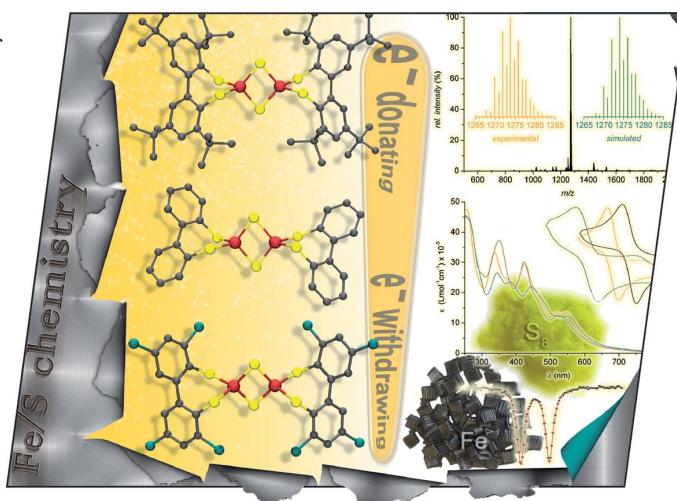


A union formed by chemical societies in Europe (ChemPubSoc Europe) has taken the significant step into the future by merging their traditional journals, to form two leading chemistry journals, the *European Journal of Inorganic Chemistry* and the *European Journal of Organic Chemistry*. Three further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

## COVER PICTURE

The cover picture shows the molecular structures of three novel 2,2'-dithiobiphenyl-ligated [2Fe-2S] clusters together with some of their characteristic spectroscopic data. Specifically tailored capping ligands with different substituents in the 3,3',5,5'-positions (*t*Bu, H, Cl) have been applied in order to examine the influence of the ligands on the electronic structures of the [2Fe-2S] cluster cores. The article by F. Meyer et al. on p. 3219ff demonstrates that the ligand modifications impose significant changes to the fundamental properties of the clusters, e.g. to their redox potentials. Electrochemical and spectroscopic data in solution and in the solid state (including X-ray structures) are discussed in detail in this contribution.



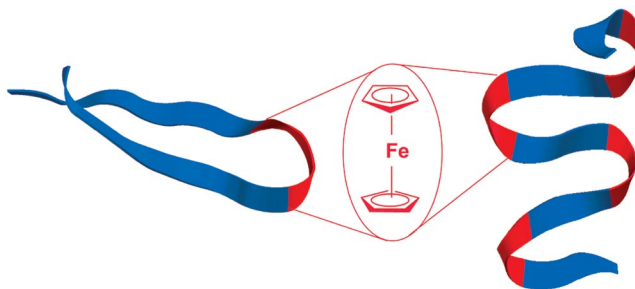
## MICROREVIEW

### Peptide Structural Mimics

A. Lataifeh, S. Beheshti,  
H.-B. Kraatz\* ..... 3205–3218

Designer Peptides: Attempt to Control Peptide Structure by Exploiting Ferrocene as a Scaffold

**Keywords:** Amino acids / Metallocenes / Peptides / Protein structures / Supramolecular chemistry



Ferrocene conjugates have emerged as highly versatile scaffolds for applications in mimicking the secondary structural motifs found in proteins. This Microreview ad-

resses the recent developments in this area, with a focus on models of  $\beta$ -sheets, turns and extended supramolecular arrangements.

## FULL PAPERS

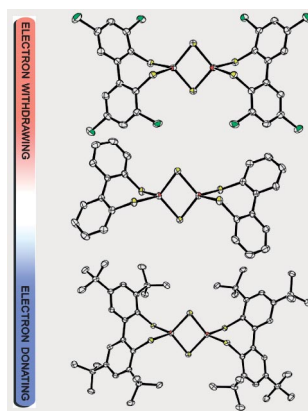
### Biomimetic [2Fe-2S] Clusters

J. Ballmann, S. Dechert, S. Demeshko,  
F. Meyer\* ..... 3219–3225



Tuning Electronic Properties of Biomimetic [2Fe-2S] Clusters by Ligand Variations

**Keywords:** Ligand effects / Bioinorganic chemistry / Iron / Sulfur / S ligands



Unusually stable biomimetic [2Fe-2S] complexes with 2,2'-dithiobiphenyl capping ligands have been developed, where variations of backbone substituents (Cl, H, *t*Bu) allow to modulate the electronic situation at the cluster core. This has been probed by a variety of spectroscopic and analytical methods (X-ray diffraction, UV/Vis and Mössbauer spectroscopy, SQUID analysis, cyclic voltammetry).

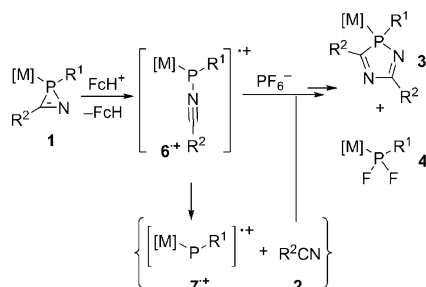
### 1,3-Dipole Chemistry

H. Helten, S. Fankel, O. Feier-Iova,  
M. Nieger, A. Espinosa Ferao,\*  
R. Streubel\* ..... 3226–3237

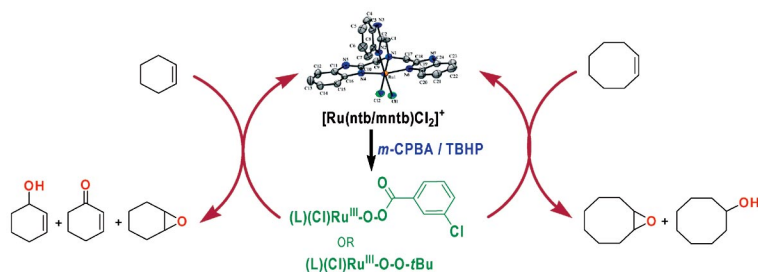


Strong Evidence for an Unprecedented Borderline Case of Dissociation and Cycloaddition in Open-Shell 1,3-Dipole Chemistry: Transient Nitrilium Phosphane-Ylide Complex Radical Cations

**Keywords:** Density functional calculations / Electron transfer / Single electron transfer reactions / Radical ions / HSAB parameters



Azaphosphirene complexes **1** undergo a surprising reaction with ferrocenium hexafluorophosphate to yield 3,5-diferrocenyl-substituted 2H-1,4,2-diazaphosphole complexes **3** and difluoro(organo)phosphane complexes **4**. DFT studies provide further evidence for a dissociation cycloaddition reaction sequence.



New mononuclear Ru<sup>III</sup> complexes have been synthesized and characterized. These complexes catalyze the allylic oxidation of cyclohexene, selective and higher epoxida-

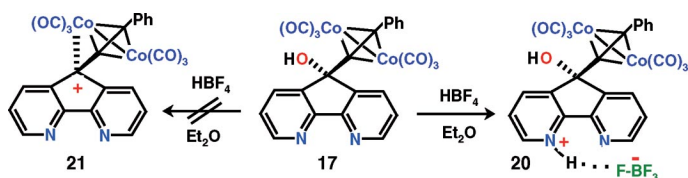
tion of cyclooctene, and the hydroxylation of alkanes. MS studies reveal the formation of ruthenium peroxido species in the catalytic reactions.

**M. Murali, R. Mayilmurugan, M. Palaniandavar\*** ..... 3238–3249

Synthesis, Structure and Spectral, and Electrochemical Properties of New Mononuclear Ruthenium(III) Complexes of Tris[(benzimidazol-2-yl)methyl]amine: Role of Steric Hindrance in Tuning the Catalytic Oxidation Activity

**Keywords:** Ruthenium(III) complexes / Electronic structure / Redox chemistry / Oxidation / Alkanes / Epoxidation / Alkenes / Ligand effects

## Metal–Nitrogen Bonds



Complexes of 4,5-diazafluoren-9-one and 9-phenylethynyl-4,5-diazafluoren-9-ol with zinc and platinum halides have been characterised. Protonation of (9-phenylethynyl-4,5-diazafluoren-9-ol)Co<sub>2</sub>(CO)<sub>6</sub> (**17**)

with HBF<sub>4</sub> does not yield a cobalt-stabilised carbocation **21**, but instead protonation occurs at the nitrogen atom to form **20**, which gives rise to an intricate hydrogen-bonding pattern.

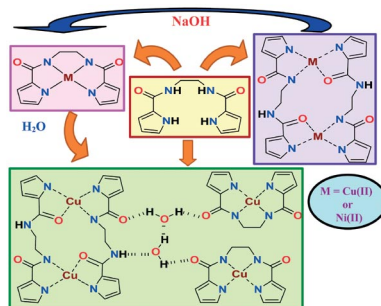
**L. Maguire, C. M. Seward, S. Baljak, T. Reumann, Y. Ortin, E. Banide, K. Nikitin, H. Müller-Bunz, M. J. McGlinchey\*** ..... 3250–3258

A Synthetic and X-ray Crystallographic Study of Zinc and Platinum Complexes of 4,5-Diazafluoren-9-one (Dafone) and Dicobalt Hexacarbonyl Derivatives of 9-Phenylethynyl-4,5-Diazafluoren-9-ol: Chelation versus Monocoordination

**Keywords:** Metal-nitrogen linkages / Asymmetric bonds / Hydrogen bonds / Coordination modes / Zinc / Platinum / Cobalt

## Multidentate N Ligand

A potential tetradentate pyrrolicarboxamide ligand, H<sub>4</sub>L<sup>1</sup>, coordinates to metal ions (M = Ni, Cu) either in a tetraanionic or trianionic fashion to afford mononuclear [M(L<sup>1</sup>)]<sup>2−</sup>, dinuclear [M<sub>2</sub>(HL<sup>1</sup>)<sub>2</sub>]<sup>2−</sup>, or adduct [{M<sub>2</sub>(HL<sup>1</sup>)<sub>2</sub>}{M(L<sup>1</sup>)}]<sup>6−</sup> complexes, respectively. Crystallographic and core-conversion studies depict several interesting features for these complexes.



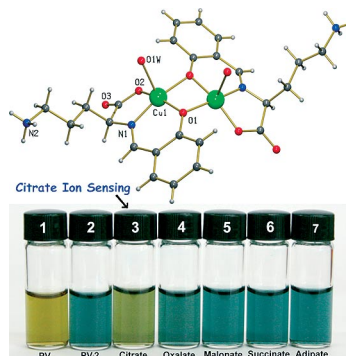
**J. Singh, G. Hundal, R. Gupta\*** ..... 3259–3265

Mononuclear and Dinuclear Ni<sup>II</sup> and Cu<sup>II</sup> Complexes with a Pyrrolicarboxamide Ligand: Core Conversions and Unusual Presence of a Dimer and Two Monomers in the Same Unit Cell

**Keywords:** N ligands / Nickel / Copper / H bonding

## Dinuclear Copper Complexes

Two chiral dimeric Cu<sup>2+</sup> complexes **1** and **2** have been prepared by a one pot method in which the L-lysine- and L-ornithine-based Schiff base ligands are generated in situ. Variable-temperature magnetic susceptibility measurements reveal strong antiferromagnetic coupling interactions. Selective citrate ion sensing was enabled through colorimetric indicator displacement assays in water at physiological pH.



**S. Khatua, K. Kim, J. Kang, J. O. Huh, C. S. Hong, D. G. Churchill\*** .... 3266–3274

Synthesis, Structure, Magnetic Properties and Aqueous Optical Citrate Detection of Chiral Dinuclear Cu<sup>II</sup> Complexes

**Keywords:** Chiral dicopper complex / Schiff bases / Magnetic properties / Structure elucidation / Citrate detection

# CONTENTS

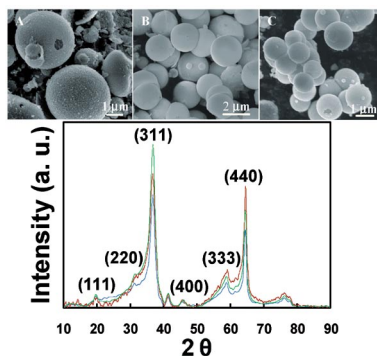
## Mesoporous Nanocrystalline Materials

C. A. Deshmane, J. B. Jasinski,  
M. A. Carreon\* ..... 3275–3281



Thermally Stable Nanocrystalline Mesoporous Gallium Oxide Phases

**Keywords:** Mesoporous materials / Gallium oxides / Nanocrystals / Thermal stability / Heterogeneous catalysis



Semicrystalline and crystalline mesoporous gallium oxide phases displaying high surface areas and unimodal pore sizes were prepared in the presence of ionic and non-ionic structure directing agents via EISA and SAHA.

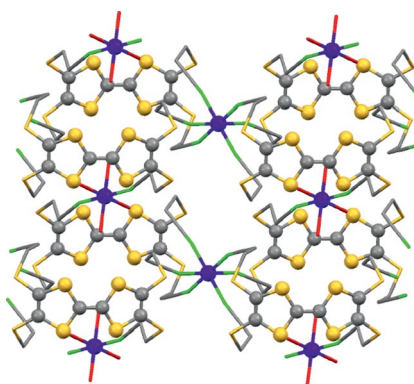
## Metal–Nitrile Polymers

J. Olivier, S. Golhen\*, R. Świątlik,  
O. Cadot, F. Pointillart,  
L. Ouahab\* ..... 3282–3290



X-ray Structures, Spectroscopic and Magnetic Studies of a Coordination Polymer Series Based on a TTF Derivative and Paramagnetic Transition Metals

**Keywords:** Polymers / Magnetic properties / Cadmium / Cobalt / Manganese / Zinc



The reaction of 2,3,6,7-tetrakis(2-cyanoethylthio)tetrathiafulvalene (TCE-TTF) with hexafluoroacetylacetonate (hfac) salts of paramagnetic ( $\text{Co}^{\text{II}}$ ,  $\text{Mn}^{\text{II}}$ ) and diamagnetic ( $\text{Zn}^{\text{II}}$ ,  $\text{Cd}^{\text{II}}$ ) ions in the presence of tetrahedral anions ( $\text{BF}_4^-$  and  $\text{ClO}_4^-$ ) afforded four isostructural salts, whose structure and properties are presented.

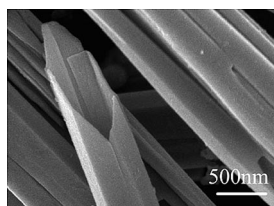
## Tellurium Nanotubes

L. Zhang,\* C. Wang, D. Wen ... 3291–3297



Preparation by Hydrothermal Techniques in a Tungstosilicic Acid Solution System and Optical Properties of Tellurium Nanotubes

**Keywords:** Nanotubes / Tellurium / Polyoxometalates



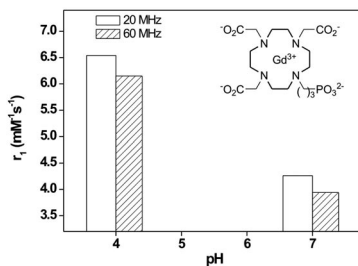
Single-crystalline tellurium nanotubes were synthesised by a simple hydrothermal, economical and green route. Tungstosilicic acid (TSA) acts as an effective reducing agent and a morphology-directing agent for tellurium nanotubes from sodium tellurate ( $\text{Na}_2\text{TeO}_3$ ) precursor powders. Te nanotubes grow along the [001] direction with excellent crystallinity and they show strong fluorescence properties.

## Ln-DO3A-Propylphosphonates

I. Mamedov,\* P. Táborský, P. Lubal,\*  
S. Laurent, L. Vander Elst, H. A. Mayer,  
N. K. Logothetis,  
G. Angelovski\* ..... 3298–3306

Relaxometric, Thermodynamic and Kinetic Studies of Lanthanide(III) Complexes of DO3A-Based Propylphosphonates

**Keywords:** Lanthanides / Phosphonates / Kinetics / Thermodynamics / Contrast agents

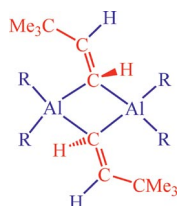


Proton relaxometric, thermodynamic and kinetic studies of two DO3A-based ligands appended with the propylphosphonate side arm and their  $\text{Ln}^{3+}$  complexes were performed. The results support possible in vivo application of these complexes.



## Hydroalumination vs. Deprotonation

Dimeric alkenyldialkylaluminum compounds were formed upon treatment of the terminal alkyne  $\text{H}-\text{C}\equiv\text{C}-\text{CMe}_3$  with dialkylaluminum hydrides. They may represent the key intermediate in the well-known *cis/trans* rearrangement of hydroalumination products. Hydrogen release and formation of alkynylaluminum compounds were observed in some cases as minor side-reactions.



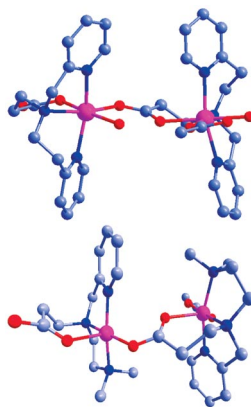
W. Uhl,\* E. Er, A. Hepp, J. Kösters,  
 M. Layh, M. Rohling, A. Vinogradov,  
 E.-U. Würthwein,  
 N. Ghavtadze ..... 3307–3316

Treatment of Terminal Alkynes  $\text{R}-\text{C}\equiv\text{C}-\text{H}$  with Dialkylaluminum Hydrides: Hydroalumination versus Deprotonation

**Keywords:** Aluminum / Hydroalumination / Vinylic compounds / Heterocycles / Alkynes

## 1D Coordination Polymers

Four new 1D coordination polymers  $[\text{Mn}^{\text{II}}(\text{L}^1\text{OO})(\text{H}_2\text{O})][\text{ClO}_4]\cdot 2\text{H}_2\text{O}$ ,  $[\text{Zn}^{\text{II}}(\text{L}^1\text{OO})][\text{ClO}_4]\cdot 2\text{H}_2\text{O}$ ,  $[\text{Cu}^{\text{II}}(\text{L}^3\text{OO})][\text{CF}_3\text{SO}_3]\cdot \text{H}_2\text{O}$ , and  $[\text{Zn}^{\text{II}}(\text{L}^3\text{OO})][\text{ClO}_4][\text{L}^1\text{OO}^- = 3-[(2-(\text{pyridine-2-yl})\text{ethyl})\{2-(\text{pyridine-2-yl})\text{-methyl}\}\text{amino}\}\text{propionate}]$ ;  $\text{L}^3\text{OO}^- = 3-[(2-(\text{pyridine-2-ylethyl})\{(\text{dimethylamino})\text{-ethyl}\}\text{amino}\}\text{propionate}]$  have been synthesized and characterized structurally and magnetically.



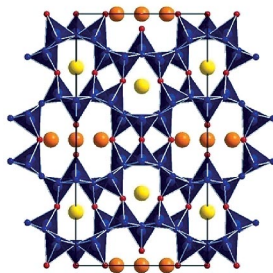
H. Arora, F. Lloret,  
 R. Mukherjee\* ..... 3317–3325

One-Dimensional Coordination Polymers of  $\text{Mn}^{\text{II}}$ ,  $\text{Cu}^{\text{II}}$ , and  $\text{Zn}^{\text{II}}$  Supported by Carboxylate-Appended (2-Pyridyl)alkylamine Ligands – Structure and Magnetism

**Keywords:** Coordination polymers / Crystal structures / Noncovalent interactions / Magnetic properties / Antiferromagnetic coupling / Carboxylate ligands / Bridging ligands / Structure elucidation

## Oxonitridoaluminosilicates

$(\text{Sr}_{1-x}\text{Ca}_x)_{(11+16y-25z)/2}(\text{Si}_{1-y}\text{Al}_y)_{16}(\text{N}_{1-z}\text{O}_z)_{25}$  ( $x \approx 0.24$ ,  $y \approx 0.18$ ,  $z \approx 0.19$ ) is a novel sialon, whose framework is built up from highly condensed layers of vertex-sharing tetrahedra. Due to the connection of these layers to a framework, further layers are generated, which contain rings of various sizes. In the cavities of the framework, Ca and Sr are distributed in a partially ordered fashion.



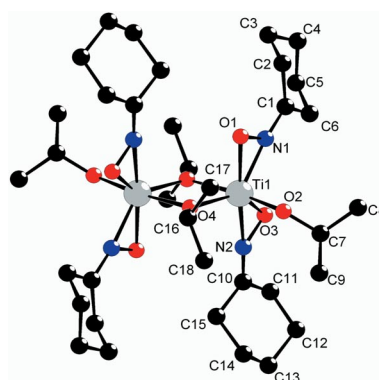
J. A. Kechele, O. Oeckler, P. J. Schmidt,  
 W. Schnick\* ..... 3326–3332

$(\text{Sr}_{1-x}\text{Ca}_x)_{(11+16y-25z)/2}(\text{Si}_{1-y}\text{Al}_y)_{16}(\text{N}_{1-z}\text{O}_z)_{25}$  ( $x \approx 0.24$ ,  $y \approx 0.18$ ,  $z \approx 0.19$ ) – A Novel Sialon with a Highly Condensed Silicate Framework

**Keywords:** Solid-state structures / Aluminosilicates / X-ray diffraction / Lattice energy calculation

## Modified Metal Alkoxides

Crystalline titanium alkoxides derivatives with one or two ketoximate ligands, as well as some partial hydrolysis products, were structurally characterized.



S. O. Baumann,\* M. Bendova, H. Fric,  
 M. Puchberger, C. Visinescu,  
 U. Schubert\* ..... 3333–3340

Ketoximate Derivatives of Titanium Alkoxides and Partial Hydrolysis Products Thereof

**Keywords:** Titanium / Oximate ligands / Metal Alkoxides / Partial hydrolysis

## CORRECTION

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- M. K. Denk\* ..... 3341    The Variable Strength of the Sulfur–Sulfur Bond: 78 to 41 kcal – G3, CBS-Q, and DFT Bond Energies of Sulfur (S<sub>8</sub>) and Disulfanes XSSX (X = H, F, Cl, CH<sub>3</sub>, CN, NH<sub>2</sub>, OH, SH)    **Keywords:** Sulfur / Radicals / Density functional calculations / Thermochemistry / Bond order / Spin density

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\* 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 21 were published online on July 10, 2009