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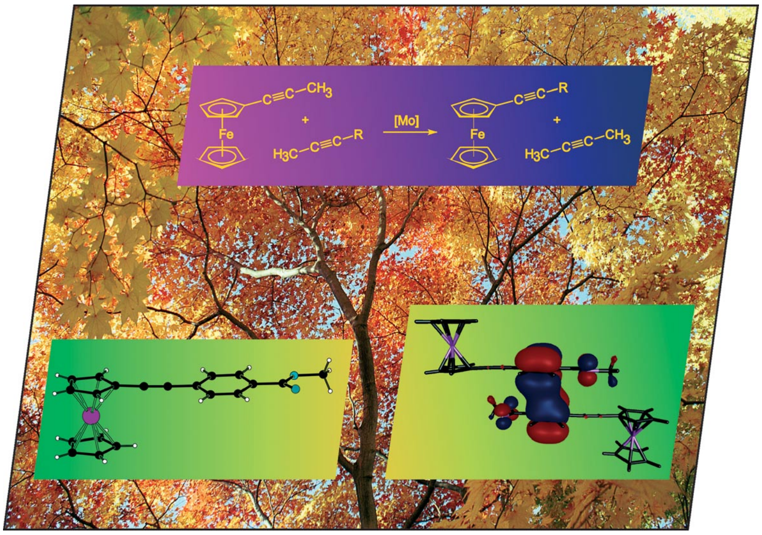
A union formed by chemical societies in Europe (ChemPubSoc Europe) has taken the significant step into the future by merging their traditional journals, to form two leading chemistry journals, the *European Journal of Inorganic Chemistry* and the *European Journal of Organic Chemistry*. Three further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

COVER PICTURE

The cover picture shows the reaction scheme for the cross-metathesis of (prop-1-yn-1-yl)ferrocene with substituted propynes effected by catalysts generated from [Mo(CO)$_6$] and halophenols, situated on a background full of typical ferrocene, autumn-like colors. The metathesis reaction affords good yields of unsymmetric ferrocenyl alkynes, thus offering a new alternative approach toward their preparation. Also shown are the crystal structure of methyl 4-[(ferrocenyl)ethynyl]benzoate and the orbital diagram of its solid-state π···π stacked dimer as calculated by DFT methods. A survey of various substrates and catalysts, results of X-ray structure analysis and DFT calculations as well as electrochemical data for a series of (phenylethynyl)ferrocenes substituted at the phenyl ring are discussed in the article by M. Kotora, P. Štěpnička et al. on p. 3911ff.



CONTENTS

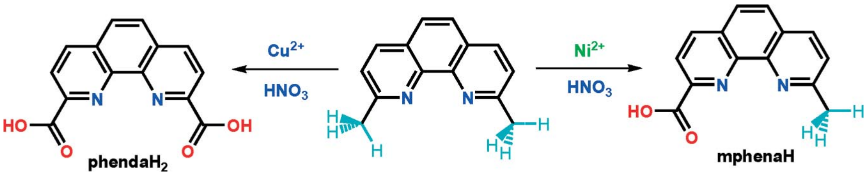
SHORT COMMUNICATION

Ligand Design

L.-L. Fan, C.-J. Li, Z.-S. Meng,
M.-L. Tong* 3905–3909

Metal-Mediated One-Step In Situ Oxidation of 2,9-Dimethyl-1,10-phenanthroline and Formation of Transition-Metal and Lanthanoid Complexes

Keywords: Copper / Nickel / Lanthanides / Oxidation / Ligand design



One-step in situ selective oxidations of 2,9-dimethyl-1,10-phenanthroline to 9-methyl-1,10-phenanthroline-2-carboxylic acid and 1,10-phenanthroline-2,9-dicarboxylic acid were carried out by utilizing HNO_3 as the oxidant in the presence of Cu^{II}, Ni^{II}, and $Cu^{II}-Ln^{III}$ salts under hydrothermal conditions.

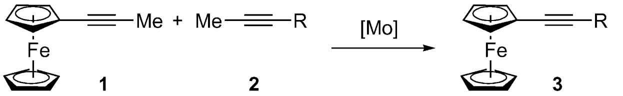
FULL PAPERS

Alkyne Metathesis

T. Bobula, J. Hudlický, P. Novák,
R. Gyepes, I. Císařová, P. Štěpnička,*
M. Kotora* 3911–3920

Mo-Catalyzed Cross-Metathesis Reaction of Propynylferrocene

Keywords: Alkynes / Metallocenes / Metathesis / Electrochemistry / X-ray diffraction



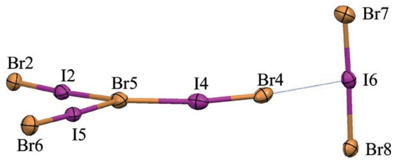
Mortreux-type catalysts promote cross metathesis of (prop-1-yn-1-yl)ferrocene (**1**) with functionalized alkynes **2** to give the corresponding alkynylferrocenes **3** with good selectivity and yields. The structures of selected products were determined by X-ray crystallography, and the results were correlated with DFT calculations. A series of alkynes $4\text{-}XC_6H_4C{\equiv}CFc$ (Fc = ferrocenyl) was studied by electrochemical methods.

Interhalides

M. C. Aragoni, M. Arca,*
F. A. Devillanova, M. B. Hursthouse,
S. L. Huth, F. Isaia, V. Lippolis,
A. Mancini, G. Verani 3921–3928

Reactions of Halogens/Interhalogens with Polypyridyl Substrates: The Case of 2,4,6-Tris(2-pyridyl)-1,3,5-triazine

Keywords: Halides / Interhalides / FT-Raman spectroscopy / X-ray crystal structures / Density functional calculations



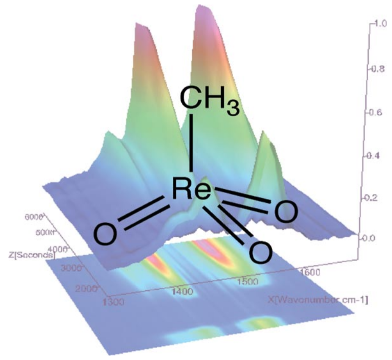
The products in the solid state obtained from the reactions between 2,4,6-tris(2-pyridyl)-1,3,5-triazine and I_2, Br_2, IBr, and ICl have been isolated and characterized. All compounds are salts containing the protonated donor counterbalanced by polyhalide anions of various complexity. In particular, $(H_3tptz^{3+})(I_3Br_4^-)(IBr_2^-)_2$ provides the first example of a planar $I_3Br_4^-$ moiety.

Catalyst Synthesis

J. K. M. Mitterpleininger, N. Szesni,
S. Sturm, R. W. Fischer,
F. E. Kühn* 3929–3934

Insights into a Nontoxic and High-Yielding Synthesis of Methyltrioxorhenium (MTO)

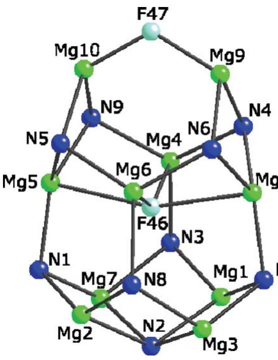
Keywords: Rhenium / Alkylzinc compounds / IR spectroscopy / Synthesis



The versatile precatalyst methyltrioxorhenium(VII) (MTO) can now be synthesized without the use of highly toxic tin organyls. Detailed insights into the synthetic procedure are given with respect to the starting materials, reagents, reaction conditions, yields and byproducts.

Magnesium Imides

A set of magnesium imides derived from fluoro- and chloro-substituted anilines have been synthesized and characterized in the solid state. Either tetrameric cubane or hexameric prismatic structures are obtained depending on the relative steric hindrance within the aggregates. In addition, a novel decametallic cage complex has been characterized as a minor side product arising from C−F bond cleavage.

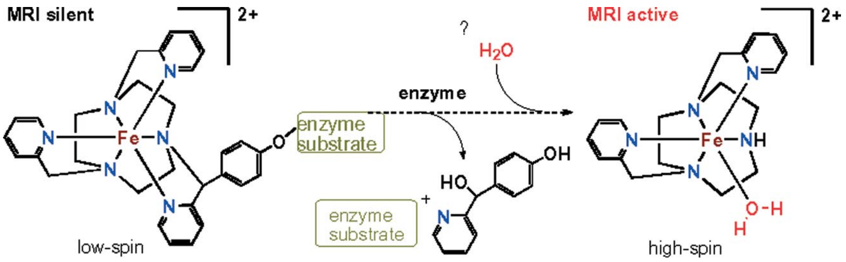


J. A. Rood, S. E. Hinman, B. C. Noll, K. W. Henderson* .... 3935−3942

The Use of Halide-Substituted Anilines for the Formation of Magnesium Imides

Keywords: Magnesium / Imides / Amides / X-ray crystallography / Aggregation

Spontaneous Complex Fragmentation



With the aim to develop a molecular imaging probe, a low-spin ferrous complex (MRI silent) was synthesized to test whether it fragments spontaneously to a paramagnetic ferrous complex (MRI active) upon enzymatic removal of a glycosyl moiety. While the underlying hexadentate ligand indeed rapidly disintegrates to a pentadentate one under physiological conditions, the metal complex does not.

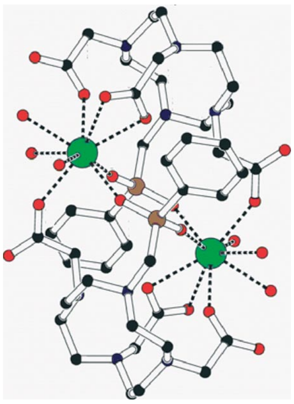
V. Stavila, Y. Stortz, C. Franc, D. Pitrat, P. Maurin, J. Hasserodt* .... 3943−3947

Effective Repression of the Fragmentation of a Hexadentate Ligand Bearing an Auto-Immolable Pendant Arm by Iron Coordination

Keywords: Iron / Macrocyclic ligands / Prodrugs / Auto-immolable spacer / Low-spin complex

Ln^{III}-dota-Type Ligands

The crystal and molecular structures of ten lanthanide complexes of 2,2′,2′′-(10-{[hydroxy(phenyl)phosphoryl]methyl}-1,4,7,10-tetraazacyclododecan-1,4,7-triyl)triacetic acid are presented in this work. These O-coordinated complexes are the first structurally characterised intermediates on the path from the ligand to the classical in-cavity N,O-coordinated complexes.



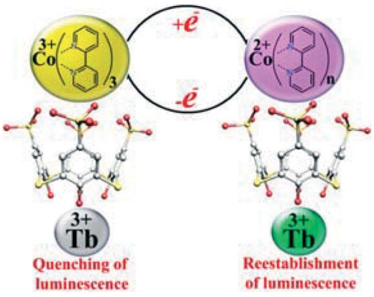
P. Vojtíšek,* J. Rohovec, J. Klimentová .... 3948−3956

Lanthanide Complexes of 2,2′,2′′-(10-{[Hydroxy(phenyl)phosphoryl]methyl}-1,4,7,10-tetraazacyclododecan-1,4,7-triyl)triacetic Acid: Structural Characterisation of Intermediates from the Proposed Complexation Mechanism in the Systems of Ln^{III}-dota-Type Ligands

Keywords: Phosphorus / Imaging agents / Lanthanides / X-ray diffraction

Redox-Switchable Co−Ln Complexes

The emission of the heterometallic $[Co(dipy)_3]^{3+}-Tb^{III}$ complex on a *p*-sulfonatothiacalix[4]arene platform can be switched on by the bulk electrochemical reduction of the Co^{III} block with further switching off by subsequent reoxidation of Co^{II}.



V. Skripacheva,* A. Mustafina,* N. Rusakova, V. Yanilkin, N. Nastapova, R. Amirov, V. Burilov, R. Zairov, S. Kost, S. Solovieva, Yu. Korovin, I. Antipin, A. Konovalov .... 3957−3963

Heterometallic $Co^{III}-Ln^{III}$ (Ln = Gd, Tb, Dy) Complexes on a *p*-Sulfonatothiacalix[4]arene Platform Exhibiting Redox-Switchable Metal-to-Metal Energy Transfer

Keywords: Heterometallic complexes / Lanthanides / Luminescence / Calixarenes

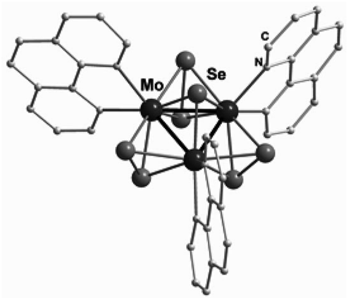
CONTENTS

Triangular Cluster Complexes

A. L. Gushchin, M. N. Sokolov,*
E. V. Peresypkina, A. V. Virovets,
S. G. Kozlova, N. F. Zakharchuk,
V. P. Fedin* 3964–3969

Crystal Structure, Electronic Structure, and Solid-State Electrochemistry of Cluster Complexes of $M_3Se_7^{4+}$ (M = Mo, W) with Noninnocent *o*-Phenanthroline and Se_2^{2-} Ligands

Keywords: Molybdenum / Tungsten / Chalcogens / Cyclic voltammetry / Electronic structure



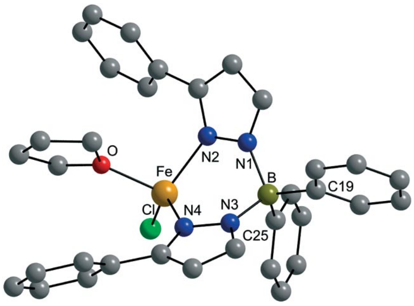
The crystal structure, electronic structure, and electrochemistry of $[M_3Se_7(o\text{-phen})_3]X_4$ (M = Mo, W) cluster complexes were investigated. Strong interactions between the X^- and Se_2 ligands of the M_3Se_7 cluster, observed in the crystal, can be described as donor–acceptor covalent bonding and are important enough to influence the redox behavior of the cluster.

Low-Coordinate Iron Complexes

M. Wagner, C. Limberg*,
B. Ziemer 3970–3976

Low-Coordinate Iron Complexes Based on Bis(pyrazolyl)borate and Their Reactivity

Keywords: Iron / Oxidation / Bidentate ligands / Coordination compounds / Pyrazole



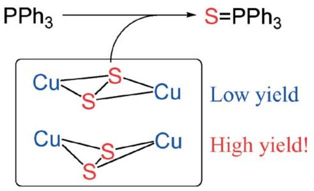
Bis(pyrazolyl)borates with bulky substituents enable the synthesis of three- and four-coordinate Fe^{II} complexes. As the BpFe units can be considered as models for the $(His)_2Fe$ moieties found in nonheme iron enzymes, attempts were also made to replace the remaining halido ligands by other residues resembling amino acids or cofactors. In the course of such studies it turned out that the BpFe core is sensitive to carboxylate functions.

(Disulfido)dicopper Complexes

Y. Kajita, J. Matsumoto, I. Takahashi,
S. Hirota, Y. Funahashi, T. Ozawa,
H. Masuda* 3977–3986

Syntheses, Characterization, and Reactivities of (μ-η^2:η^2-Disulfido)dicopper(II) Complexes with *N*-Alkylated *cis,cis*-1,3,5-Triaminocyclohexane Derivatives

Keywords: Disulfide / Dicopper complexes / Triaminocyclohexane / Dihedral angles



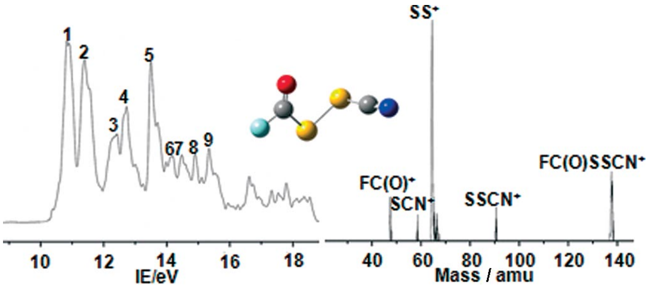
The syntheses and characterization of novel (μ-η^2:η^2-disulfido)dicopper complexes with *N*-alkylated *cis,cis*-1,3,5-triaminocyclohexane derivatives are described and their reactivities are discussed in terms of the dihedral angle of the two CuS_2 planes in the $Cu_2(S_2)$ structure.

Properties of FC(O)SSCN

S. Tong, L. Du, L. Yao, M. Ge,*
C. O. Della Védova 3987–3995

Gas-Phase Generation, Structure, Spectroscopy, and Quantum Chemical Calculations of Fluorocarbonylsulfur Thiocyanate, FC(O)SSCN

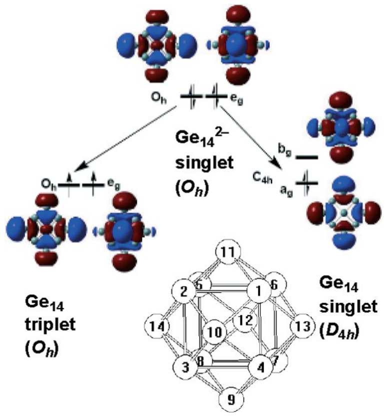
Keywords: Structures / Ionization and dissociation processes / Photoelectron spectroscopy / Theoretical calculations



Fluorocarbonylsulfur thiocyanate was generated from a gas–solid reaction of FC(O)SCl on the surface of finely powdered AgSCN. The reaction products were detected and characterized by photoelectron spectroscopy and photoionization mass spectrometry. The geometrical and electronic structures of FC(O)SSCN were investigated by theoretical calculations and PES experiments.

14-Atom Bare Germanium Clusters

Density functional theory (DFT) at the hybrid B3LYP level has been applied to the germanium clusters $Ge_{14}z$ (z = −8, −6, −4, −2, 0, +2, +4) starting from seven different initial configurations. An O_h omnicapped cube structure is the most stable for Ge_{14}^{2-} followed by a hexagonal antiprism structure with a relative energy of 42.7 kcal/mol. Structures derived from the omnicapped cube are also the global minima for Ge_{14} and Ge_{14}^{2+}. Structures based on the D_{6h} hexagonal wheel are also found.



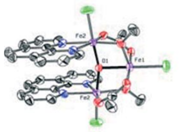
R. B. King,* I. Silaghi-Dumitrescu, M. M. Uţă .... **3996−4003**

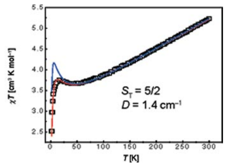
Beyond the Icosahedron: A Density Functional Theory Study of 14-Atom Germanium Clusters

Keywords: Germanium / Metal clusters / Density functional theory

A μ_3-Oxido Trinuclear Iron Cluster

The synthesis, crystal structure and magnetochemical characterization of the new μ-oxido cluster $[Fe_3(\mu_3\text{-}O)(\mu_2\text{-}CH_3O)_2(\mu_2\text{-}CH_3COO)_2(phen)_2Cl_3]$ is reported. The core of the complex is an isosceles triangle with a rare T-shaped geometry. Magnetic studies revealed an antiferromagnetically exchanged S_T = 5/2 ground-state spin with a positive D value of about 1.5 cm^{-1}.





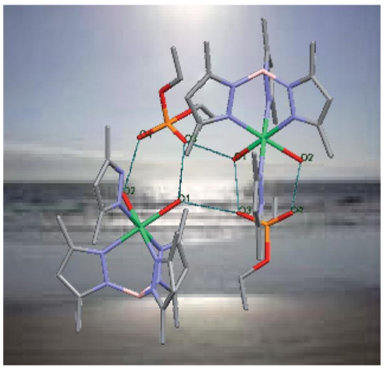
P. Alborés,* E. Rentschler* .... **4004−4011**

A T-Shaped μ_3-Oxido Trinuclear Iron Cluster with High Easy-Plane Anisotropy: Structural and Magnetic Characterization

Keywords: Polynuclear complexes / Magnetic properties / DFT calculations / (μ-Oxido)iron core / Easy-plane anisotropy

Hydrogen-Bonding Interactions

Nickel(II) complexes containing hydrotris(3,5-dimethylpyrazolyl)borate and phosphate esters were prepared and fully characterized. X-ray crystallographic studies reveal that the phosphate ester anions are hydrogen bonded to the pyrazole moieties or to the O−H groups of water molecules. Their behavior in solution was investigated by 1D and 2D ^{1}H NMR spectroscopic techniques.



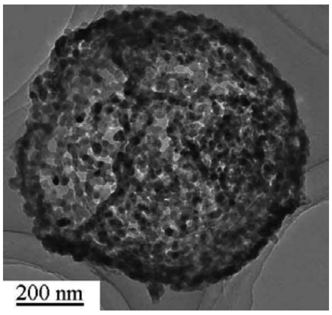
M. D. Santana,* L. López-Banet, G. García, L. García, J. Pérez,* M. Liu .... **4012−4018**

Hydrogen Bonding and Anion Binding in Structures of Tris(pyrazolyl)boratenickel(II) and Phosphate Esters

Keywords: Hydrogen bonds / Nickel / NMR spectroscopy / Receptors / Solid-state structures / Phosphates

Hollow Spheres

$CoFe_2O_4$ hollow spheres with sizes ranging from 600 nm to 1 μm were prepared through hydrothermal carbonization, followed by calcination. XRD, TEM, HRTEM, SEM, N_2 adsorption−desorption, XPS, IR, and TG techniques were used to characterize the product in detail, and the magnetic properties were also investigated.



Y. Meng, D. Chen,* X. Jiao ... **4019−4023**

Synthesis and Characterization of $CoFe_2O_4$ Hollow Spheres

Keywords: Nanostructures / Template synthesis / Magnetic materials / Mesoporous materials

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* Author to whom correspondence should be addressed.

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