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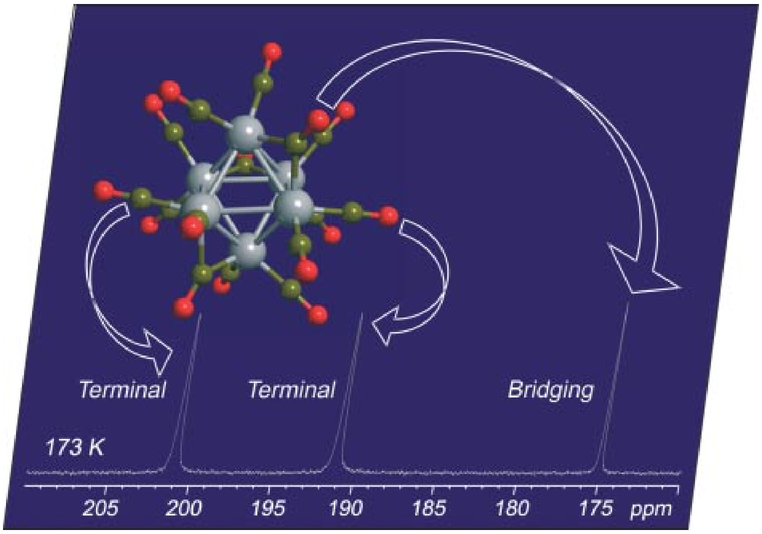
The EUChemSoc Societies have taken the significant step into the future by merging their traditional journals, to form two leading chemistry journals, the *European Journal of Inorganic Chemistry* and the *European Journal of Organic Chemistry.* Three further EUChemSoc Societies (Austria, Czech Republic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

COVER PICTURE

The cover picture shows the structure and the ^{13}C NMR spectrum of $[Ir_6(CO)_{15}]^{2-}$ at 173 K. It features an unprecedented μ_2-bridging carbonyl low frequency shift; the resonances of the terminal μ_1-carbonyl groups are placed at higher frequencies. This unusual trend has been explained by combined use of DFT calculations and solid-state NMR parameters, such us chemical shift tensors and shielding anisotropies. The scalar and *S*pin-*O*rbit (SO) relativistic two-component *Z*ero-*O*rder *R*egular *A*pproximation (ZORA) methods have been employed in the geometry optimization and NMR chemical shift calculations, respectively. The large SO contribution (26.6 ppm) to the ^{13}C chemical shifts of the μ_2-bridging CO groups accounts for the position of the experimentally observed resonance. This work outlines the importance of the SO evaluation in cases of atoms connected to heavy metal atoms. Details are discussed in the article by L. Garlaschelli, R. Gobetto et al. on p. 3487ff.



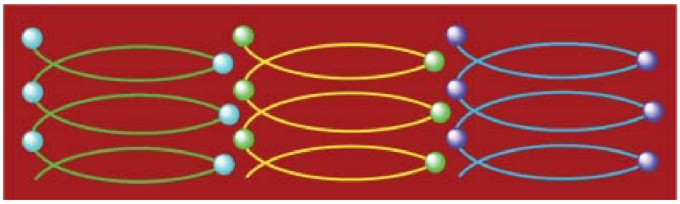
MICROREVIEW

Chirality Transfer

C. He, Y. G. Zhao, D. Guo,* Z. H. Lin, C. Y. Duan* **3451–3463**

Chirality Transfer through Helical Motifs in Coordination Compounds

Keywords: Helical structures / Chirality / Building intermediates / Conformational chirality



This microreview describes the design of helicates and the structural features that are necessary for chirality transfer. The extension of chirality from one-dimensional to three-dimensional chiral polymers in complicated chiral architectures is also described.

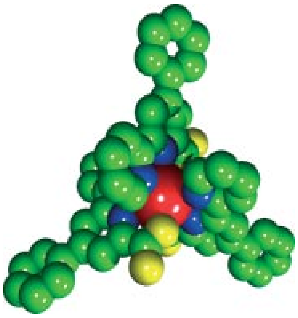
SHORT COMMUNICATIONS

Luminescent Lanthanide Complexes

G. S. Kottas, M. Mehlstäubl, R. Fröhlich, L. De Cola* **3465–3468**

Highly Luminescent, Neutral, Nine-Coordinate Lanthanide(III) Complexes

Keywords: Lanthanides / Luminescence / Sensitizers / Energy transfer / Carboxylate ligands



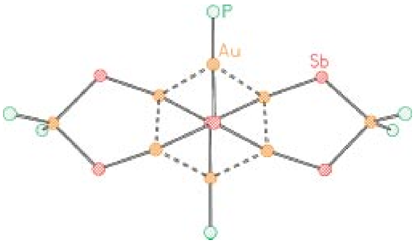
A simple approach to synthesize small and neutral, but highly luminescent lanthanide complexes has been used.

Bridging Antimony Ligands

D. Fenske,* A. Rothenberger, S. Wieber **3469–3471**

Synthesis and Characterization of a Gold Complex Containing $[SbPh]^{2-}$ and $[SbPh_2]^-$ Anions as Bridging Ligands

Keywords: Bridging ligands / Aurophilicity / Antimony / Gold / Group 15 ligands



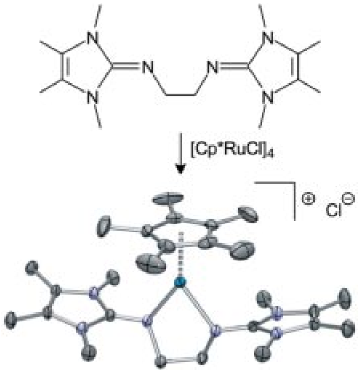
The synthesis and structural characterization of the gold antimony complex $[Au_8(SbPh)_2(SbPh_2)_4(PEt_3)_6]$ is reported. The Au^I ions show weak aurophilic interactions and are bridged by $[SbPh]^{2-}$ and $[SbPh_2]^-$ anions.

Coordinative Unsaturation

D. Petrovic, T. Glöge, T. Bannenberg, C. G. Hrib, S. Randoll, P. G. Jones, M. Tamm* **3472–3475**

Synthesis and Reactivity of 16-Electron Pentamethylcyclopentadienyl–Ruthenium(II) Complexes with Bis(imidazolin-2-imine) Ligands

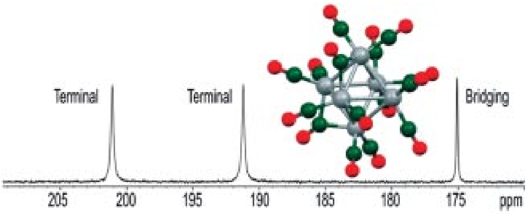
Keywords: Ruthenium / Cyclopentadienyl ligands / N ligands / 16-electron complexes / Coordinative unsaturation



The syntheses of stable 16-electron ruthenium half-sandwich complexes bearing bis(imidazolin-2-imine) ligands are presented and their stabilities are ascribed to the strong π-electron releasing capability of the imine ligand on the basis of experimental results and DFT calculations.

FULL PAPERS

Unprecedented μ_2-CO Shift



Terminal or bridging CO peak in Ir cluster? The unusual chemical shift of the bridging carbonyl ligands in $[Ir_6(CO)_{15}]^{2-}$ is explained by a combined use of solid-state NMR parameters and DFT calculations.

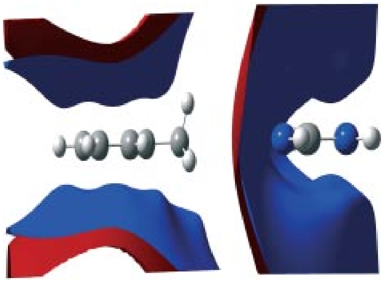
**M. R. Chierotti, L. Garlaschelli,*
R. Gobetto,* C. Nervi, G. Peli, A. Sironi,
R. Della Pergola 3477–3483**

An Unusual Carbonyl Chemical Shift in a Carbonylhexairidium Cluster: A Combined Solid-State NMR and DFT Approach

Keywords: NMR spectroscopy / DFT calculations / Carbonyl cluster / Iridium / Chemical shift tensors / Shielding anisotropy

DNA Cleavage

DNA binding and cleavage reactions in the presence of copper(II) terpyridine complexes were investigated, and the effect of the substituent on the terpyridine ring was explained by computational studies.



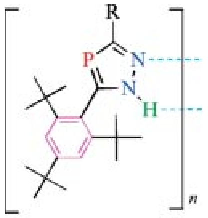
**V. Uma, M. Elango,
B. U. Nair* 3484–3490**

Copper(II) Terpyridine Complexes: Effect of Substituent on DNA Binding and Nuclease Activity

Keywords: Copper / Tridentate ligands / DNA binding / Nuclease activity

Phosphorus Heterocycles

[2+3] Cycloaddition of phosphaalkynes with trimethylsilyldiazomethane derivatives proceeds in spite of the presence of a bulky Mes* (= 2,4,6-tBu$_3$C$_6$H$_2$) group which exceedingly stabilizes the C≡P moiety. The corresponding [2+3] adducts, 1,2,4-diazaphospholes, show dimer or trimer structure connected by hydrogen bonds. The first observed trimer structure of 1,2,4-diazaphosphole includes effects of the bulky aryl group enhancing the molecular aggregation by the CH–π interaction.



n = 2 (R = SiMe$_3$)
3 (R = H)

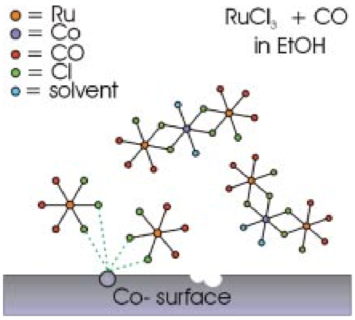
**S. Ito,* H. Miyake,
M. Yoshifuji* 4911–3496**

1,3-Dipolarophile Character of an Extremely Bulky Phosphaalkyne Mes*C≡P (Mes* = 2,4,6-tBu$_3$C$_6$H$_2$) Leading to the Formation of 1,2,4-Diazaphospholes with Unique Hydrogen Bonding Properties

Keywords: Heterocycles / Phosphaalkynes / Cycloaddition / Hydrogen bonds / DFT calculations / X-ray crystallography

Carbonylation on Metal Surfaces

The reductive carbonylation of ruthenium and osmium halides in the presence of cobalt and iron surfaces has been used for synthesis of mixed-metal complexes. Linear, dimetallic, chlorido-bridged, trinuclear complexes $[M_2Cl_2(\mu\text{-}Cl)_4(CO)_6M'(L)_2]$ (M = Ru, Os; M′ = Fe, Co; L = CH$_3$CH$_2$OH, H$_2$O) were obtained through the interaction between reducing RuCl$_3$ or OsCl$_3$ and the oxidizing solid metal surface.



**M. Jakonen, P. Hirva, T. Nivajärvi,
M. Kallinen, M. Haukka* 3497–3588**

Surface-Assisted Synthesis and Behavior of Dimetallic Mixed-Metal Complexes $[M_2Cl_2(\mu\text{-}Cl)_4(CO)_6M'(L)_2]$ (M = Ru, Os; M′ = Fe, Co; L = CH$_3$CH$_2$OH, H$_2$O)

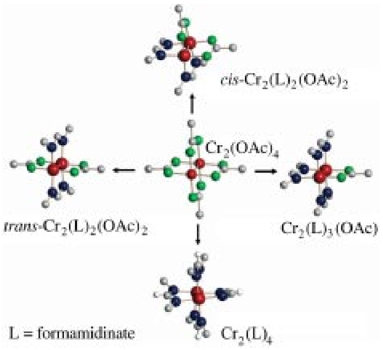
Keywords: Ruthenium / Osmium / Cobalt / Iron / Synthesis design

Chromium Complexes

F. A. Cotton, Z. Li, C. A. Murillo* **3509–3513**

Precursors for Assembly of Supramolecules Containing Quadruply Bonded Cr_2^{4+} Units: Systematic Preparation of Cr_2(formamidinate)$_n$(acetate)$_{4-n}$ (n = 2–4)

Keywords: Metal–metal bonds / Supramolecular chemistry / Chromium / Corner piece precursors



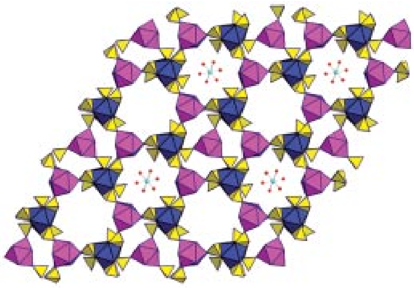
Quadruply bonded dichromium complexes with a mixed set of ligands having different labilities, Cr_2(formamidinate)$_n$(acetate)$_{4-n}$ (n = 2–4), were synthesized to serve as corner-piece precursors for assembly of large molecules by selective substitution of the labile acetate groups by polydentate dianions.

Mixed-Valence Compounds

B. M. Casari,* V. Langer **3514–3518**

New Open-Framework Mixed-Valence Chromium(III) Cerium(III)/(IV) Sulfate: $CrCe^{III}{}_7Ce^{IV}{}_6(HSO_4)_6(SO_4)_{21}\cdot75H_2O$

Keywords: Mixed-valent compounds / Lanthanides / Cerium sulfate / X-ray diffraction



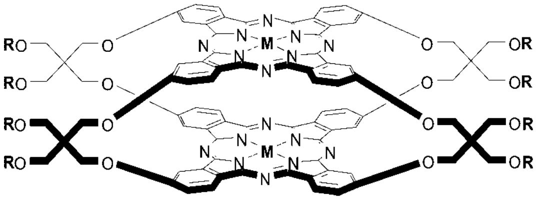
The cerium atoms, interlinked by sulfate groups, extend to form layers held together by hydrogen-bonding contacts. Perpendicular to these layers there are 10 Å wide channels.

Cofacial Bismetallophthalocyanine

M. Özer, A. Altındal, A. R. Özkaya, B. Salih, M. Bulut, Ö. Bekaroğlu* **3519–3526**

Synthesis, Characterization, and Electrochemical and Electrical Properties of Novel Pentaerythritol-Bridged Cofacial Bismetallophthalocyanines and Their Water-Soluble Derivatives

Keywords: Phthalocyanines / Cofacial configuration / Synthesis / Cyclic voltammetry / Thermopower



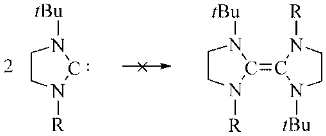
Novel cofacial bismetallophthalocyanines were synthesized at 300 °C. The resulting Pcs accommodating four pentaerythritol monoacetal side groups were hydrogenated. The target water-soluble cofacial bismetallophthalocyanines were obtained by heating suspensions of the compounds bearing the eight OH side groups in aqueous KOH.

Wanzlick Carbenes

M. K. Denk,* A. Hezarkhani, F.-L. Zheng **3527–3534**

Steric and Electronic Effects in the Dimerization of Wanzlick Carbenes: The Alkyl Effect

Keywords: Carbenes / Thiourea / Thermochemistry / Dimerization / Enetetramine / Steric hindrance / DFT calculations / Steric effects / Electronic effects



R	ΔG° [kcal]
R = Me	–0.9
R = Et	+2.1
R = *i*Pr	+4.5
R = *t*Bu	+25.5

The study of Wanzlick carbenes with mixed *N*-alkyl substitution reveals the relative importance of electronic and steric effects preventing dimerization to the respective enetetramines.

Sulfur Imides

The structure of (*Z*)-$CF_3CF_2N{=}SCl_2$ is determined by X-ray diffraction analysis at low temperature. The central sulfur(+IV)−imide bond is well described by the NBO analysis model as a semipolar $S^+{-}N^-$ bond with strong hyperconjugative interactions.

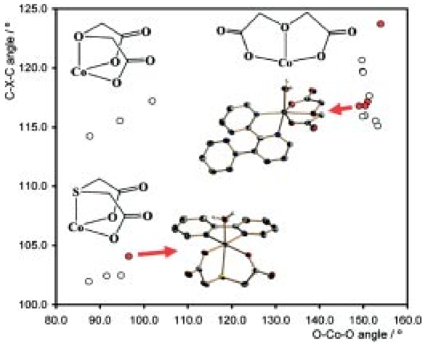
N. L. Robles, R. M. S. Álvarez,
E. H. Cutin, C. O. Della Védova,*
M. F. Erben, R. Boese, H. Willner,
R. Mews .... 3535−3542

Anomeric Interactions in Pentafluoroethylimidosulfurous Dichloride, $CF_3CF_2N{=}SCl_2$: Structural, Conformational and Configurational Properties in the Gaseous and Condensed Phases

Keywords: Imides / Conformation analysis / Structural analysis / Hyperconjugation / Sulfur

Multidentate Ligands

The general stereochemical features of cobalt thiodiacetate and oxydiacetate complexes are illustrated on the basis of the available structural data and some new crystal structures presented in this paper (red dots).



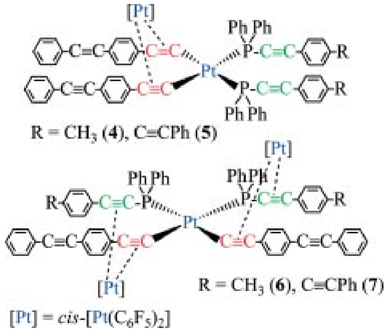
A. Grirrane, A. Pastor, E. Álvarez,
C. Mealli, A. Ienco, P. Rosa,
A. Galindo* .... 3543−3552

Thiodiacetate and Oxydiacetate Cobalt Complexes: Synthesis, Structure and Stereochemical Features

Keywords: Cobalt / Thiodiacetate / Oxydiacetate / Tridentate Ligands / Coordination modes

Alkynylplatinum Complexes

The platinum complexes *cis*-$[\{Pt(PPh_2C{\equiv}CR)_2(\mu\text{-}\eta^1{:}\eta^2\text{-}C^{\alpha},C^{\beta}\text{-}C{\equiv}CC_6H_4C{\equiv}CPh)_2\}Pt(C_6F_5)_2]$ (**4**, **5**) and $[\{Pt(\mu\text{-}\eta^1{:}\eta^2\text{-}C^{\alpha},C^{\beta}\text{-}C{\equiv}CC_6H_4C{\equiv}CPh)_2(\mu\text{-}1\kappa P{:}2\eta^2\text{-}C^{\alpha},C^{\beta}\text{-}PPh_2C{\equiv}CR)_2\}\{Pt(C_6F_5)_2\}_2]$ (**6**, **7**) stabilized by double ethynyltolan or mixed ethynyltolan/(arylalkynyl)phosphane bridging systems, respectively, have been synthesised from *cis*-$[Pt(C{\equiv}CC_6H_4C{\equiv}CPh)_2(PPh_2C{\equiv}CR)_2]$ by treatment with *cis*-$[Pt(C_6F_5)_2(thf)_2]$.



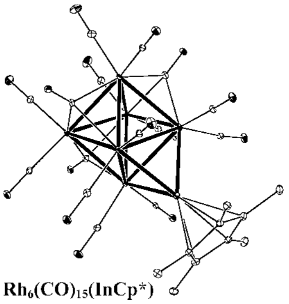
A. García, E. Lalinde,*
M. T. Moreno .... 3553−3560

Ethynyltolan Platinum Complexes with (Arylalkynyl)phosphane Ligands

Keywords: Alkyne ligands / Phosphane ligands / Platinum / X-ray diffraction

InCp* Coordination Chemistry

Reaction of the hexanuclear carbonyl rhodium cluster $Rh_6(CO)_{15}(NCMe)$ with InCp* complex under mild conditions results in the formation of $Rh_6(CO)_{16-x}(InCp^*)_x$, x = 1−2 clusters.



$Rh_6(CO)_{15}(InCp^*)$

E. V. Grachova,* G. Linti ..... 3561−3564

Reactivity of InCp* Towards Transition Metal Carbonyl Clusters: Synthesis and Structural Characterization of the $Rh_6(CO)_{16-x}(InCp^*)_x$ Mixed-Metal Cluster Compounds, x = 1−2

Keywords: Rhodium / Indium / Cluster compounds

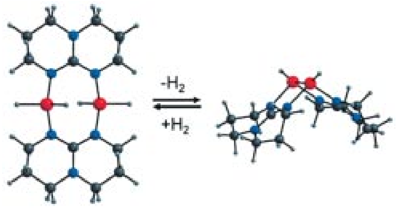
CONTENTS

H_2 Elimination Reactions

O. Ciobanu, H.-J. Himmel* 3565–3572

Repeated Dihydrogen Elimination from Boranes and Gallanes Stabilized by Guanidine-Type Bases: A Quantum Chemical Study Motivated by Recent Experimental Results

Keywords: Hydrides / Group 13 elements / Quantum chemical calculations / Hydrogen storage



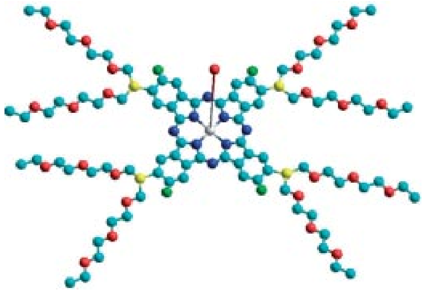
The thermodynamic properties of repeated H_2 eliminations from guanidine-stabilized group 13 element hydrides are analysed on the basis of quantum chemical calculations. Some of these reactions might be interesting for hydrogen storage and/or olefin hydrogenation.

Oxotitanium Phthalocyanines

D. Atilla, M. Durmuş, Ö. Yılmaz,
A. G. Gürek, V. Ahsen,
T. Nyokong* 3573–3581

Synthesis, Photophysical and Photochemical Properties of Poly(oxyethylene)-Substituted Phthalocyaninato Oxotitanium(IV) Complexes

Keywords: Phthalocyanine / Titanium / Quantum yields / Singlet oxygen / Fluorescence



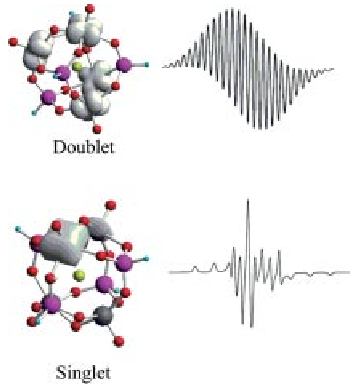
The synthesis, photophysical and photochemical properties of tetra- and chlorotetrapoly(oxyethylene)-substituted oxotitanium(IV) phthalocyanines are reported for the first time. The complexes show high singlet oxygen quantum yields, which make them useful for PDT applications.

Vanadium Organophosphonates

N. H. Thong, J. K. Jabor, R. Stößer,
M. Meisel,* B. Ziemer 3582–3593

Localization and Delocalization of Spin Density in Mixed-Valence (V^{IV}/V^{V}) $[(V_2O_3)_2(PhPO_3)_4\subset F]^{-n}$ (n = 1, 2): Theoretical and Experimental Studies

Keywords: Adsorption / DFT calculation / ESR / Hyperfine structure / Vanadium / Cage compounds



DFT calculations were carried out to determine the energies and spin-density distribution for the cage $[(V_2O_3)_2(PhPO_3)_4\subset F]^{-n}$ structures with the symmetries D_{2d}, C_{2v}, and C_s. The calculated hyperfine coupling constants are in a good agreement with those determined by ESR spectroscopy. A proposal is given for the localization/delocalization of spin density based on thermally driven fluctuations of the cage geometry or alternatively by hopping of the unpaired electron inside the cage.