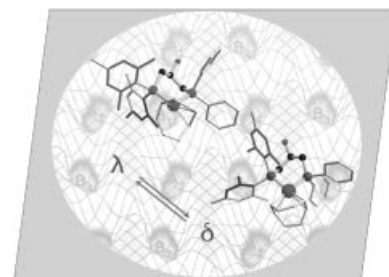


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COVER PICTURE

The cover picture shows two conformations of the chiral chelate cation $[\{\kappa\text{-P}(\text{Mes})_2\text{CH}_2\text{CH}(\text{OH})\text{CH}_2\text{-}\kappa\text{-P}(\text{Ph})_2\}\text{Rh}(\eta^4\text{-COD})]^+$ which is active as an enantioselective hydrogenation catalyst. The δ - and λ -twist conformations of the six-membered diphosphane chelate cycle are shown together with a projection of the hypersurface relevant to the transition between these enantiomeric forms. The hypersurface is generated by force field calculations. The specific force field is derived by refinement of the relevant force field parameters by genetic algorithms on the basis of eleven compounds of this type. The predictions made by this model are in almost quantitative agreement with the experimental data: The λ -form is calculated to be $3.1 \text{ kJ}\cdot\text{mol}^{-1}$ more stable than the δ -form (experimental: $3.4 \text{ kJ}\cdot\text{mol}^{-1}$). The $\delta \rightleftharpoons \lambda$ transition is predicted to be accompanied by a coupled rotation of the mesityl groups (color code in the cover picture) in full agreement with the experimental results. The upper threshold of the activation barrier of the transition is calculated to be $69.1 \text{ kJ}\cdot\text{mol}^{-1}$; the experimental value is $64.4 \text{ kJ}\cdot\text{mol}^{-1}$. This novel approach to molecular modeling is described in the article by G. Huttner et al. on p. 3111 ff. The quantitative NMR analysis of the structure and dynamics of compounds containing six-membered diphosphane chelate cycles is presented in the accompanying article by G. Huttner et al. on p. 3129 ff.



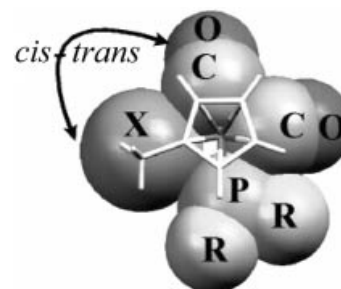
MICROREVIEW

Contents

3067 N. J. Coville,* D. C. Leventis

Organometallic Chemistry: Structural Isomerization Reactions in Confined Environments

Keywords: Isomerization / Solid-state reactions /
 Surfaces / Organometallic chemistry /
 Rhenium

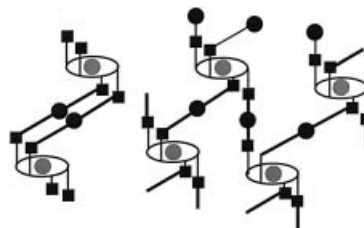


SHORT COMMUNICATIONS

3079 B. Zimmer, V. Bulach, M. W. Hosseini,*
A. De Cian, N. Kyritsakas

1- and 2-D Coordination Networks Based on Porphyrin and Copper: an Example of Supramolecular Isomerism

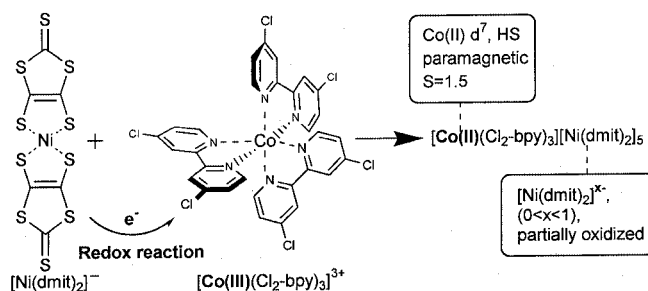
Keywords: Porphyrin / Pyridine / Isonicotinoyl / Coordination network / Copper / Atropo-isomerism



3083 M. J. J. Mulder, J. G. Haasnoot,
D. J. Stufkens, L. H. Tjeng, H.-J. Lin,
C.-T. Chen, J. Reedijk*

A New Synthetic Strategy for Magnetic Metal Bis(dithiolene) Based Conductors

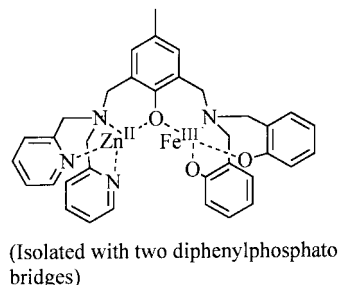
Keywords: Redox chemistry / Conducting materials / X-ray absorption spectroscopy / EPR spectroscopy / Raman spectroscopy



3087 C. Belle,* I. Gautier-Luneau, L. Karmazin,
J.-L. Pierre, S. Albedyhl, B. Krebs,
M. Bonin

Regio-Directed Synthesis of a Zn^{II}Fe^{III} Complex from an Unsymmetrical Ligand and Its Relevance to Purple Acid Phosphatases

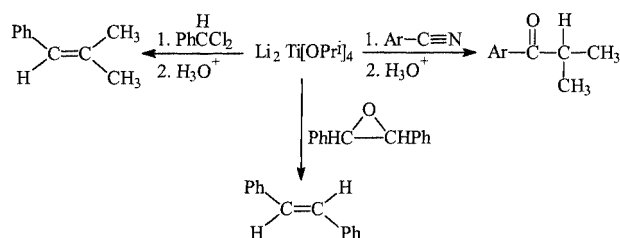
Keywords: Heterometallic complexes / Zinc / Iron / Unsymmetrical ligands / Phosphatases



3091 J. J. Eisch,* J. N. Gitua

Astonishing Alkylation and Unusual Reduction Reactions of Anionic Titanium(II) Isopropoxide Complexes: Evidence for SET Processes in Transition-Metal Oxidative Additions

Keywords: Titanium / Subvalent compounds / Oxidative addition / Alkylation / Electron transfer



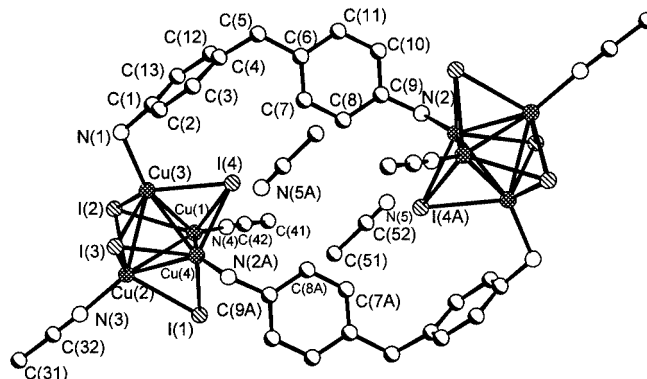
FULL PAPERS

3097 R.-H. Wang, M.-C. Hong,* J.-H. Luo,
R. Cao,* J.-B. Weng



The First Two Novel Metallamacrocycles Constructed from Cubane-Like Cu_4I_4 Cluster Units and Ditopic Diamines

Keywords: Amine ligands / Copper / Metallacycles / X-ray diffraction

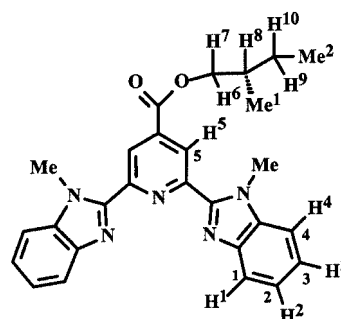


3101 G. Muller, J. P. Riehl, K. J. Schenk,
G. Hopfgartner, C. Piguet, J.-C. G. Bünzli*



Lanthanide Triple Helical Complexes with a Chiral Bis(benzimidazole)pyridine Derivative

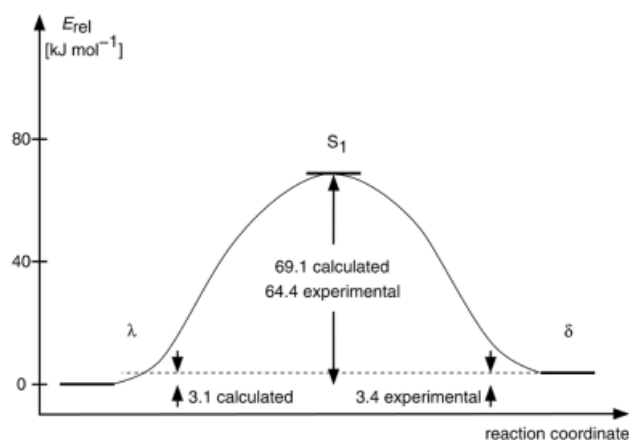
Keywords: Lanthanides / Tridentate ligands / Chirality / Luminescence / Stability constants



3111 V. Schulz, A. Frick, G. Huttner*

How to Model the Conformational Behaviour of Saturated Diphosphane Chelate Cycles: The Conformational Rearrangement Processes of $[\{\kappa\text{-PAR}_2\text{CH}_2\text{CH}(\text{OH})\text{CH}_2\text{-}\kappa\text{-PAR}'_2\}\text{Rh}(\eta^4\text{-COD})]^+$

Keywords: Rhodium / Phosphane ligands / Chelates / Molecular modelling / Conformation analysis

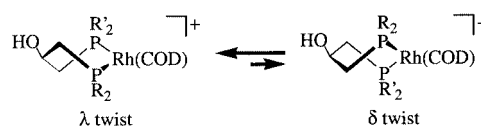


3129 A. Frick, V. Schulz, G. Huttner*



Interconversion of δ and λ Forms of Six-Membered Chelate Cycles – A Quantitative NMR Spectroscopic Study of (Diphosphane)rhodium Compounds

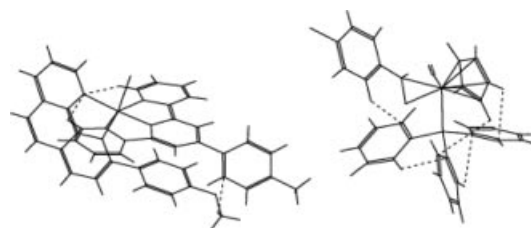
Keywords: Conformational analysis / Diphosphanes / Rhodium / Kinetics / Thermodynamics



3148 H. Suezawa,* T. Yoshida, Y. Umezawa,
S. Tsuboyama, M. Nishio*

CH/ π Interactions Implicated in the Crystal Structure of Transition Metal Compounds – A Database Study

Keywords: Hydrogen bonds / Noncovalent interactions / π interactions / Supramolecular chemistry



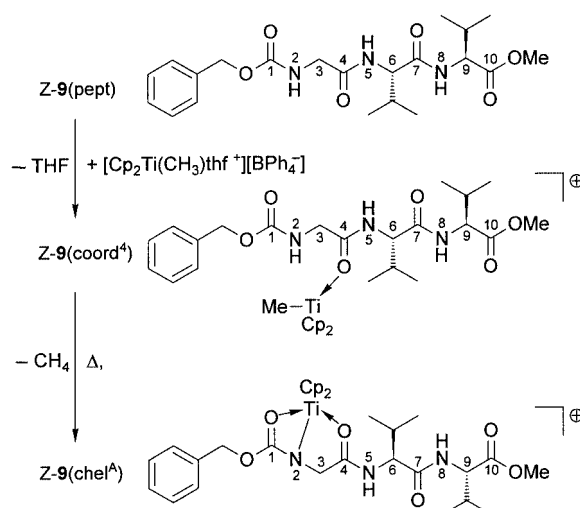
CH/ π interactions disclosed in crystal structure of transition metal compounds

3156 D. Harmsen, G. Erker,* R. Fröhlich,
G. Kehr



Reaction of $[(\text{Cp}_2\text{TiCH}_3)(\text{THF})^+][\text{BPh}_4^-]$ with Tripeptide Derivatives: Formation of Cationic (Peptide)titanocene Complexes

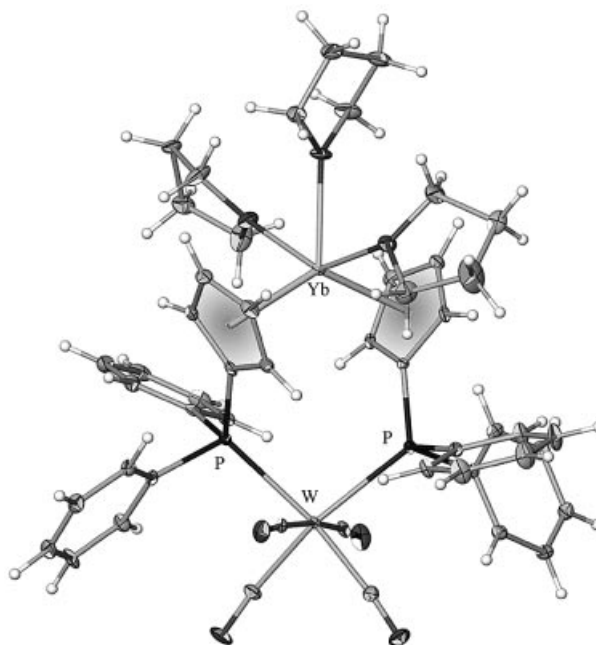
Keywords: Bioinorganic chemistry / Peptides / Metallocenes / Titanium / Cations



3172 K. Müller-Buschbaum,* G. B. Deacon,
C. M. Forsyth

$[\text{Yb}(\text{THF})_3(\text{C}_5\text{H}_4\text{PPh}_2)_2\text{W}(\text{CO})_4] \cdot 0.5\text{THF}$ and $[\text{Yb}(\text{THF})(\text{C}_5\text{H}_4\text{PPh}_2)_2(\mu\text{-OC})\text{W}(\text{CO})_3]$: Two New Heterobimetallic Complexes Containing Yb^{II} and W^0

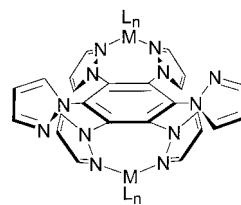
Keywords: Heterometallic complexes / Ytterbium / Tungsten / Carbonyl ligands



- 3178** A. M. Guerrero, F. A. Jalón,*
B. R. Manzano, R. M. Claramunt,
M. D. Santa María, C. Escolástico,
J. Elguero, A. M. Rodríguez,
M. A. Maestro, J. Mahía

Variety in the Coordination Modes of the Ligand Hexakis(pyrazol-1-yl)benzene (Hpzb) to Pd^{II}, Pt^{II} and Cu^I Centres

Keywords: N ligands / Conformational analysis / Palladium / Platinum / Copper / Coordination chemistry

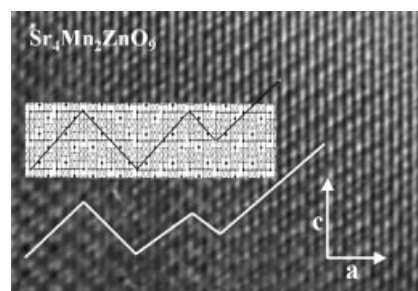


ML_n = Pd(C₆F₅)₂; [Pd(η³-C₄H₇)]⁺; Cu(PMe₃)⁺

- 3190** M. Hernando,* K. Boulahya, M. Parras,
J. M. González-Calbet

Synthesis, Microstructural Characterisation and Magnetic Study of Two New One-Dimensional Members of the (A₃ZnMnO₆)_α (A₃Mn₃O₉)_β Homologous Series (A = Ba, Sr)

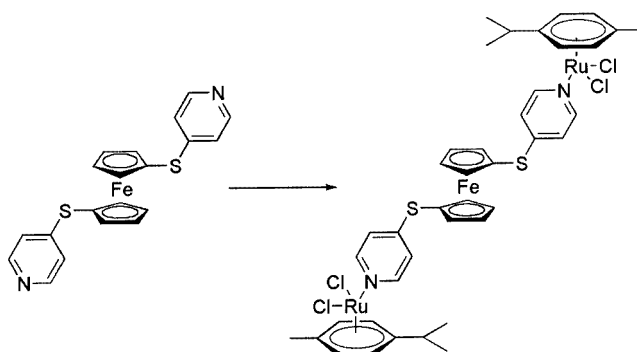
Keywords: Electron diffraction / Electron microscopy / One-dimensional oxides / Magnetic properties / Twinned microstructure



- 3197** R. Horikoshi, T. Mochida,* R. Torigoe,
Y. Yamamoto

Preparation and Electrochemical Properties of Polynuclear Organometallic Complexes Derived from Ferrocene-Containing Bidentate Ligands

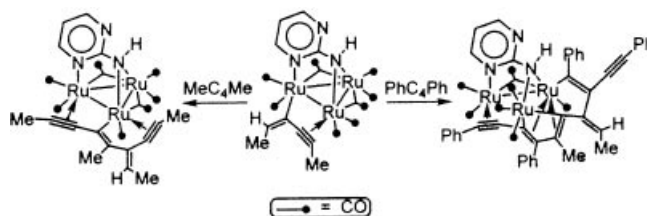
Keywords: Bridging ligands / Cyclic voltammetry / Ruthenium / Rhodium / Iridium / Metallocenes



- 3204** J. A. Cabeza,* I. del Río, M. Moreno,
S. García-Granda, M. Pérez-Priede,
V. Riera

Reactivity of a Triruthenium Ynenyl Cluster Complex with Diynes: Cluster-Mediated Combination of up to Three Substituted Butadiyne Molecules into a Carbon-Rich Hydrocarbyl Ligand

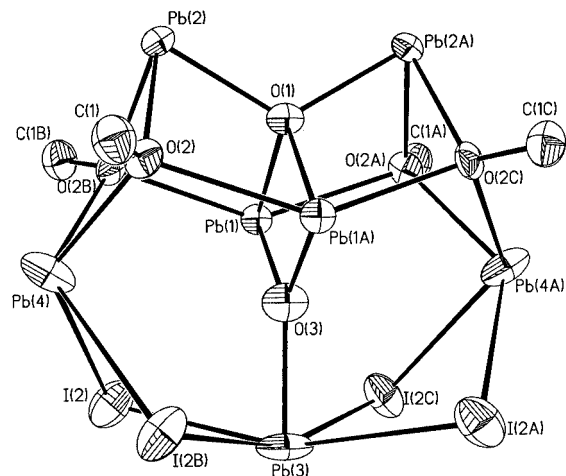
Keywords: Ruthenium / Clusters / Alkynes / C-C bond formation / N ligands



3210 Y.-J. Shi, Y. Xu, X.-T. Chen,* Z. Xue,
X.-Z. You*

Formation and Structure of the Novel Hepta-nuclear Lead(II) Oxo Cluster $[\text{Pb}_7(\mu_3\text{-O})(\mu_4\text{-O})-(\mu_3\text{-OMe})_4(\mu_2\text{-I})_4]\text{I}_2$ with an Unprecedented Cage Structure

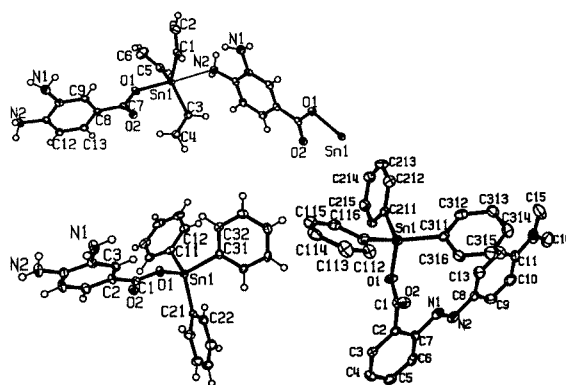
Keywords: Lead / Cluster compounds / Alkoxides / Oxo ligands / Crystal structure



3214 F. P. Pruchnik,* M. Bańbuła, Z. Ciunik,
H. Chojnacki, M. Latocha, B. Skop,
T. Wilczok, A. Opolski, J. Wietrzyk,
A. Nasulewicz

Structure, Properties and Cytostatic Activity of Triorganotin (Aminoaryl)carboxylates

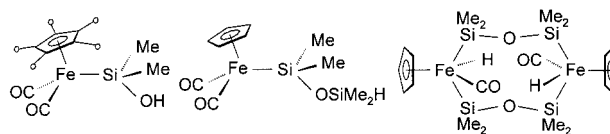
Keywords: Tin / Cytostatic agents / Antitumor activity / O ligands



**3235 W. Malisch,* M. Hofmann, G. Kaupp,
H. Käß, J. Reising**

Si–H-Functionalized Ferriodisiloxanes: Synthesis from the Ferriodimethylsilanol $C_5R_5(OC)_2Fe-SiMe_2OH$ ($R = H, Me$) and Photoinduced Transformation into μ_2 -Disiloxanediyl-Bridged Dinuclear Iron Complexes

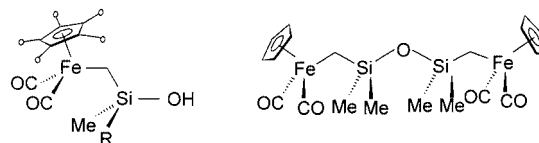
Keywords: Iron / Metallacycles / Oxidative addition / Silicon / Siloxanes



**3242 W. Malisch,* M. Hofmann, M. Nieger,
W. W. Schöller, A. Sundermann**

Synthesis, Structural Characterization and Reactivity of the (Ferriomethyl)silanols $C_5R_5(OC)_2Fe-CH_2-SiMe(R')OH$ ($R = H, Me$; $R' = Me, Ph$)

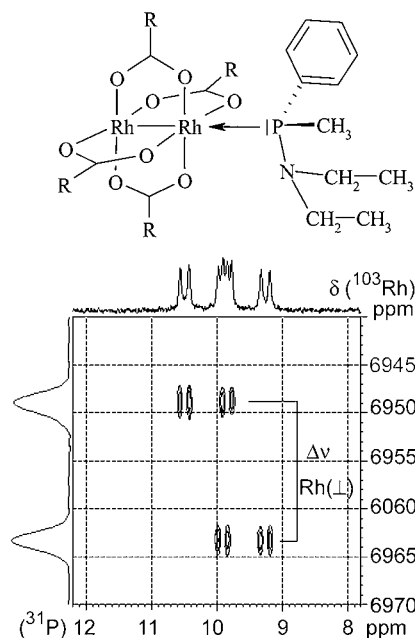
Keywords: Silicon / Iron / Oxygenation / (Metalloalkyl)silanols / Density functional calculations



**3253 D. Magiera, W. Baumann, I. S. Podkorytov,
J. Omelanczuk, H. Duddeck***

Stable $Rh_2(MTPA)_4$ Phosphane Adducts – The First Example of *P*-Chirality Recognition by ^{103}Rh NMR Spectroscopy

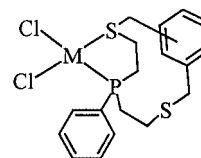
Keywords: Phosphanes / Rhodium / NMR spectroscopy / Chirality / Chiral discrimination



**3258 L. Escribe,* J. A. Muñoz, R. Kivekäs,
R. Sillapää, J. Casabó**

Synthesis, Characterisation and Reactivity towards Pd^{II} and Pt^{II} of *ortho*-, *meta*- and *para*-Xylyl-Based Phosphorus-Containing Macrocycles

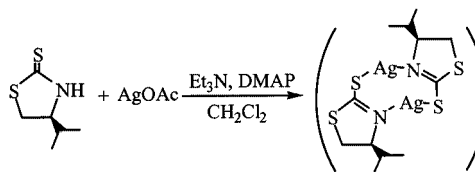
Keywords: Macrocycles / Palladium, Platinum / S ligands / Phosphanes



3264 M. Shi,* J.-K. Jiang, G.-L. Zhao

A Novel Chiral Silver(I) Complex from the Reaction of Thiazolidinethione with AgOAc

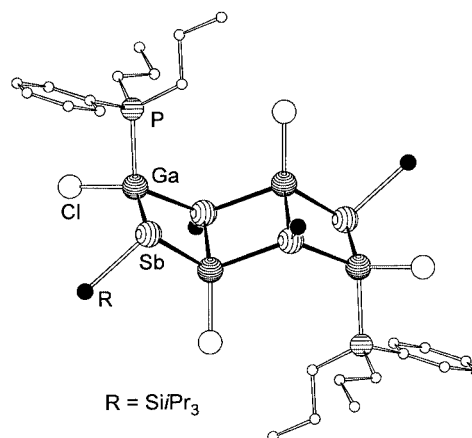
Keywords: Silver / Cluster compounds / S ligands / Structure elucidation



3268 C. von Hänisch,* P. Scheer, B. Rolli

Cyclic and Polycyclic Gallium-Antimony Compounds: Synthesis and Crystal Structures of $[\text{GaCl}(\text{PnPr}_2\text{Ph})(\text{SbSiPr}_3)]_2$ and $[(\text{GaCl})_4(\text{SbSiPr}_3)_4(\text{PnPr}_2\text{Ph})_2]$

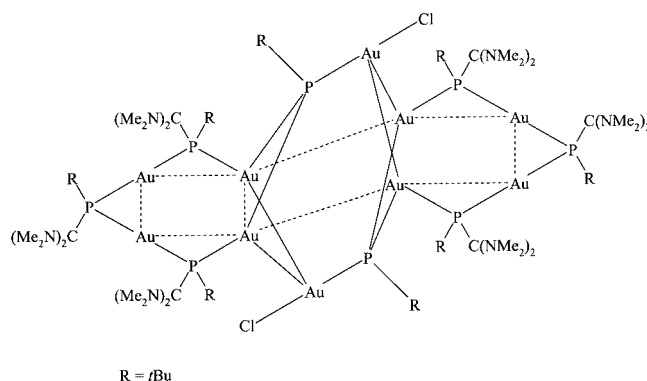
Keywords: Gallium / Antimony / Polycycles / Heterocycles / Semiconductors



3272 L. Weber,* U. Lassahn, H.-G. Stammer, B. Neumann, K. Karaghiosoff

Synthesis and Structure of the Decanuclear Gold(I) Cluster Cation $[\text{Au}_8(\text{AuCl})_2\{\mu_3\text{-P}(\text{tBu})\}_2\{\mu\text{-P}(\text{tBu})=\text{C}(\text{NMe}_2)_2\}_6]^{4+}$ with Bridging Phosphaalkene and Phosphanediide Ligands

Keywords: Cluster compounds / Gold / Phosphaalkenes / Phosphinidenes

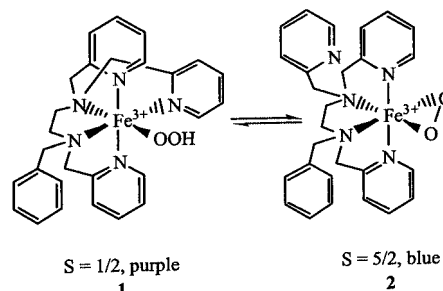


3278 O. Horner,* C. Jeandey, J.-L. Oddou, P. Bonville, C. J. McKenzie, J.-M. Latour



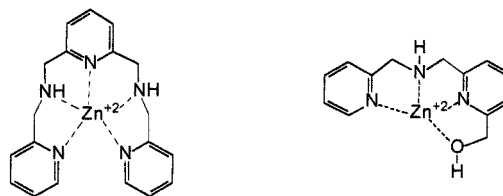
Hydrogenperoxo- $[(\text{bztpen})\text{Fe}(\text{OOH})]^{2+}$ and Its Deprotonation Product Peroxo- $[(\text{bztpen})\text{Fe}(\text{O}_2)]^+$, Studied by EPR and Mössbauer Spectroscopy – Implications for the Electronic Structures of Peroxo Model Complexes

Keywords: EPR spectroscopy / Iron / Mössbauer spectroscopy / Peroxo ligands



3284 T. Darbre,* C. Dubs, E. Rusanov,
H. Stoeckli-Evans

Syntheses of Zinc Complexes with Multidentate Nitrogen Ligands: New Catalysts for Aldol Reactions



Keywords: Aldol reaction / Catalysis / N ligands / N,O ligands / Zinc

3292 S. Dalai, P. S. Mukherjee, G. Rogez,
T. Mallah,* M. G. B. Drew,
N. R. Chaudhuri*

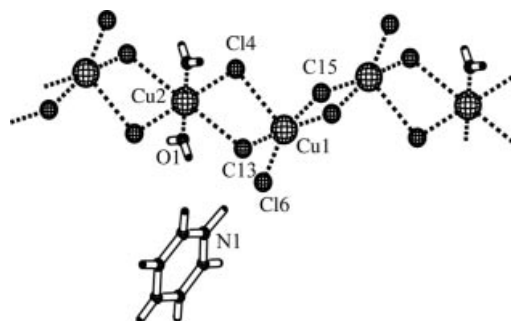
Synthesis, Crystal Structures, and Magnetic Properties of Two New 1D Copper(II) Coordination Polymers Containing Fumarate(−2) and Chelating N,N′-Donor as Ligands



Keywords: Coordination polymers / Copper / Magnetic properties / N ligands

3298 M. Czugler, L. Kótai,* B. Sreedhar,*
A. Rockenbauer, I. Gács, S. Holly

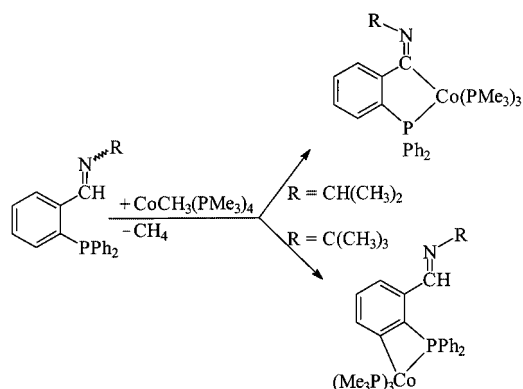
The Effect of HCl on the Copper(II) Chloride/Pyridine/Water System: Synthesis, Properties and Crystal Structure of [(pyH)₂CuCl₄] and [(pyH)₂Cu₃Cl₈(H₂O)₂]_n



Keywords: Copper / IR spectroscopy / EPR spectroscopy / Hydrogen bonds

3305 H.-F. Klein,* R. Beck, U. Flörke,
H.-J. Haupt

Steric Control of Cyclometallation Reactions in Schiff-Base Complexes of Cobalt(I) Containing an Anchoring Diphenylphosphanyl Group

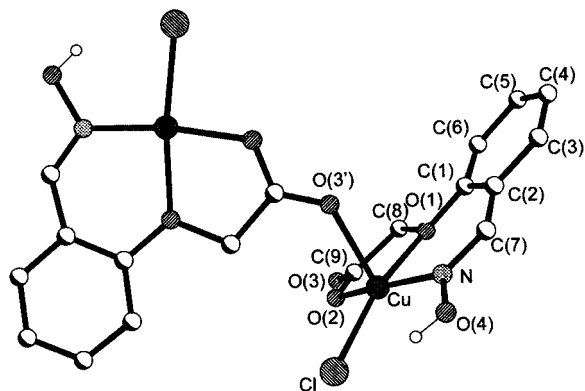


Keywords: Cyclometallation / Cobalt / P ligands / Schiff bases / Regioselectivity

- 3313** S. Shova,* Gh. Novitchi, M. Gdaniec,
A. Caneschi, D. Gatteschi, L. Korobchenko,
V. K. Voronkova, Yu. A. Simonov, C. Turta

Helical 1D Coordination Polymers – Structure and Magnetic Properties of *catena*-Poly[chloro-(μ-(2-[(hydroxyimino)methyl]phenoxy)acetato-*N,O,O,O'*)copper(II)]

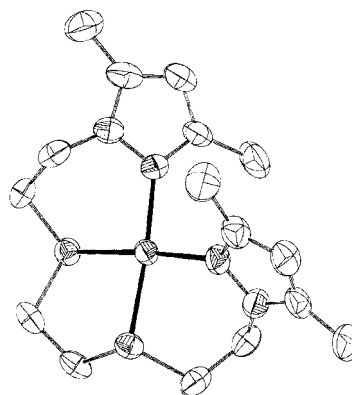
Keywords: Copper / EPR spectroscopy / Magnetic properties / N ligands / O Ligands



- 3319** J. García-Antón, J. Pons,* X. Solans,
M. Font-Bardia, J. Ros*

Synthesis of New Pd^{II} Complexes Containing Thioether–Pyrazole Hemilabile Ligands – Structural Analysis by ¹H and ¹³C NMR Spectroscopy and Crystal Structures of [PdCl₂(bdo)] and [Pd(bdo)](BF₄)₂ [bdo = 1,8-Bis(3,5-dimethyl-1-pyrazolyl)-3,6-dithiaoctane]

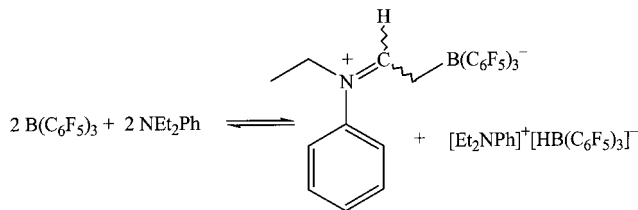
Keywords: Hemilabile ligands / N ligands / Palladium / S ligands



- 3328** N. Millot, C. C. Santini,* B. Fenet,
J. M. Basset

Formation and Characterization of Zwitterionic Stereoisomers from the Reaction of B(C₆F₅)₃ and NEt₂Ph: (*E*)- and (*Z*)-[EtPhN⁺=CHCH₂-B⁻(C₆F₅)₃]

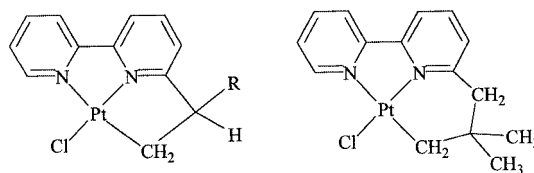
Keywords: Boranes / Aniline / Zwitterions / NMR spectroscopy



- 3336** A. Zucca,* S. Stoccoro, M. A. Cinellu,
G. Minghetti, M. Manassero, M. Sansoni

Metallation of Unactivated Methyl Groups – Platinum(II) Derivatives with 6-Alkyl-2,2'-bipyridines

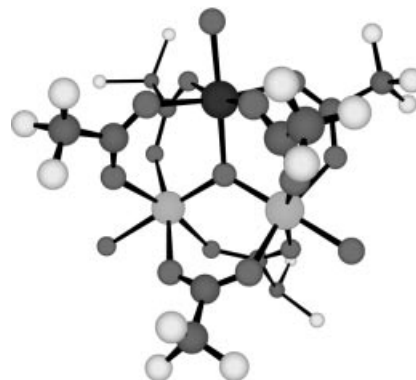
Keywords: Platinum / N ligands / Cyclometallation



- 3347** K. S. Gavrilenko, A. Vértés, G. Vanko,
L. F. Kiss, A. W. Addison,*
T. Weyhermüller, V. V. Pavlishchuk*

Synthesis, Magnetochemistry, and Spectroscopy
of Heterometallic Trinuclear Basic Trifluoro-
acetates $[\text{Fe}_2\text{M}(\mu_3\text{-O})(\text{CF}_3\text{COO})_6(\text{H}_2\text{O})_3]\cdot\text{H}_2\text{O}$
(M = Mn, Co, Ni)

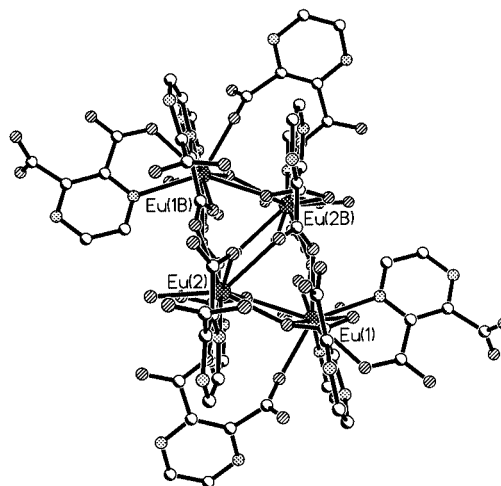
Keywords: Heterometallic complexes / Carboxylate
ligands / Magnetic properties / Iron /
Manganese / Cobalt / Nickel / Trinuclear
complexes



- 3356** X.-J. Zheng, L.-P. Jin,* S.-Z. Lu

Hydrothermal Syntheses, Structures, and
Properties of First Examples of Lanthanide(III)
2,3-Pyrazinedicarboxylates with Three-Dimen-
sional Framework

Keywords: Hydrothermal synthesis / Lanthanides /
Coordination polymer / N ligands /
O ligands



- 3365** Index 2002

Editorial staff and publishers express their thanks to all authors, referees, and readers for their continued trust, support, and interest over the past year and wish them a prosperous 2003.