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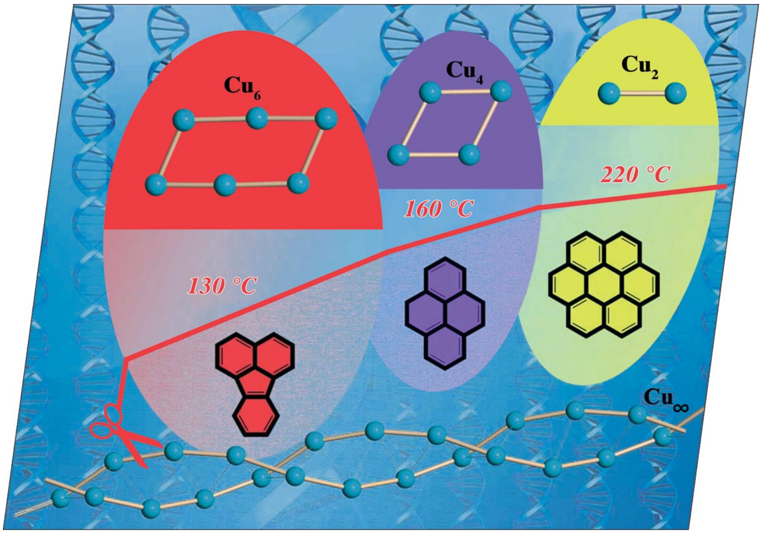
# COVER PICTURE

**The cover picture shows** the cleavage of an infinite copper(I) helix into discrete $Cu_n$ fragments of decreasing nuclearity ($n$ = 6, 4, 2) as a result of the increase in temperature of the gas-phase reactions with polyarenes. Details are discussed in the article by Yu. Sevryugina and M. A. Petrukhina on p. 219ff.



# CONTENTS

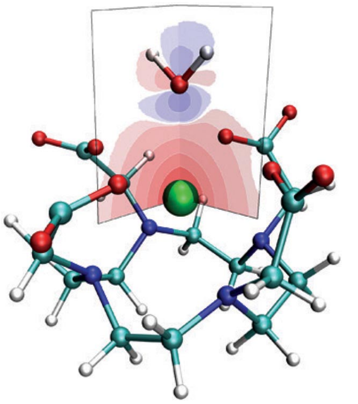
## MICROREVIEW

### MRI Contrast Agents

**O. V. Yazyev, L. Helm* ............. 201–211**

Nuclear Spin Relaxation Parameters of MRI Contrast Agents – Insight from Quantum Mechanical Calculations

**Keywords:** Relaxivity / Hyperfine interactions / Quantum chemistry / Gadolinium / MRI contrast agent



Fundamental parameters for nuclear spin relaxation such as quadrupole coupling constants and hyperfine interaction tensors can be obtained from quantum chemical calculations combined with molecular dynamics simulations. Recent results are reviewed on the $Gd^{3+}$ ion in aqueous solution and on the MRI contrast agent $[Gd(DOTA)(H_2O)]^-$.

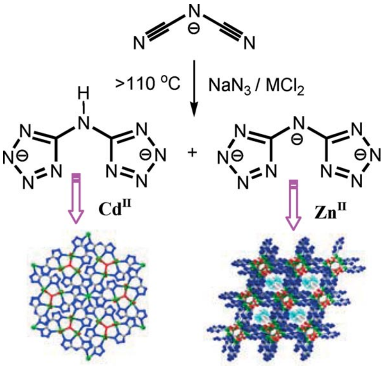
## SHORT COMMUNICATION

### Microporous MOFs

**L.-L. Zheng, H.-X. Li, J.-D. Leng,**
**J. Wang, M.-L. Tong* ............... 213–217**

Two Photoluminescent Metal–Organic Frameworks Constructed from $Cd_3(\mu_3\text{-}OH)$ Cluster or 1D $Zn_5(\mu_3\text{-}OH)(\mu\text{-}OH)_2$ Chain Units and In Situ Formed Bis(tetrazole)amine Ligands

**Keywords:** Cadmium / Zinc / Amines / Cluster compounds / MOFs / Photoluminescence



Two photoluminescent coordination polymers with triangular $[Cd_3(\mu_3\text{-}OH)]^{5+}$ cluster subunits or 1D $[Zn_5(\mu_3\text{-}OH)_2(\mu\text{-}OH)_2]_n{}^{6n+}$ chain subunits bridged by a bis(tetrazole)amine ligand generated in situ were obtained from the hydrothermal reactions of $CdCl_2{\cdot}2.5H_2O$ or $ZnCl_2$, sodium dicyanamide, and sodium azide.

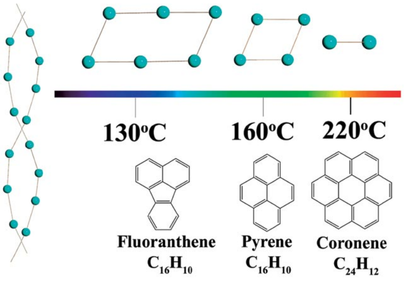
## FULL PAPERS

### Thermal Copper Helix Fragmentation

**Yu. Sevryugina,**
**M. A. Petrukhina* .................... 219–229**

Breaking Infinite $Cu^I$ Carboxylate Helix Held by Cuprophilicity into Discrete $Cu_n$ Fragments ($n$ = 6, 4, 2)

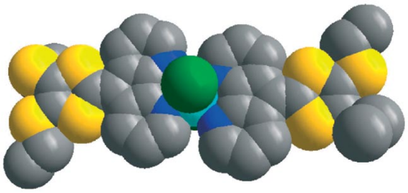
**Keywords:** Copper(I) carboxylate / Gas-phase reactions / Polyaromatic hydrocarbons



Controlled cleavage of the infinite copper(I) double-helical chain into discrete $Cu_n$ fragments of decreasing nuclearity ($n$ = 6, 4, and 2) has been achieved as a result of the successive temperature increase of the gas-phase co-deposition reactions.

## Diazafluorenes

Both *trans*- and *cis*-metal complexes with diazafluorene ligands were characterized crystallographically. The results show that intermolecular charge transition is enhanced when metal ions are coordinated, and these metal complexes exhibit negative $\lambda$ NLO properties and are self-defocusing samples.



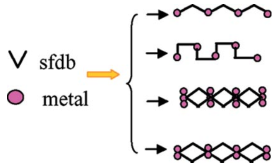
**Q.-Y. Zhu, W. Lu, Y. Zhang, G.-Q. Bian, J. Gu, X.-M. Lin, J. Dai* ......... 230–238**

Syntheses, Crystal Structures, and Optical Properties of Metal Complexes with 4′,5′-Diaza-9′-(4,5-disubstituted-1,3-dithiol-2-ylidene)fluorene Ligands

**Keywords:** Metal complexes / Crystal structure / Optical properties / Dithioles / Fluorenes

## Luminescent Coordination Polymers

Seven metal–organic coordination polymers are synthesized hydrothermally and structurally characterized by single-crystal X-ray diffraction analyses. They show various 1D chain structures, and weak hydrogen bonding and π···π stacking contacts link the discrete 1D chains to form high-dimensional supramolecular architectures in **3**–**7**. Compounds **1**, **2**, and **4**–**7** show blue luminescence at room temperature.



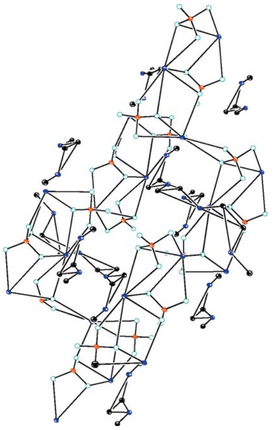
**X.-L. Chen, L. Gou, H.-M. Hu,* F. Fu, Z.-X. Han, H.-M. Shu, M.-L. Yang, G.-L. Xue, C.-Q. Du ................. 239–250**

New Examples of Metal Coordination Architectures of 4,4′-Sulfonyldibenzoic Acid: Syntheses, Crystal Structure and Luminescence

**Keywords:** Coordination modes / O ligands / Materials science / Organic–inorganic hybrid composites / Luminescence

## Metal Tetrahydridoborate Complexes

The structures of coordination compounds of $MBH_4$ (M = Li, Na, K) depend on the $MBH_4$:ligand ratio. Thus, while $LiBH_4(L)_3$ complexes are mostly monomolecular, association is observed for 1:2 and 1:1 compounds. Tetraglyme forms double strands with $NaBH_4$, whereas complexes of $LiBH_4$ with pyridines are mononuclear and a chain structure is found for $NaBH_4py_3$. $MeHN\text{-}NH_2$ reacts with $LiBH_4$ to form a salt but a chain structure is generated in $LiBH_4(H_3N\text{-}NHPh)_2$. The three-dimensional array of $NaBH_4(morpholine)_2$ contains mono-, bi- and tridentate $BH_4$ groups.

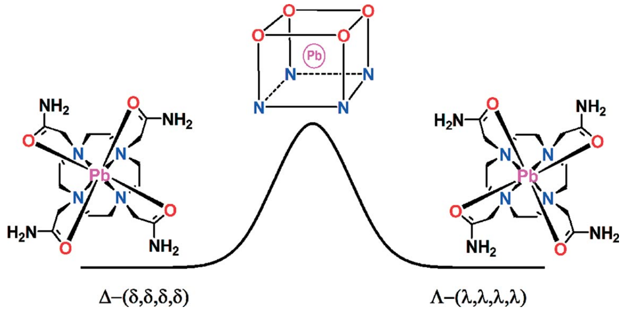


**J. C. Gálvez Ruiz, H. Nöth,* M. Warchhold ........................... 251–266**

Coordination Compounds of Alkali Metal Tetrahydroborates with Ethers and Amines

**Keywords:** Alkali metals / Hydroborates / Amines / X-ray structures

## Lead(II) Complexation



The lead(II)-binding properties of 1,4,7,10-tetrakis(carbamoylmethyl)-1,4,7,10-tetraazacyclododecane (DOTAM) have been investigated. An inverted-square antiprismatic octacoordinate complex with a stereochemically inactive $6s^2$ lone pair is formed both in the solid state and in solution. Stopped-flow kinetic measurements enabled unraveling of the formation process of the lead(II) complex.

**F. Cuenot, M. Meyer,* E. Espinosa, A. Bucaille, R. Burgat, R. Guilard,* C. Marichal-Westrich ................ 267–283**

New Insights into the Complexation of Lead(II) by 1,4,7,10-Tetrakis(carbamoylmethyl)-1,4,7,10-tetraazacyclododecane (DOTAM): Structural, Thermodynamic, and Kinetic Studies

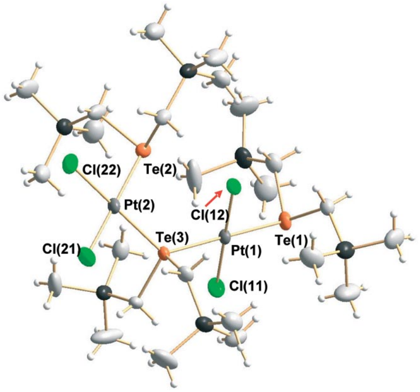
**Keywords:** Lead / Macrocyclic ligands / X-ray diffraction / NMR spectroscopy / Reaction mechanisms

## Telluroether Complexes

**L. Vigo, R. Oilunkaniemi,***
**R. S. Laitinen*** ......................... **284–290**

Formation and Characterization of Platinum and Palladium Complexes of Bis(trimethylsilylmethyl)tellane

**Keywords:** Bis(trimethylsilylmethyl)tellane / Platinum complexes / Palladium complexes / X-ray diffraction / NMR spectroscopy



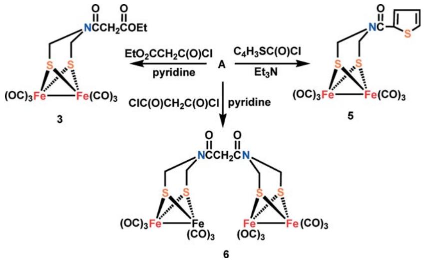
In addition to the mononuclear complexes $[MCl_2\{Te(CH_2SiMe_3)_2\}_2]$ (M = Pt, Pd), the reactions of $[MCl_2(NCPh)_2]$ (M = Pt, Pd) and $Te(CH_2SiMe_3)_2$ afford dinuclear $[Pt_2Cl_4\{\mu\text{-}Te(CH_2SiMe_3)_2\}\{Te(CH_2SiMe_3)_2\}_2]$ and $[Pd_2(\mu\text{-}Cl)_2Cl_2\{Te(CH_2SiMe_3)_2\}_2]$. The platinum complex shows a bridging telluroether ligand and both *cis*-Cl– and *trans*-Cl–platinum centers.

## Functionalized ADT Complexes

**L.-C. Song,* L.-X. Wang, B.-S. Yin,**
**Y.-L. Li, X.-G. Zhang, Y.-W. Zhang,**
**X. Luo, Q.-M. Hu** .................... **291–297**

The *N*-Acylated Derivatives of Parent Complex $[\{(\mu\text{-}SCH_2)_2NH\}Fe_2(CO)_6]$ as Active Site Models of Fe-Only Hydrogenases: Synthesis, Characterization, and Related Properties

**Keywords:** Bioinorgnic chemistry / Iron / Electrochemistry / Hydrogenase models



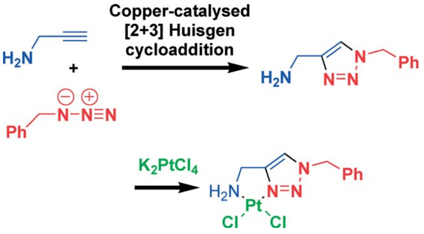
Eight *N*-acylated diiron azadithiolates as H-cluster models were prepared by direct acylation of the $[\{(\mu\text{-}SCH_2)_2NH\}Fe_2(CO)_6]$ (**A**) complex or by functional transformation of the initially acylated products. Also reported are three crystal structures and the electrochemical properties for some of the acylated products.

## Click Chelators

**A. Maisonial, P. Serafin,**
**M. Traïkia, E. Debiton,* V. Théry,**
**D. J. Aitken,* P. Lemoine,* B. Viossat,**
**A. Gautier*** ............................... **298–305**

Click Chelators for Platinum-Based Anticancer Drugs

**Keywords:** Click chemistry / Platinum / Chelates / Cancer



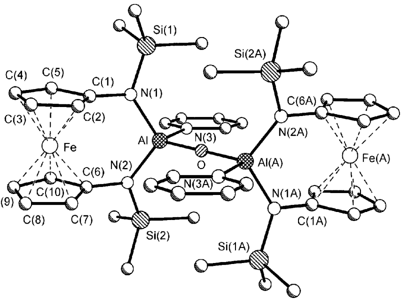
Triazoles from "click chemistry" are convenient ligands for the formation of platinum complexes that exhibit cytotoxicity against breast cancer cells lines.

## Dialuminoxanes

**B. Wrackmeyer,* E. V. Klimkina,**
**W. Milius** ................................. **306–311**

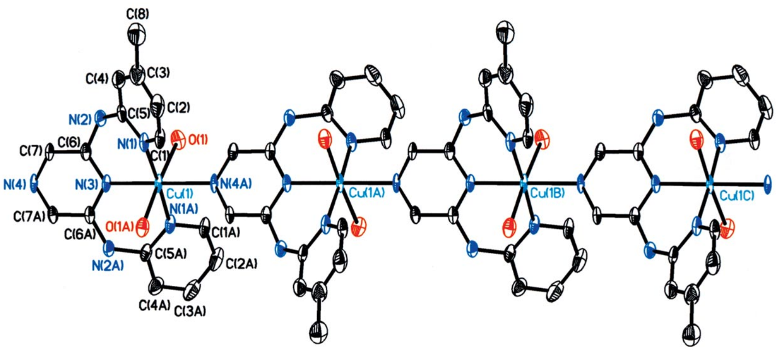
A Pyridine-Stabilized Alumoxane Containing Two 1,3,2-Diazaalumina[3]ferrocenophane Units

**Keywords:** Aluminum / Amides / Alumoxanes / NMR spectroscopykeywords



The first example of a structurally characterized bis(amino)dialuminoxane was isolated as a side product, and its structure was established by NMR spectroscopy in solution and by X-ray structural analysis in the solid state. It exists in the solid state in two modifications, either with a linear Al–O–Al or a bent Al–O–Al unit.

## Ligand Design



Four unsymmetrical pyrazine- and/or 4-picoline-modulated *N*,*N′*-bis(α-pyridyl)-2,6-diaminopyridine ligands were synthesized and their 1D copper(II) complexes studied. Complexes that had zigzag 1D structures displayed weak ferromagnetic coupling, whereas those that had straight 1D structures showed antiferromagnetic interaction.

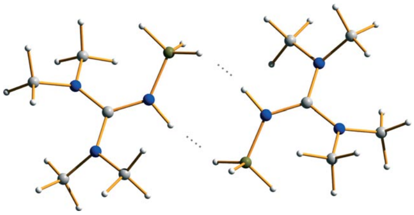
**W.-Z. Wang, R. H. Ismayilov, G.-H. Lee,**
**H.-T. Wang, R.-R. Wang,**
**S.-M. Peng* .............................. 312–321**

Control of Structure and Magnetic Interaction Through Ligand Design: One-Dimensional Complexes from Ferromagnetic to Antiferromagnetic Coupling

**Keywords:** Coordination polymers / Copper / N ligands / Ligand design / Magnetic interactions

## Boron Hydrides

The synthesis of the borane adduct 1,1,3,3-tetramethylguanidine–borane, $H_3B{\cdot}N(H)C(NMe_2)_2$, was achieved, and a detailed comparison of the bonding properties in amine– and guanidine–borane adducts on the basis of quantum chemical calculations is discussed.



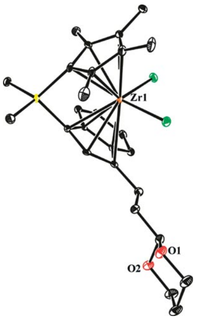
**O. Ciobanu, S. Leingang, H. Wadepohl,**
**H.-J. Himmel* .......................... 322–329**

The 1,1,3,3-Tetramethylguanidine–Borane Adduct: Theoretical Comparison of the Bonding Properties in Amine– and Guanidine–Borane Adducts

**Keywords:** Boron hydrides / Dissociation energy / Guanidine adducts / Hydrogen bonding / Quantum chemical calculations

## Heterocyclic-Modified Metallocenes

Several bis(indenyl)- and *ansa*-indenylcyclopentadienyl zirconocenes bearing heterocyclic rings containing potential oxygen donor atoms were prepared, which are capable of bonding to acidic sites on the surface of magnesium chloride.



**P. J. Aragón Sáez, F. Carrillo-Hermosilla,***
**E. Villaseñor, A. Otero,* A. Antiñolo,**
**A. M. Rodríguez ........................ 330–337**

Heterocycle-Substituted Indenes as Precursors for Supported Zirconocene Catalysts

**Keywords:** Metallocenes / Zirconium / Heterocycles / Polymerization