands  $(\text{Me}_3\text{Si})_2\text{C}=\text{PN}(\text{1-Ada})\text{PPh}_2$  with dichlorides of palladium and platinum occurs with carbene-like insertion of both phosphaalkene phosphorus atoms into  $\text{M}-\text{Cl}$  bonds, leading to molecular chelate complexes with metallasubstituted *P*-chloroylide functions: the coordinated phosphaalkene P atoms behave as Lewis acids towards the chloride ions.

## FULL PAPERS

CH<sub>3</sub>ReO<sub>3</sub> (MTO) forms adducts with bidentate Lewis bases. The formation, stability and catalytic activity of the complexes depend on the functional groups attached to the Lewis base ligands.



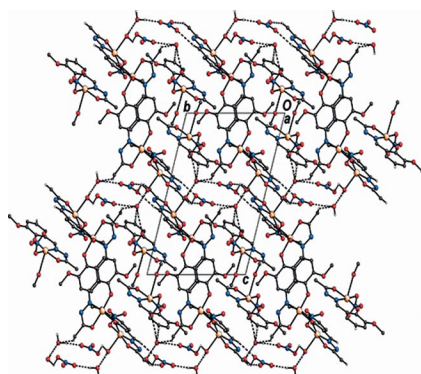
### Adducts with Methyltrioxidorhenium

M.-D. Zhou, K. R. Jain, A. Günyar,  
P. N. W. Baxter, E. Herdtweck,  
F. E. Kühn\* ..... 2907–2914

Bidentate Lewis Base Adducts of Methyltrioxidorhenium(VII): Ligand Influence on Catalytic Performance and Stability

**Keywords:** Lewis bases / Epoxidation / Biphasic catalysis / Rhenium / Methyltrioxidorhenium (MTO)

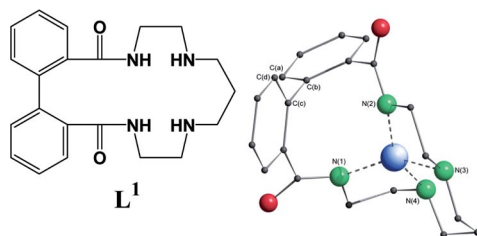
On the basis of hydrogen-bonding interactions, a new potentially tetradentate ONOO donor hydrazone ligand in a rare singly phenoxo-bridged copper(II) (1) and a doubly phenoxo-bridged manganese(II) (2) coordination complex can form two unusual 3D supramolecular architectures.



A. Ray, C. Rizzoli, G. Pilet, C. Desplanches,  
E. Garribba, E. Rentschler,  
S. Mitra\* ..... 2915–2928

Two New Supramolecular Architectures of Singly Phenoxo-Bridged Copper(II) and Doubly Phenoxo-Bridged Manganese(II) Complexes Derived from an Unusual ONOO Donor Hydrazone Ligand: Syntheses, Structural Variations, Cryomagnetic, DFT, and EPR Studies

**Keywords:** Supramolecular chemistry / Structure elucidation / Density functional calculations / N,O ligands / Hydrogen bonds / Bridging ligands



Cu<sup>II</sup> complexes of new dioxo macrocycles were characterized in solution. With L<sup>1</sup>, a neutral copper complex [CuL<sup>1</sup>H<sub>2</sub>] is obtained at physiological pH. The pro-

tonation constants for the ligands and the complexation constants for the complexes were determined. The process of complexation was investigated.

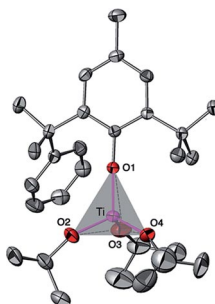
### Complexation Process of Cu Complexes

I. Déchamps-Olivier, C. Cadiou,  
D. Harakat, T. Roisnel, F. Chuburu,\*  
J. Hodacova, S. Koskova ..... 2929–2941

Thermodynamic and Structural Investigations on the Complexation Process of Dioxo Macrocyclic Ligands: Towards Neutral Copper Complexes at Physiological pH

**Keywords:** Macrocyclic ligands / Thermodynamics / UV/Vis spectroscopy / Copper

Functionalized mono- and dinuclear mono(aryloxido)titanium(IV) complexes were prepared. Evidence for the hemilabile behaviour of the CH<sub>2</sub>NMe<sub>2</sub>-substituted aryloxido ligand is discussed. Interesting activities for the selective dimerization of ethylene to 1-butene [2100 g/gTi/h, selectivity C<sub>4</sub><sup>=</sup>(α) = 92% (99+%) were observed.



J.-B. Cazaux, P. Braunstein, L. Magna,\*  
L. Saussine,\*  
H. Olivier-Bourbigou ..... 2942–2950

Mono(aryloxido)Titanium(IV) Complexes and Their Application in the Selective Dimerization of Ethylene

**Keywords:** Dimerization / O ligands / Hemilability / Titanium / Structure–activity relationships

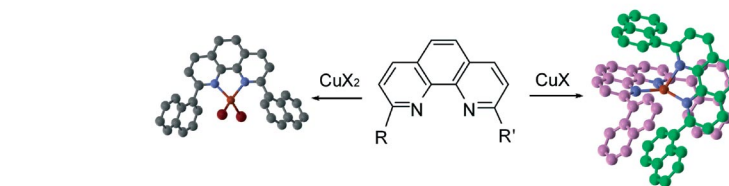
# CONTENTS

## Four-Coordinate Copper Complexes

P. Yang, X.-J. Yang,\* B. Wu\*... 2951–2958

Synthesis, Structure, and Spectroscopic and Electrochemical Properties of Copper(II/I) Complexes with Symmetrical and Unsymmetrical 2,9-Diaryl-1,10-phenanthroline Ligands

**Keywords:** Copper / Structure elucidation / Electrochemistry / N ligands



A series of four-coordinate copper(II) and copper(I) complexes,  $[\text{CuX}_2\text{L}]$  (1–6) and  $[\text{CuL}_2](\text{CuX}_2)$  (7–12) ( $\text{X} = \text{Cl}, \text{Br}$ ;  $\text{L} = 2\text{-R-9-R'-1,10-phenanthroline}$ , dpp:  $\text{R} = \text{R}'$

$= \text{Ph}$ ; npp:  $\text{R} = \text{naphthyl}$ ,  $\text{R}' = \text{Ph}$ ; dnp:  $\text{R} = \text{R}' = \text{naphthyl}$ ) were synthesized and their redox properties were studied.

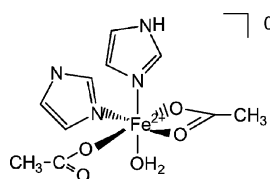
## Bioinorganic Chemistry

O. Horner,\* J.-L. Oddou, C. Jeandey, I. Michaud-Soret, J.-M. Mouesca ..... 2959–2966



Detailed Mössbauer Characterization of  $\text{Fe}^{2+}$  Fur, the Active Form of the Ferric Uptake Regulation Protein from *E. coli* and Density Functional Calculations on Some Related Models

**Keywords:** Moessbauer spectroscopy / Density functional calculations / Iron / Bioinorganic chemistry / Protein models



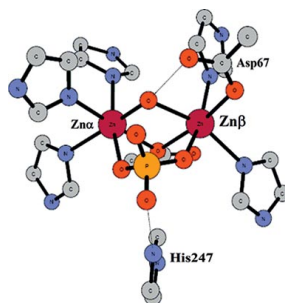
The  $\text{Fe}^{2+}$  center of iron-substituted ferric uptake regulation protein (Fur) has been fully characterized by Mössbauer spectroscopy and parameters, as estimated by density functional theory calculations for structural models of the active center, compared to the experimental data. The model with a (3O,2N,1O) coordination ( $\Delta E_Q > 0$ ) is found to be a better representation of the environment around the iron center in  $\text{EC-Fe}^{2+}\text{Fur}$ .

## Enzymatic RNA Hydrolysis

R.-Z. Liao, F. Himo,\* J.-G. Yu,\* R.-Z. Liu ..... 2967–2972

Theoretical Study of the RNA Hydrolysis Mechanism of the Dinuclear Zinc Enzyme RNase Z

**Keywords:** Enzyme catalysis / Metalloenzymes / Dinuclear zinc enzymes / Density functional calculations / Hydrolysis / Reaction mechanisms / Zinc



Density functional theory was used to investigate the reaction mechanism of the dinuclear zinc enzyme RNase Z (see picture), catalyzing the removal of tRNA 3'-end trailer.

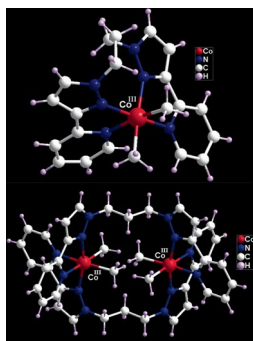
## Dialkylcobalt(III) Complexes

V. Mishra, H. Mishra, R. Mukherjee\* ..... 2973–2980



Generation and Properties of  $\text{Co}^{\text{I}}/\text{Ni}^{\text{I}}$  Species Stabilized by a Tetradentate Pyridylpyrazole Ligand: Crystal Structures of Dialkyl- $\text{Co}^{\text{III}}$  Complexes

**Keywords:** Cobalt / Nickel / Redox chemistry / EPR spectroscopy / Nitrogen heterocycles / N ligands / Chelates

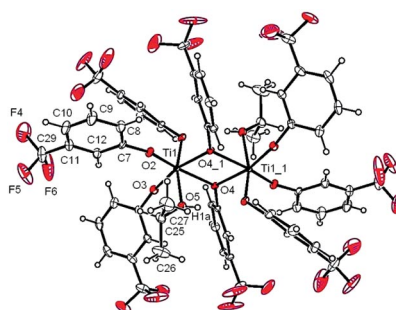


$\text{Co}^{\text{I}}$  and  $\text{Ni}^{\text{I}}$  species stabilized by 2,2'-[propane-1,3-diylbis(1*H*-pyrazole-1,3-diyl)]dipyridine have been generated and characterized.



## Ti-Catalyzed Polymerization

The synthesis of a variety of aryloxy compounds and benzyloxy derivatives of  $\text{Ti}^{\text{IV}}$  is reported. Their utility in the polymerization of  $\epsilon$ -caprolactone and  $\delta$ -valerolactone is described.



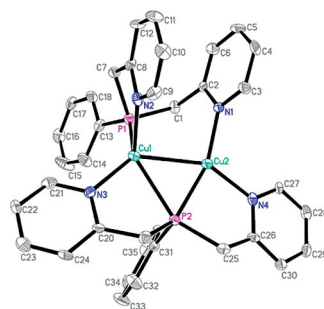
**R. R. Gowda, D. Chakraborty,\*  
V. Ramkumar** ..... 2981–2993

New Aryloxy and Benzyloxy Derivatives of Titanium as Catalysts for Bulk Ring-Opening Polymerization of  $\epsilon$ -Caprolactone and  $\delta$ -Valerolactone

**Keywords:** Titanium(IV) /  $\epsilon$ -Caprolactone /  $\delta$ -Valerolactone / Polymerization / Titanium / Lactones

## Coordination Modes

Reaction of phenylbis(pyrid-2-ylmethyl)phosphane and bis(pyrid-2-ylmethyl)phenylphosphonite with silver(I) and copper(I) salts affords a series of discrete molecules where the ligands coordinate in different fashions that span from terminally bonding to bridging two metal centers, thus inducing short metal–metal contacts.



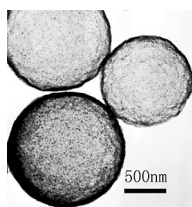
**F. Hung-Low, A. Renz,  
K. K. Klausmeyer\*** ..... 2994–3002

The Variable Binding Modes of Phenylbis(pyrid-2-ylmethyl)phosphane and Bis(pyrid-2-ylmethyl) Phenylphosphonite with  $\text{Ag}^{\text{I}}$  and  $\text{Cu}^{\text{I}}$

**Keywords:** N,P ligands / Silver / Metal-metal interactions / Coordination modes

## Magnetic Hollow Carbon Spheres

A rapid one-step, template-free, and continuous strategy leads to high-density magnetite ( $\text{Fe}_3\text{O}_4$ ) nanoparticles located in carbon hollow microspheres (MCHMs) in which  $\text{Fe}_3\text{O}_4$  nanoparticles are uniformly dispersed in the shells of carbon hollow microspheres.



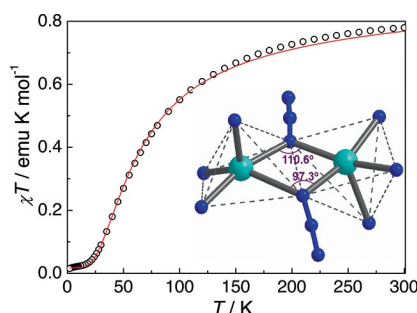
**R. Zheng, X. Meng,  
F. Tang\*** ..... 3003–3007

High-Density Magnetite Nanoparticles Located in Carbon Hollow Microspheres with Good Dispersibility and Durability: Their One-Pot Preparation and Magnetic Properties

**Keywords:** Materials science / Nanostructures / Magnetic properties / Hollow spheres / Iron / Magnetite

## Magnetic Exchange

In a doubly bridged  $\text{Cu}^{\text{II}}$  complex, two end-on azido bridges occupying the equatorial positions exhibit widely different Cu–N–Cu angles. Combined experimental and theoretical studies reveal that the two azido bridges propagate ferro- and antiferromagnetic coupling, respectively, and compete to give rise to a controlled antiferromagnetic interaction.



**Q.-X. Jia, M.-L. Bonnet, E.-Q. Gao,\*  
V. Robert\*** ..... 3008–3015

Competing Large and Small Angles in a Double End-On Azido Copper(II) Binuclear Complex: A Combined Experimental and Theoretical Study of Magnetic Interactions

**Keywords:** Ab initio calculations / Azides / Copper / Density functional calculations / Magnetic properties

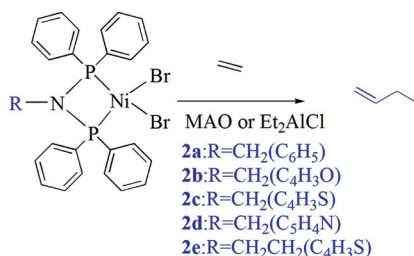
# CONTENTS

## Nickel Ethylene Oligomerization

K. Song, H. Gao,\* F. Liu, J. Pan, L. Guo,  
S. Zai, Q. Wu\* ..... 3016–3024

Syntheses, Structures, and Catalytic Ethylene Oligomerization Behaviors of Bis-(phosphanyl)aminenickel(II) Complexes Containing *N*-Functionalized Pendant Groups

**Keywords:** Oligomerization / Nickel / Structure–activity relationships / P,P ligands



In the presence of methylaluminoxane, bis-(phosphanyl)amine complexes of nickel(II) showed high activity for ethylene oligomerization and high selectivities for dimer and linear  $\alpha$ -olefins at low temperature. At high temperature, the nickel catalysts decomposed rapidly and underwent Friedel–Crafts alkylation of toluene with ethylene and the olefin oligomers.

\* Author to whom correspondence should be addressed.

Supporting information on the WWW (see article for access details).

If not otherwise indicated in the article, papers in issue 19 were published online on June 18, 2009