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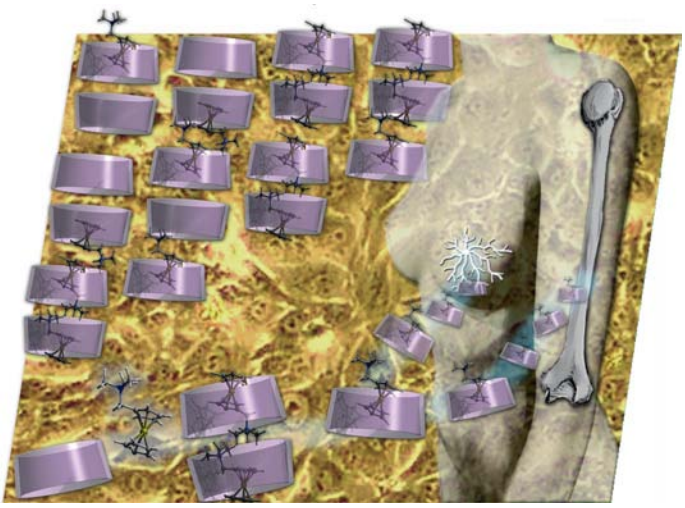
COVER PICTURE

The cover picture shows the structural model of an inclusion complex isolated after co-dissolution of β-cyclodextrin and trimethyl(ferrocenylmethyl)ammonium iodide in ethanol/water. A combination of crystallography and theoretical calculations showed that β-cyclodextrin molecules form dimers stacked into infinite channels that accommodate the guest cations inside. The pure guest and the inclusion compound are cytotoxic against the breast adenocarcinoma cell line MDA-MB-231 but exhibit negligible activity on the osteosarcoma MG-63 cell line. Details are discussed in the article by S. S. Braga, I. S. Gonçalves et al. on p. 4955ff.



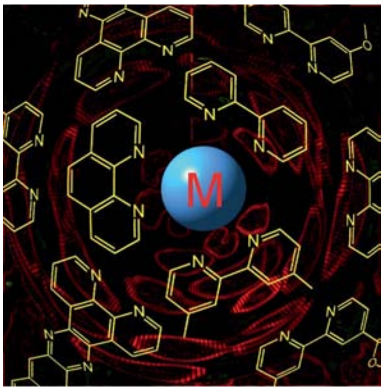
MICROREVIEW

Anticancer Polypyridyl Complexes

L. Salassa* **4931–4947**

Polypyridyl Metal Complexes with Biological Activity

Keywords: Metal complexes / Polypyridyl ligands / Transition metals / Drug design / Antitumor agents



Metal polypyridyl complexes are widely studied in coordination chemistry and have been employed in a wide range of applications, from catalysis to chemical biology. However, their use as potential anticancer agents has not been fully explored. This review highlights recent examples of metal polypyridyl complexes studied for their enzyme-inhibition and cytotoxicity properties.

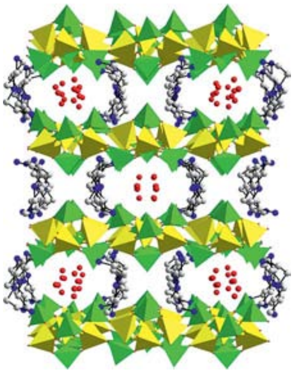
SHORT COMMUNICATION

Layered Beryllium Phosphites

J. Wang, D. Luo, X. Luo, Y. Chen, Z. Lin* **4949–4953**

Open-Framework Beryllium Phosphites with Layered Structures

Keywords: Hydrothermal synthesis / Structure elucidation / Open frameworks / Beryllium / Phosphites



Three new beryllium phosphite solids have been prepared in the presence of different amine molecules as the structure-directing agents. These compounds represent the first examples of open-framework beryllium phosphites with layered structures.

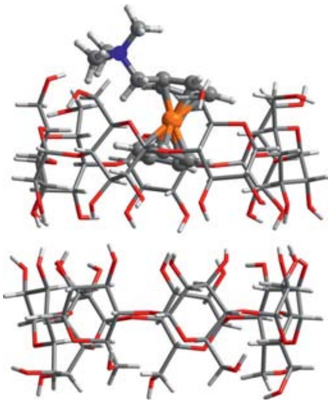
FULL PAPERS

Ferrocene–Cyclodextrin Complexes

S. M. Bruno, J. A. Fernandes, J. Marques, S. C. Neto, P. J. Ribeiro-Claro, M. Pillinger, F. A. A. Paz, M. P. M. Marques, S. S. Braga,* I. S. Gonçalves* **4955–4963**

Structural Studies and Cytotoxicity of Trimethyl(ferrocenylmethyl)ammonium Iodide Encapsulated in β-Cyclodextrin

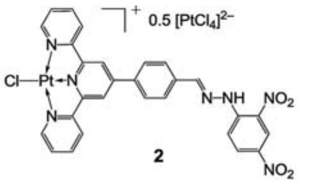
Keywords: Inclusion complexes / Host-guest systems / Cyclodextrins / Ferrocene derivatives / Structure elucidation / Density functional calculations / Cytotoxicity / Medicinal chemistry

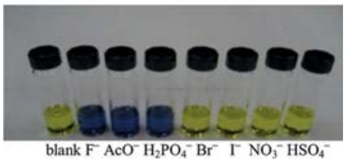


The title inclusion complex was characterized by various techniques, including powder and single-crystal XRD. Using the structural model derived from these data as a starting point, DFT calculations led to a model of the crystal structure with 2:1 (host/guest) and 2:2 adducts. Encapsulation of the ferrocene derivative in β-cyclodextrin enhances its antitumor activity towards a breast adenocarcinoma line.

Anion Sensing

Terpyridine derivative **1**, bearing 2,4-dinitrophenylhydrazone, and its platinum chloride complex **2** exhibit drastic color change as well as quenching of emission intensity and triplet transient absorption upon addition of F^-, AcO^-, or $H_2PO_4^-$ anions. Deprotonation of the hydrazone NH group is demonstrated to be the mechanism for the anion sensing.





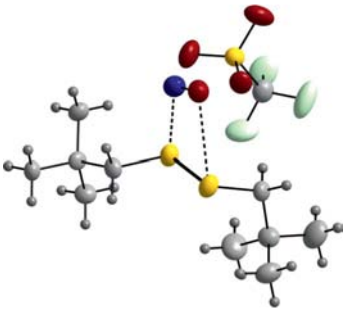
B. Zhang, Y. Li, W. Sun* **4964–4969**

Anion-Sensitive 2,4-Dinitrophenylhydrazone-Containing Terpyridine Derivative and Its Platinum Chloride Complex

Keywords: Terpyridine derivatives / Platinum / Photophysics / Sensors / Transient absorption

Diorgano Dichalcogenide Adducts

Two new dimethyl diselenide–iodine adducts have been synthesized as well as the first diorgano disulfide–nitrosonium adduct. Crystal structures and theoretical analysis (DFT) of the reaction of the NO^+ cation with R_2S_2 and the di-*neo*-pentyl disulfide nitrosonium charge transfer adduct are presented.

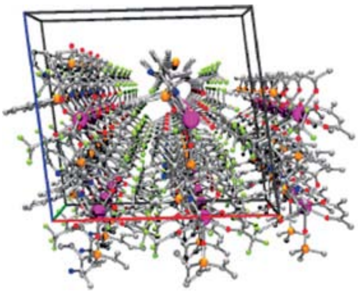


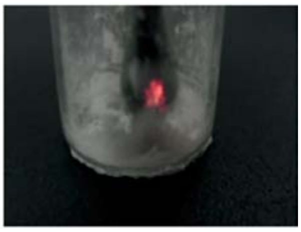
B. Mueller, T. T. Takaluoma,
R. S. Laitinen, K. Seppelt* **4970–4977**

Syntheses and Structures of Two Dimethyl Diselenide–Diiodine Adducts and the First Well Characterized Diorgano Disulfide–Nitrosonium Adduct

Keywords: Main group elements / Density functional calculations / Iodine / Chalcogens / Diorgano dichalcogenides / Nitrosonium

Lanthanide Coordination Polymers





We report on characteristic triboluminescence form a europium(III) coordination polymer crystal with non-centrosymmetric *Cc* structure suitable for piezoelectricity, shown in the figure. Triboluminescence is observed upon breaking, even at ambient temperature and in daylight. The remarkable triboluminescence phenomenon and geometrical structure of lanthanide coordination polymer are demonstrated.

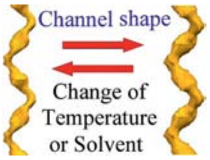
Y. Hasegawa,* R. Hieda, K. Miyata,
T. Nakagawa, T. Kawai* **4978–4984**

Brilliant Triboluminescence of a Lanthanide Coordination Polymer with Low-Vibrational-Frequency and Non-Centrosymmetric Structural Networks

Keywords: Luminescence / P ligands / Lanthanides / Metal–organic frameworks / Europium

Structural Flexibility of MOFs

Structural parameters of a row of coordination polymers gradually varied depending on the temperature or size of solvent molecules in the voids. This can be considered as a model of changes occurring at desolvation of the polymers or adsorption of guests. Sorption capacity of these compounds is of the order methanol < ethanol < *n*-hexane < *n*-octane. This is consistent with hydrophobic channels.



R. A. Polunin, S. V. Kolotilov,
M. A. Kiskin, O. Cador, S. Golhen,
O. V. Shvets, L. Ouahab,*
Z. V. Dobrokhotova, V. I. Ovcharenko,
I. L. Eremenko,* V. M. Novotortsev,
V. V. Pavlishchuk* **4985–4992**

Structural Flexibility and Sorption Properties of 2D Porous Coordination Polymers Constructed from Trinuclear Heterometallic Pivalates and 4,4′-Bipyridine

Keywords: Polymers / Porous materials / Adsorption / Structural flexibility / Hydrophobic interactions / Solvent effects

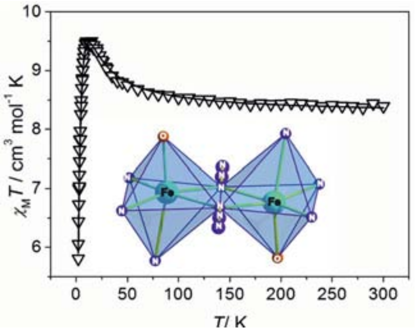
CONTENTS

Bridged Iron(III) Dimers

S. Naiya, M. G. B. Drew, C. Diaz*, J. Ribas, A. Ghosh* 4993–4999

Synthesis, Crystal Structure, and Magnetic Properties of a Very Rare Double μ-1,1-Azido- and a μ-1,1-(OMe)-Bridged Fe^{III} Dimer Containing a N,N,O-Donor Tridentate Schiff Base Ligand

Keywords: Iron / Schiff bases / Magnetic properties / N,N,O ligand / Azido bridges



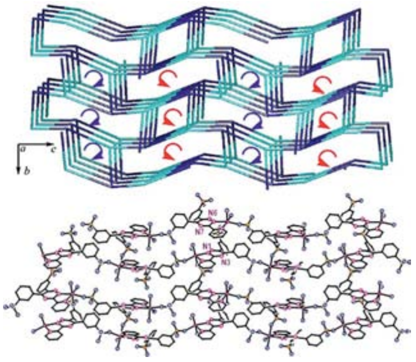
A very rare μ-1,1-azido-bridged and a μ-OMe-bridged dinuclear Fe^{III} compound with a tridentate N,N,O-donor Schiff base have been synthesized and characterized structurally. The former is only the third example of μ-1,1-azido bridges in Fe^{III}. The variable-temperature magnetic studies show that the former is ferromagnetically and the latter antiferromagnetically coupled.

MOF Material

A. O. Ibrahim, Y. Zhou,* F. Jiang, L. Chen, X. Li, W. Xu, O. O. E. Onawumi, O. A. Odunola, M. Hong* 5000–5005

An Unusual (10,3)-d MOF Material with Nanoscale Helical Cavities and Multifunctionality

Keywords: Metal-organic frameworks / Helical structures / Nanostructures / Nonlinear optics / Magnetic properties / Manganese / Copper / Sorption / Carbon dioxide fixation



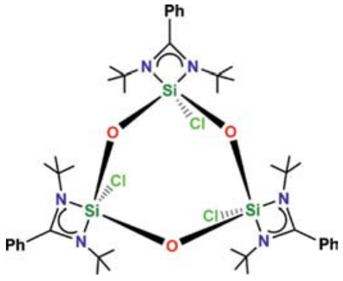
A (10,3)-d metal-organic framework, $[Mn_2(pdtd)_2(H_2O)_4]_n \cdot 5nH_2O$ (**1**), containing the asymmetrical 3-(2-pyridyl)-5,6-diphenyl-1,2,4-triazine-P,P′-disulfonate ligand (pdtd) was constructed. XRD analysis revealed that **1** is an acentric structure possessing exposed uncoordinated nitrogen atoms within helical cavities. **1** exhibits multifunctionality: nonlinear optical activity, CO_2 sorption, and magnetic coupling.

Silylene Chemistry

A. Jana, R. Azhakar, S. P. Sarish, P. P. Samuel, H. W. Roesky,* C. Schulzke, D. Koley 5006–5013

Reactions of Stable Amidinate Chlorosilylene and [1+4]-Oxidative Addition of N-Heterocyclic Silylene with *N*-Benzylideneaniline

Keywords: Boron / Silicon / Chlorosilylene / Cycloaddition / Spiro compounds / Density functional calculations



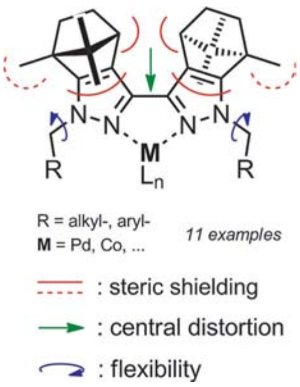
The reaction of $PhC(NtBu)_2SiCl$ (**L**) with N_2O afforded the trimer $\{PhC(NtBu)_2Si(O)Cl\}_3$ (**1**), containing a Si_3O_3 six-membered ring. Treatment of **L** with $B(C_6F_5)_3$ and 9-BBN {9-borobicyclo[3.3.1]nonane} yielded the chlorosilylene–boron adducts **L**·$B(C_6F_5)_3$ (**2**) and **L**·9-BBN (**3**). The reaction of $CH\{(C{=}CH_2)(CMe)(2,6\text{-}iPr_2\text{-}C_6H_3N)_2\}Si$ (**L′**) with *N*-benzylideneaniline afforded the [1+4]-cycloaddition product **4**.

Rigid Ligands

M. J. Spallek, S. Stockinger, R. Goddard, F. Rominger, O. Trapp* 5014–5024

Bulky and Modular 3,3′-Bipyrazoles as Ligands: Synthesis, Characterization, and Catalytic Activity of Pd Complexes

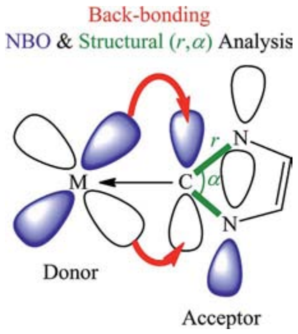
Keywords: Homogeneous catalysis / Palladium / N ligands / Rigid ligands



A sterically bulky 3,3′-bipyrazole ligand class was synthesized in excellent yields using camphor as a building block. The highly modular nature of the system gave rise to a series of 11 new ligands with tunable steric and electronic properties. The derived catalysts with increasing electron-donating properties revealed higher conversions in Cu-free Wacker oxidations of terminal alkenes.

Backbonding in NHC Complexes

DFT calculations have been used to analyze metal-to-ligand backbonding in a range of model transition metal complexes of N-heterocyclic carbenes. Two new methods of analysis have been introduced. The first is structural, and the second uses the perturbative natural bond orbital (NBO) method. Both methods lead to the firm conclusion that backbonding is significant in these compounds.



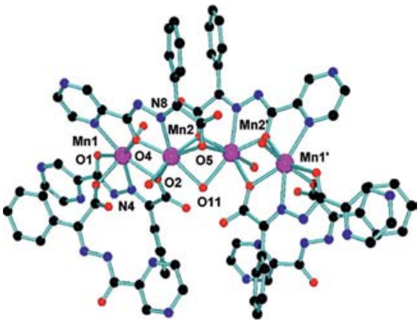
A. Comas-Vives,*
J. N. Harvey* **5025–5035**

How Important Is Backbonding in Metal Complexes Containing N-Heterocyclic Carbenes? Structural and NBO Analysis

Keywords: NBO analysis / Density functional calculations / Backbonding / Carbene ligands / Second-order perturbative analysis / Donor–acceptor systems

Multifunctional Hydrazone Ligands

Multifunctional polytopic hydrazone ligands form polymetallic complexes with μ-O (hydrazone, carboxylate) and μ-N,N (triazole) bridging, leading to spin–spin interactions between the metal centres with examples of antiferromagnetic and ferromagnetic exchange.



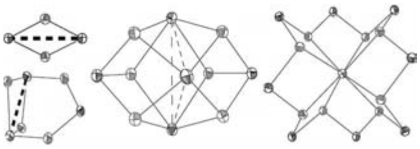
P. J. Bettle, L. N. Dawe, M. U. Anwar,
L. K. Thompson* **5036–5042**

Dinuclear, Tetranuclear and Chain (Mn^{II}, Co^{II}) Complexes of Multifunctional Hydrazone Ligands – Structural and Magnetic Studies

Keywords: Hydrozone ligands / Magnetic properties / Cobalt / Manganese

Manganese Cluster Compounds

Four Mn or mixed Mn/Ce clusters at high oxidation states were prepared by the reaction of Mn^{2+} salts where $(NH_4)_2[Ce(NO_3)_6]$ was used as an oxidizing agent. These complexes possess inorganic cores that have topologies that range from the rhomb, the triangle, and the nonplanar loop to the trigonal bipyramid. The four complexes possess distinctly different magnetic properties.



C.-B. Ma,* M.-Q. Hu, H. Chen,
C.-N. Chen,* Q.-T. Liu **5043–5053**

A New Family of Homo- and Heterometallic Manganese Complexes at High Oxidation States Derived from the Oxidation of Mn^{II} with Ce^{IV}: Syntheses, Structures, and Magnetic Properties

Keywords: Manganese / Cerium / Cluster compounds / Magnetic properties

CORRECTION

Keywords: Calcium / Iron / Arsenic / Superconductors / Intermetallic phases / Solid-state reactions / Thermal stability

Synthesis and Thermal Stability Studies of $CaFe_4As_3$

T. Yi, A. P. Dioguardi, P. Klavins,
N. J. Curro, L. L. Zhao, E. Morosan,
S. M. Kauzlarich* **5054**

* Author to whom correspondence should be addressed.

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