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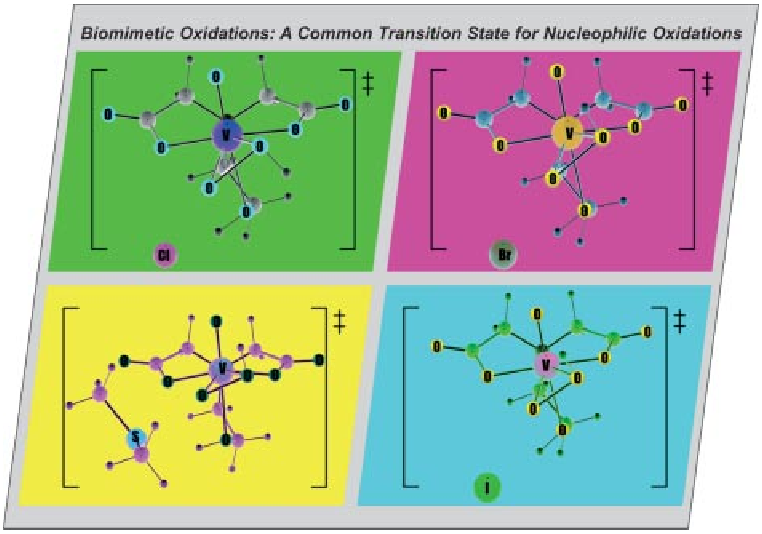
The EUChemSoc Societies have taken the significant step into the future by merging their traditional journals, to form two leading chemistry journals, the *European Journal of Inorganic Chemistry* and the *European Journal of Organic Chemistry.* Three further EUChemSoc Societies (Austria, Czech Republic and Sweden) are Associates of the two journals.

COVER PICTURE

The cover picture shows four substrates (Cl^-, Br^-, I^-, and dimethyl sulfide) that all pass through nearly identical transition states when oxidized by (hydroperoxido)(oxido)vanadium(V) 2,2′-[(2-hydroxyethyl)imino]diacetate [VO(OOH)Hheida]. The differences in the physical properties of the substrate are represented by the changes in the color scheme for each panel. Despite the different "colors", certain features of the transition states are always maintained, such as: nearly linear substrate peroxo oxygen bond angles, nucleophilic attack of the substrate on the unprotonated peroxo oxygen atom, and nearly complete hydroperoxo oxygen bond. This work lays the foundation for the development of more effective and potentially stereoselective catalysts based on the biomimetic catalyst V(OOH)Hheida. Details of this computational study can be found in the article by V. L. Pecoraro, and L. De Gioia on p. 515ff.



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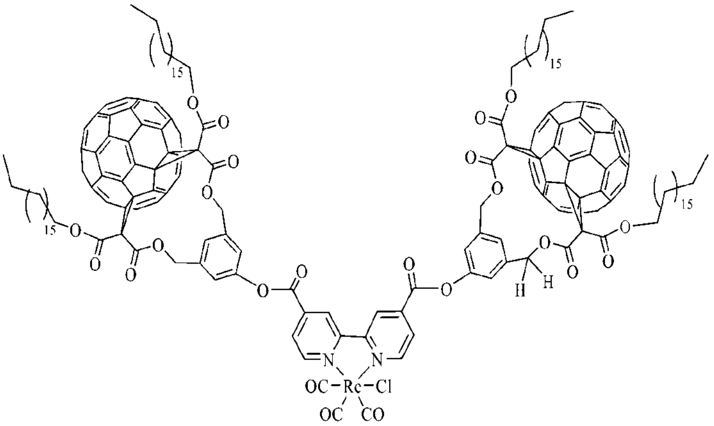
SHORT COMMUNICATIONS

Metal Complex−Fullerene Hybrids

H. D. Lee, S. K. Oh, C. S. Choi, K.-Y. Kay* .... 503−508

A Novel Amphiphilic Re^I Complex with Bis(fullerene)-Substituted Bipyridine Ligands: Synthesis, Electrochemistry, and Langmuir Film

Keywords: Rhenium / Fullerenes / Bipyridines / Cyclic voltammetry / Langmuir films



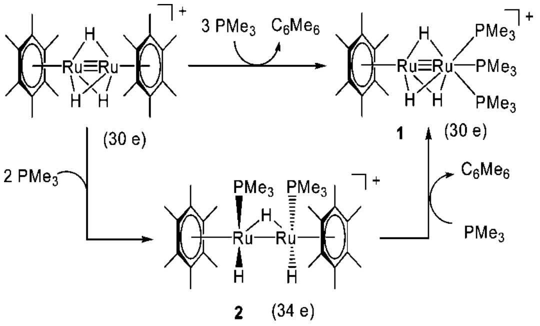
An amphiphilic fullerene (C_{60}) derivative with a (bipyridine)tricarbonylrhenium(I) chloride polar head group has been prepared. The Langmuir film of this compound has been characterized by its surface pressure versus molecular area isotherm and Brewster angle microscopy (BAM) observations.

Diruthenium Cations

M. J.-L. Tschan, F. Chérioux, B. Therrien, G. Süss-Fink* .... 509−513

A Surprising Reaction of Trimethylphosphane with the Unsaturated Diruthenium Complex $[(\eta^6\text{-}C_6Me_6)_2Ru_2(\mu_2\text{-}H)_3]^+$: Synthesis and Molecular Structure of the Cations $[(\eta^6\text{-}C_6Me_6)Ru_2(PMe_3)_3(\mu_2\text{-}H)_3]^+$ and $[(\eta^6\text{-}C_6Me_6)_2Ru_2(PMe_3)_2(\mu_2\text{-}H)(H)_2]^+$

Keywords: Ruthenium complexes / Arene complexes / Phosphane ligands / Hydrido ligands



The dinuclear cation $[(\eta^6\text{-}C_6Me_6)_2Ru_2(\mu_2\text{-}H)_3]^+$ reacts at 80 °C with trimethylphosphane to give, with substitution of a C_6Me_6 ligand by three PMe_3 ligands, the complex $[(\eta^6\text{-}C_6Me_6)Ru_2(PMe_3)_3(\mu_2\text{-}H)_3]^+$. The intermediary complex $[(\eta^6\text{-}C_6Me_6)_2Ru_2(PMe_3)_2(\mu_2\text{-}H)(H)_2]^+$ has been isolated at 20 °C as the tetrafluoroborate salt.

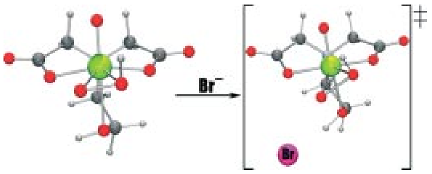
FULL PAPERS

Mechanism of Biomimetic Oxidations

C. J. Schneider, G. Zampella, C. Greco, V. L. Pecoraro,* L. De Gioia* .... 515−523

Mechanistic Analysis of Nucleophilic Substrates Oxidation by Functional Models of Vanadium-Dependent Haloperoxidases: A Density Functional Theory Study

Keywords: Peroxido ligands / Tripodal ligands / Oxidation / Vanadium / Density functional calculations



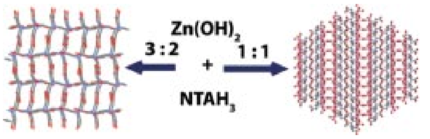
Density functional theory has been used to investigate the structural, electronic, and reactivity properties of an established functional model for vanadium dependent haloperoxidases, $K[VO(O_2)Hheida]$ ($Hheida^{2-}$ = 2,2′-[(2-hydroxyethyl)imino]diacetate).

ZnO Nanoparticles

H. Thakuria, B. M. Borah, G. Das* **524–529**

ZnO Nanoparticles From a Metal-Organic Framework Containing Zn^{II} Metallacycles

Nitrilotriacetic acid (H_3NTA) reacts in the solid phase with zinc hydroxide (1:1) to form a 3D ladder-like metal-organic framework that forms wurtzite ZnO nanoparticles when heated above 600 °C. The same reaction with an excess of zinc hydroxide gives a mixed coordination network that gives ZnO microwires upon decomposition at around 500 °C.



Keywords: Metallacycles / Tripodal ligands / Hydrogen bonds / Metal-organic frameworks / Nanoparticles

Copper Redox Reactions

A. Burg,* E. Maimon, H. Cohen, D. Meyerstein* **530–536**

Ligand Effects on the Chemical Activity of Copper(I) Complexes: Outer- and Inner-Sphere Oxidation of Cu^{I}L

outer sphere:

$$\mathrm{Cu^{I}L^{+} + [(cyclam)Ni^{III}(SO_4)_2]^{-} \longrightarrow Cu^{II}L^{2+} + [(cyclam)Ni^{II}(SO_4)_2]^{2-}}$$

$$\mathrm{Cu^{I}L^{+} + {}^{*}Cu^{II}L^{2+} \longrightarrow Cu^{II}L^{2+} + {}^{*}Cu^{I}L^{+}}$$

$$\boldsymbol{k(\mathrm{Cu^{+}_{aq}}) > k([\mathrm{Cu^{I}L}]^{+})}$$

inner sphere:

$$\mathrm{Cu^{I}L^{+} + [(NH_3)_5Co^{III}Cl]^{2+} \longrightarrow products}$$

$$\boldsymbol{k(\mathrm{Cu^{+}_{aq}}) > k([\mathrm{Cu^{I}L}]^{+})}$$

Ligand effects on the kinetics of reduction by Cu^I by the outer- and inner-sphere mechanisms were studied. The results indicate that acetonitrile and alkenes should not be used as solvents for $[Cu^IL]^+$ redox-catalyzed processes. The results suggest that [Cu^I(2,5,8,11-tetraaza-2,5,8,11-tetramethyldodecane)]$^+$ is expected to be a good catalyst for such processes.

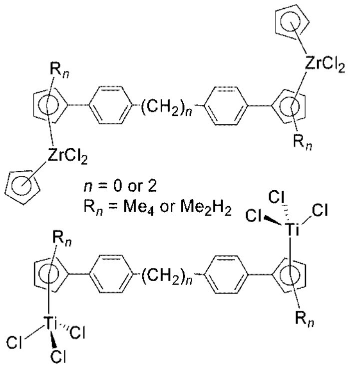
Keywords: Copper / Electron self exchange rate constant / Outer-sphere mechanism / Inner-sphere mechanism

Dinuclear Olefin Polymerization Catalysts

S. K. Kim, H. K. Kim, M. H. Lee, S. W. Yoon, Y. Han, S. Park, J. Lee, Y. Do* **537–545**

Dinuclear Metallocenes with a Modulated Biphenylene Bridge for Olefin Polymerization

Well-defined novel dinuclear zirconocenes show comparable catalytic activity in ethylene polymerization and produce PE with increased molecular weight. In case of syndiotactic polystyrene preparation with the dinuclear half titanocenes, the decrease in the molecular weight and the activity was recognized as polymerization behavior.



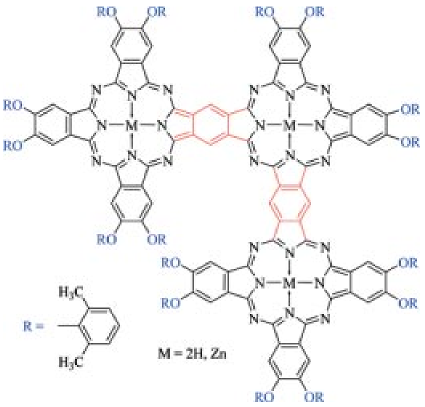
Keywords: Homogeneous catalysis / Metallocenes / Olefins / Polymerization / Titanium / Zirconium

Trinuclear Phthalocyanines

S. G. Makarov, O. N. Suvorova, C. Litwinski, E. A. Ermilov, B. Röder, O. Tsaryova, T. Dülcks, D. Wöhrle* **546–552**

Linear and Rectangular Trinuclear Phthalocyanines

Linear and rectangular trinuclear metal-free and zinc(II) phthalocyanines showing absorptions up to 940 nm with extinction coefficients of up to around 700000 M^{-1} cm^{-1} have been synthesized. Their electronic-absorption and fluorescence spectra have been recorded and compared to those of the corresponding mono- and dinuclear phthalocyanines.



Keywords: Phthalocyanines / NIR absorption / UV/Vis spectroscopy

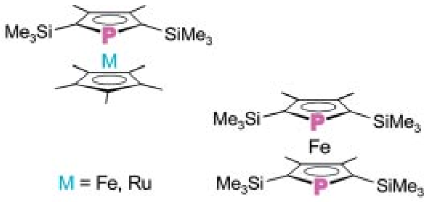
CONTENTS

Phosphametallocenes

R. Loschen, C. Loschen, W. Frank, C. Ganter* .... 553−561

Synthesis, Structure and Reactivity of Trimethylsilyl-Substituted Phosphametallocenes

Keywords: Metallocenes / P ligands / Silicon / Phosphaferrocenes / Conformation analysis



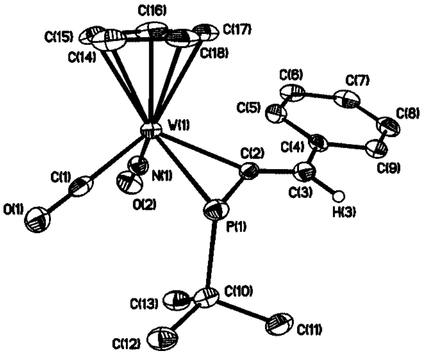
Phosphametallocenes with sterically demanding Me_3Si groups have been prepared from the respective phospholyl anion and were characterized by X-ray diffraction. For complex **8** the barrier for internal ring−ring rotation was determined by low-temperature NMR spectroscopy and the result was confirmed by DFT calculations.

Inversely Polarized Phosphaalkenes

L. Weber,* G. Noveski, T. Braun, H.-G. Stammler, B. Neumann .... 562−567

Synthesis of the η^2-1-Phosphaallene Complexes $[(\eta^5\text{-}C_5H_5)(CO)(NO)W\{\eta^2\text{-}R^1P{=}C{=}C(R^2)H\}]$ (R^1 = *t*Bu, Cy; R^2 = Ph, H) from $[(\eta^5\text{-}C_5H_5)(CO)(NO)W{=}C{=}C(R^2)H]$ (R^2 = Ph, H) and Inversely Polarized Phosphaalkenes $R^1P{=}C(NMe_2)_2$ (R^1 = *t*Bu, Cy), and Their Structure

Keywords: Vinylidene complexes / Phosphaallene complexes / Phosphaalkenes / Tungsten



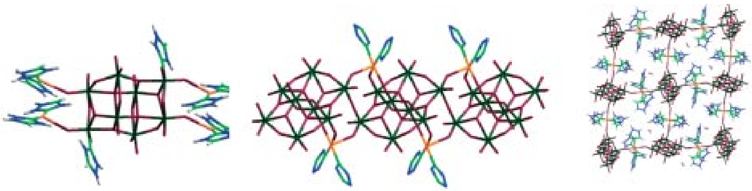
The reaction of vinylidene complexes $[(\eta^5\text{-}C_5H_5)(CO)(NO)W{=}C{=}C(H)R^1]$ (R^1 = Ph,H) with the phosphaalkenes $R^2P{=}C(NMe_2)_2$ (R^2 = *t*Bu, *c*-C_6H_{11}) affords the novel η^2-1-phosphaallene complexes $[\eta^2\text{-}\{R^1P{=}C{=}C(H)R^2\}W(CO)(NO)(\eta^5\text{-}C_5H_5)]$.

Templated Octamolybdates

K. Pavani, S. E. Lofland, K. V. Ramanujachary, A. Ramanan* .... 568−578

The Hydrothermal Synthesis of Transition Metal Complex Templated Octamolybdates

Keywords: Solvothermal synthesis / Molybdenum / Supramolecular chemistry / Organic−inorganic hybrid composites



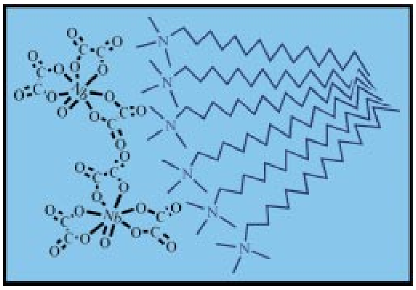
The present work demonstrates the role of a transition metal complex and temperature in influencing the hydrothermal crystallization of octamolybdate cluster based solids with varying dimensionality. The crystal structures are rationalized in terms of supramolecular interactions between soluble molecular precursors.

A Niobium Sol−Gel Precursor

M. A. Bizeto, V. R. L. Constantino* .... 579−584

Niobium Oxide Mesophases Obtained by Self-Assembly of an Aqueous Soluble Niobium Complex Precursor and Organic Templates

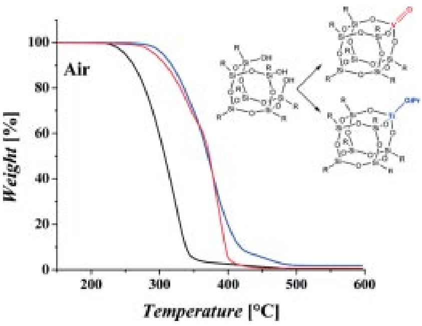
Keywords: Niobium / Mesophases / Organic−inorganic hybrid composites / Template synthesis / Sol−gel synthesis



The ammonium trioxalato(oxido)niobate is evaluated as a water-soluble inorganic precursor for the sol−gel-like synthesis of organized niobium oxide mesophases using organic templates as structure-directing agents. The benefits of using this precursor are the low cost, easy handling, and the opportunity to recycle the starting material directly from the niobium oxide.

Metal-Containing Isobutylsilsesquioxanes

Metal isobutylsilsesquioxanes containing Ti^{IV} and V^{V} prepared by direct corner-capping of a trisilanolisobutylsilsesquioxane precursor. The hybrid inorganic–organic nature of these compounds and the possibility of dispersing catalytically active metal centres in a highly efficient way within organic matrices have been investigated by dispersing these compounds in a polypropylene matrix by melt blending.

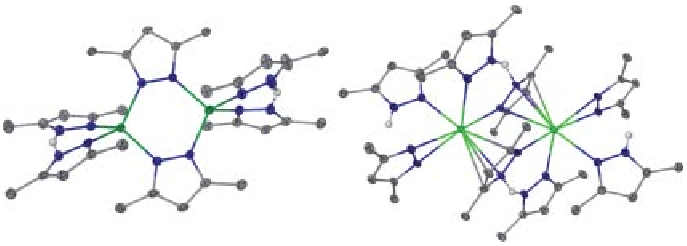


F. Carniato, E. Boccaleri,*
L. Marchese, A. Fina, D. Tabuani,
G. Camino **585–591**

Synthesis and Characterisation of Metal Isobutylsilsesquioxanes and Their Role as Inorganic–Organic Nanoadditives for Enhancing Polymer Thermal Stability

Keywords: Silsesquioxanes / Titanium / Vanadium / Polymers / Nanocomposites

Pyrazolate Complexes



Stabilization through hydrogen bonding between neutral pyrazole and anionic pyrazolato ligands is the main structure-determining force in a group of novel alkaline earth and rare earth metal diisopropylpyrazolates.

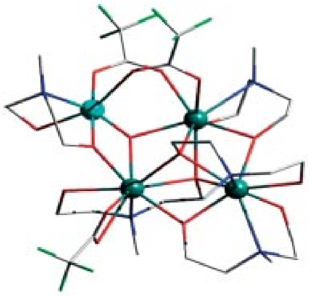
J. Hitzbleck, G. B. Deacon,
K. Ruhlandt-Senge* **592–601**

Structural Trends in Alkaline Earth and Rare Earth Metal 3,5-Diisopropylpyrazolates

Keywords: Alkaline earth metals / Lanthanoids / N ligands / Coordination modes

Coordination Modes

The versatility in the bonding modes of the trifluoroacetate ligand is reflected in the X-ray structures of the complexes $[Y_3Cu(\eta^3\text{-}OH)(mdeaH)_5(TFA)_3](TFA)_2(H_2O)$ (**1**) and $[Ba_3(mdeaH_2)_4(TFA)_6]_{1\infty}$ (**2**), where it acts not only in a terminal (η^1 and η^2) or bridging-chelating (μ,η^2 and $\mu_3\text{-}\eta^2{:}\eta^2{:}\eta^1$) manner but also as a counterion. The unique $\mu_3\text{-}\eta^2(O,O'){:}\eta^2(O,F){:}\eta^1(O)$ bonding mode in **2** shows the metal···F interaction, observed for the first time for a TFA ligand.



1

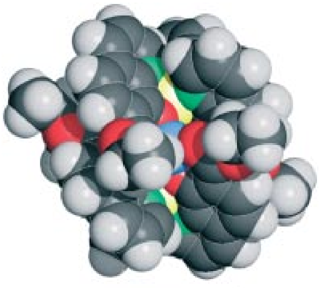
S. Mishra,* J. Zhang,
L. G. Hubert-Pfalzgraf, D. Luneau,
E. Jeanneau **602–608**

The Interplay between Yttrium and Barium or Copper Trifluoroacetates and *N*-Methyldiethanolamine: Synthesis of a Heterometallic Y_3Cu Trifluoroacetate Complex and a Homometallic Ba-TFA 1D Polymer

Keywords: Heterometallic complexes / Yttrium / Copper / Barium / N,O ligands

Metallosupramolecular Chemistry

Hierarchical self-assembly is an appropriate tool in order to obtain oligonuclear coordination compounds. In the presented example, lithium cations act as a "glue", which connects simple mononuclear complexes to supramolecular aggregates.



$[Li_3(ligand)_6Ni_2]^+$

M. Albrecht,* M. Fiege, M. Baumert,
M. de Groot, R. Fröhlich, L. Russo,
K. Rissanen **609–616**

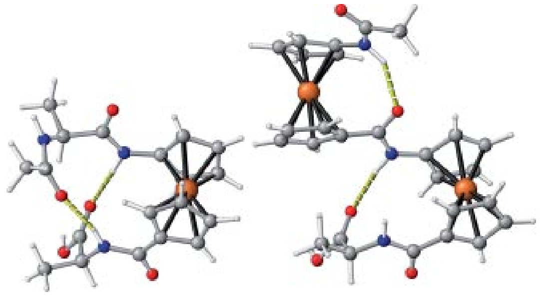
Hierarchical, Lithium-Templated Assembly of Helicate-Type Complexes: How Versatile Is This Reaction?

Keywords: Dinuclear complexes / Helicates / Hierarchical assembly / Chelate ligands / N,O ligands

CONTENTS

Ferrocene Peptides

Keywords: Conformation analysis / Hydrogen bonds / Metallocenes / Molecular modelling / Solid-phase synthesis



The development of solid-phase peptide synthesis for ferrocene amino acids, conformational analyses of the peptides, on-bead oxidation procedures and on-bead binding assays paves the way for devising selective redox-controlled receptor and transporter systems, which, by synthetic design, are amenable to parallel solid-phase peptide synthesis and on-bead oxidation and screening assays.