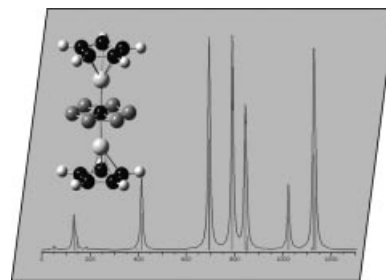


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COVER PICTURE

The cover picture shows the structure and IR spectrum of a novel triple-decker complex $(C_5H_5)Fe(B_6C)Fe(C_5H_5)$ obtained by density functional calculations. Similar results on a series of $(C_nH_n)M(B_6X)M(C_nH_n)$ ($M = Fe, Ru, Mn, Re$; $X = B, C, N$; $n = 5, 6$) complexes containing planar hexacoordinate carbon or other nonmetal atoms at the centers of the B_6X middle-deckers were also obtained. Natural orbital analyses indicate that the nonmetal centers X follow the octet rule in these complexes, and effective $d-\pi$ coordination interactions exist between the partially filled Fe 3d orbitals and the delocalized π orbitals of the three parallel ligands. This work provides strong theoretical evidence to facilitate future experimental characterization of the long-sought planar hexacoordinate carbon atom and expands the structural domain of traditional sandwich-type transition-metal complexes. Details are discussed in the article by S.-D. Li et al. on p. 2567 ff.



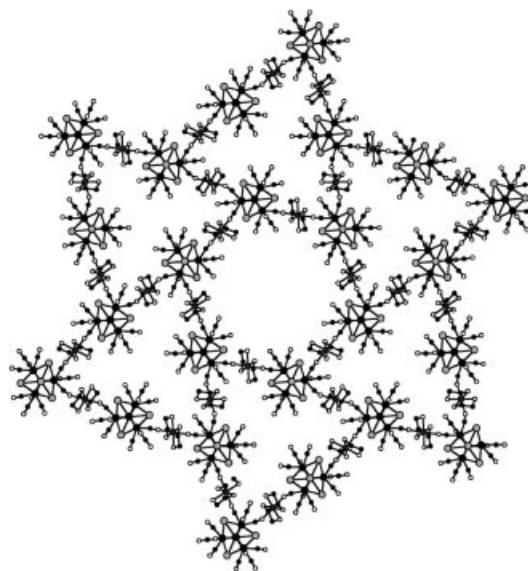
MICROREVIEW

Contents

2533 **O. A. Efremova, Y. V. Mironov,***
 V. E. Fedorov

Design of Cyano-Bridged Coordination Polymers Based on Tetrahedral Rhenium Cluster Cyanide Complexes and 3d Transition Metals

Keywords: Cluster compounds / Cyanides / N ligands / Rhenium / Transition metals

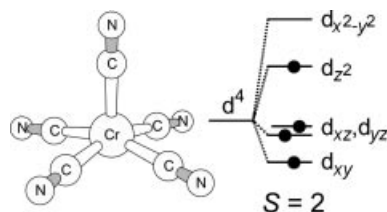


SHORT COMMUNICATIONS

2551 R. J. Deeth*

A Theoretical Rationale for the Formation, Structure and Spin State of Pentacyanochromate(II)

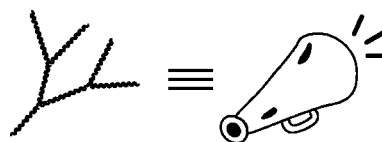
Keywords: Density functional theory / Ligand field theory / Angular overlap model / COSMO / Solvation effects



2556 C.-O. Turrin, A. Maraval, G. Magro, V. Maraval, A.-M. Caminade,* J.-P. Majoral*

First Example of Dendrons as Topological Amplifiers

Keywords: Dendrons / Dendrimers / Macrocycles / Phosphorus / NMR spectroscopy

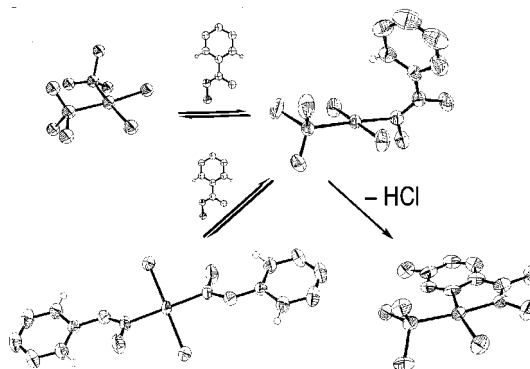


2561 S. Otto,* A. Chanda, P. V. Samuleev, A. D. Ryabov*



DFT-Verified Crystallographic Mechanism of Cycloplatination

Keywords: Platinum / C-H activation / Metallacycles / X-ray diffraction / Density functional calculations

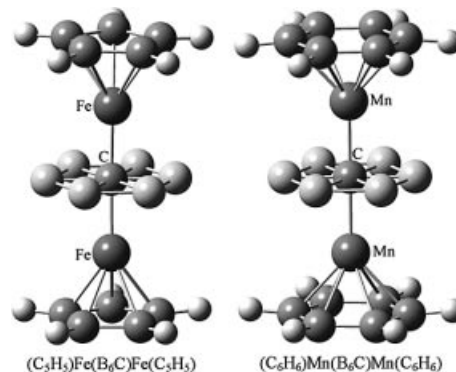


FULL PAPERS

2567 S.-D. Li,* C.-Q. Miao, G.-M. Ren, J.-C. Guo

Triple-Decker Transition-Metal Complexes $(C_nH_n)M(B_6C)M(C_nH_n)$ ($M = Fe, Ru, Mn, Re$; $n = 5, 6$) Containing Planar Hexacoordinate Carbon Atoms

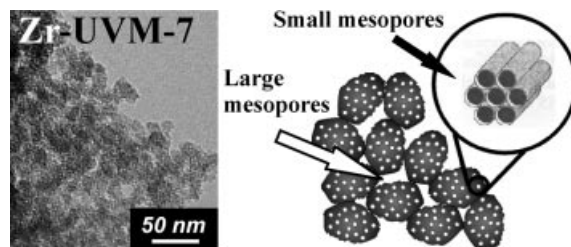
Keywords: Planar hexacoordinate carbon / Triple-decker transition-metal complexes / Density functional theory / Geometric structures / Electronic structure / IR spectroscopy



- 2572** D. Ortiz de Zárate, A. Gómez-Moratalla,
C. Guillem, A. Beltrán, J. Latorre,
D. Beltrán, P. Amorós*

High-Zirconium-Content Nano-Sized Bimodal Mesoporous Silicas

Keywords: Mesoporous materials / Zirconia / Surfactants / Nanoparticles / Bimodal porous materials

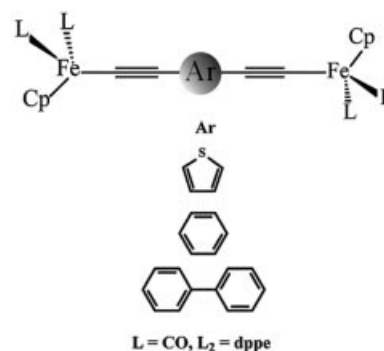


- 2582** L. Medei, L. Orian, O. V. Semeikin,
M. G. Peterleitner, N. A. Ustynyuk,
S. Santi,* C. Durante, A. Ricci, C. Lo Sterzo*



A Joint Experimental and Computational Study on the Electronic Communication in Diethynyl-aryl-Bridged $(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\eta^2\text{-dppe})$ and $(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2$ Units

Keywords: Mixed-valence compounds / Iron / Electron transfer / Electronic communication / Ethynylaryl bridging ligand

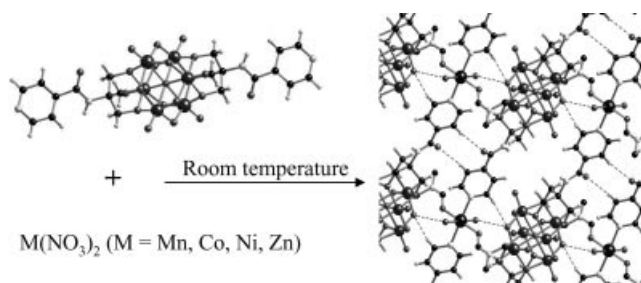


- 2598** J. W. Han, K. I. Hardcastle, C. L. Hill*



Redox-Active Coordination Polymers from Esterified Hexavanadate Units and Divalent Metal Cations

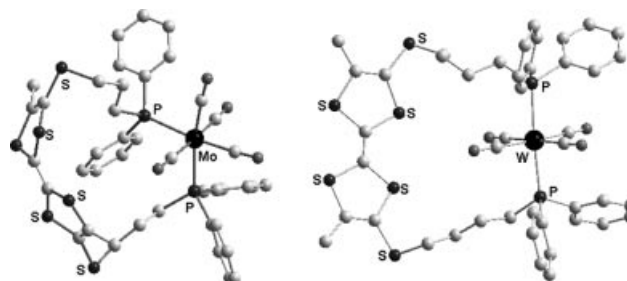
Keywords: Polyoxometalates / Coordination polymers / Vanadium



- 2604** G. Gachot, P. Pellon, T. Roisnel, D. Lorcy*

Redox-Active 17- and 19-Membered Metallamacrocycles Incorporating Tetrathiafulvalene

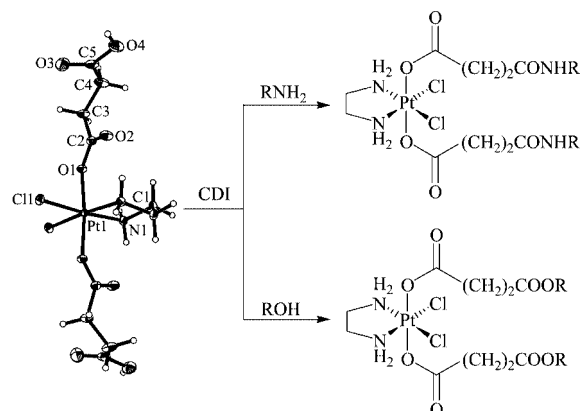
Keywords: Metallamacrocycle / Tetrathiafulvalene / Diphosphane ligands / Molybdenum / Tungsten



2612 M. Reithofer, M. Galanski,* A. Roller,
B. K. Keppler

An Entry to Novel Platinum Complexes: Carboxylation of Dihydroxoplatinum(IV) Complexes with Succinic Anhydride and Subsequent Derivatization

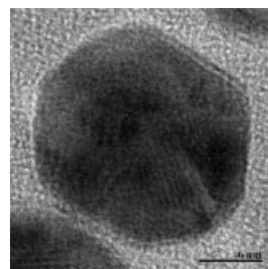
Keywords: Antitumor agents / Bioinorganic chemistry / Carboxylate ligands / Drug design / Platinum



2618 M. J. Richardson,* J. H. Johnston,
T. Borrmann

Monomeric and Polymeric Amines as Dual Reductants/Stabilisers for the Synthesis of Gold Nanocrystals: A Mechanistic Study

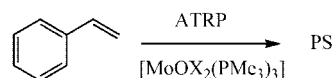
Keywords: Amines / Nanostructures / Phase diagram / Colloids



2624 J. A. Mata, S. Maria, J.-C. Daran, R. Poli*

Synthesis and Characterization of $\text{MoOI}_2(\text{PMe}_3)_3$ and Use of $\text{MoOX}_2(\text{PMe}_3)_3$ ($\text{X} = \text{Cl}, \text{I}$) in Controlled Radical Polymerization

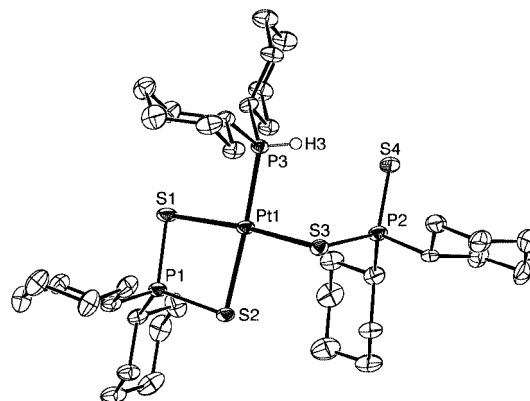
Keywords: Molybdenum / Oxido ligands / Phosphane ligands / Halide exchange / Atom transfer radical polymerization



2634 V. Gallo, M. Latronico, P. Mastrorilli,*
C. F. Nobile, G. Ciccarella, U. Englert

Stepwise Sulfuration of the Terminal Phosphido Complex *trans*-[PtCl(PHCy₂)₂(PCy₂)]: Synthesis of [Pt($\kappa^2\text{S}, \text{S}'\text{-PS}_2\text{Cy}_2$)(PHCy₂)₂]Cl and [Pt($\kappa^2\text{S}, \text{S}'\text{-PS}_2\text{Cy}_2$){ $\kappa\text{P-P(S)Cy}_2$ }(PHCy₂)] and Crystal Structure of [Pt($\kappa^2\text{-S}, \text{S-PCy}_2\text{S}_2$)($\kappa\text{-S-PCy}_2\text{S}_2$)(PHCy₂)]

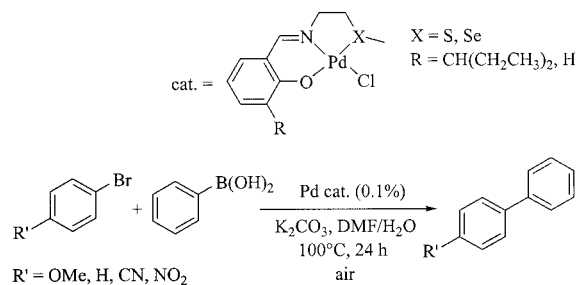
Keywords: Platinum / Terminal phosphides / Phosphanyl sulfides / Phosphanyldithioates / Phosphorus



2642 I. D. Kostas,* B. R. Steele,* A. Terzis,
S. V. Amosova, A. V. Martynov,
N. A. Makhaeva

New Palladium Complexes with S- or Se-Containing Schiff-Base Ligands as Efficient Catalysts for the Suzuki–Miyaura Cross-Coupling Reaction of Aryl Bromides with Phenylboronic Acid under Aerobic Conditions

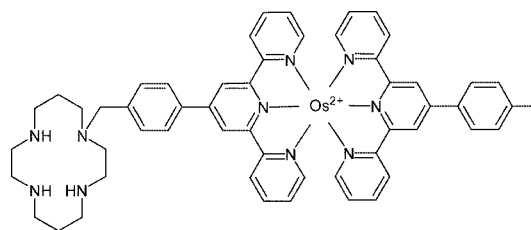
Keywords: Homogeneous catalysis / Suzuki / C–C coupling / Schiff bases / Tridentate ligands



2647 J. V. Ros-Lis, R. Martínez-Máñez,* J. Soto,
C. McDonagh, A. Guckian

A Prospective Study of the Use of the [Os(tpy)₂]²⁺ (tpy = 2,2';6':2''-Terpyridine) Core as Signalling Scaffolding for the Development of Chemical Sensors

Keywords: Chemosensors / Osmium terpyridines / Macrocyclic ligands / Fluorescent probes / Thin films

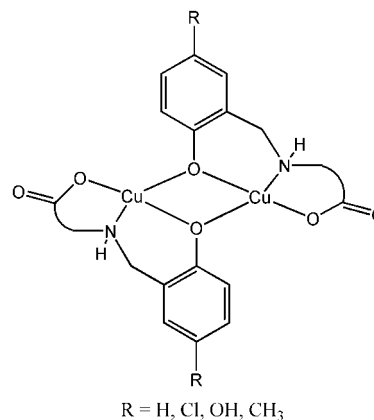


2656 B. Sreenivasulu, F. Zhao, S. Gao,
J. J. Vittal*



Synthesis, Structures and Catecholase Activity of a New Series of Dicopper(II) Complexes of Reduced Schiff Base Ligands

Keywords: Biomimetic studies / Copper / Reduced Schiff-base complexes / Tridentate ligands / Catecholase activity / Magnetic properties

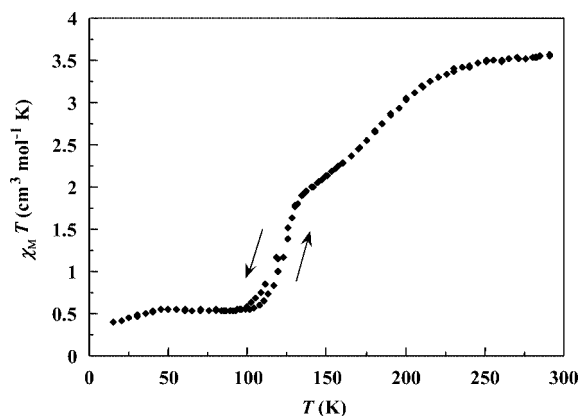


2671 G. S. Matouzenko,* D. Luneau, G. Molnár,
N. Ould-Moussa, S. Zein, S. A. Borshch,
A. Bousseksou, F. Averseng



A Two-Step Spin Transition and Order–Disorder Phenomena in the Mononuclear Compound [Fe(Hpy-DAPP)](BF₄)₂

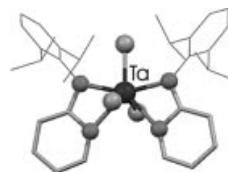
Keywords: Density functional calculations / Iron / Magnetic properties / Mössbauer spectroscopy / N ligands / Spin crossover



2683 A. Noor, W. Kretschmer, R. Kempe*

Synthesis and Structure of Trialkyltantalum Complexes Stabilized by Aminopyridinato Ligands

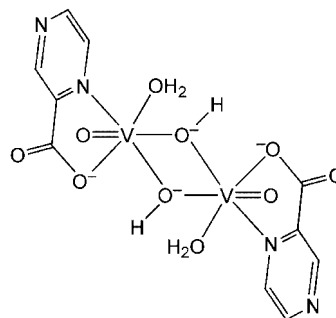
Keywords: Amido ligands / Aminopyridinato ligands / N ligands / Olefin polymerization / Tantalum



**2690 E. Garribba,* G. Micera,*
E. Lodyga-Chruscinska, D. Sanna**

Oxovanadium(IV) Complexes with Pyrazine-carboxylic Acids: The Coordinating Properties of Ligands with the (N_{aromatic} , COO^-) Donor Set

Keywords: Vanadium / N,O ligands / Isomers / Magnetic properties / EPR spectroscopy

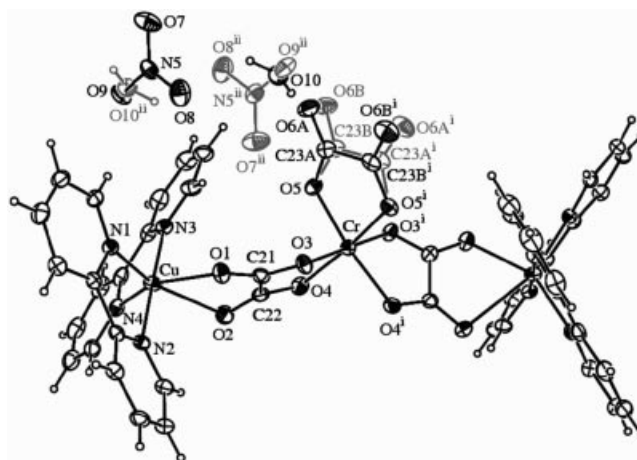


**2701 M. Jurić, P. Planinić, N. Brničević,*
D. Milić, D. Matković-Čalogović, D. Pajić,
K. Zadro**



New Heterometallic (Cu^{II} and Cr^{III}) Complexes – First Crystal Structure of an Oxalate-Bridged Ferromagnetically Coupled [$\text{Cu}^{\text{II}}\text{Cr}^{\text{III}}\text{Cu}^{\text{II}}$] System

Keywords: Crystal structure / Copper complexes / Chromium complexes / Oxalate bridges / Ferromagnetic interaction



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