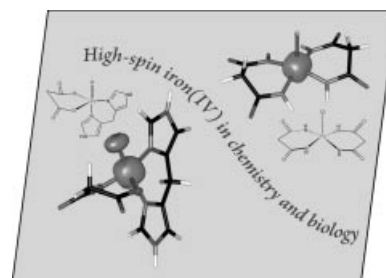


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COVER PICTURE

The cover picture shows DFT-optimized models of a non-heme high-spin iron(IV)-oxo intermediate and of Collins' stable high-spin Fe^{IV} complex. A. Ghosh, P. R. Taylor and co-workers show in their article on p. 4555ff. that these species, although both are high-spin Fe^{IV} , exhibit radically different electronic configurations and spin density profiles (green). Moreover, the authors present some of the first high-level ab initio calculations aimed at benchmarking the triplet-quintet energy difference for Fe^{IV} species.



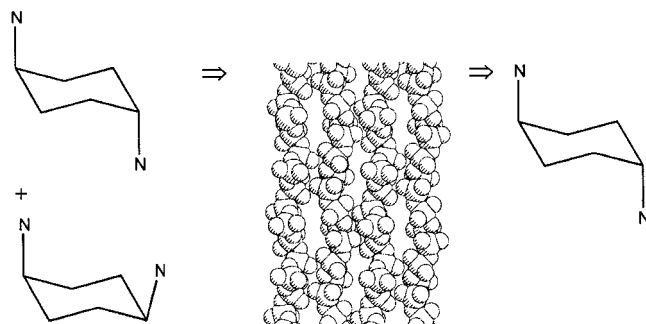
SHORT COMMUNICATIONS

Contents

4547 Y. Xu,* W. Fan, S. P. Elangovan,
 M. Ogura, T. Okubo*

$[\text{Ge}_9\text{O}_{14}(\text{OH})_{12}](\text{C}_6\text{N}_2\text{H}_{16})_2 \cdot \text{H}_2\text{O}$: A Novel Germanate with Ge–O Helical Chains Formed by Hydrothermal Synthesis that Can Separate *trans* and *cis* Isomers in Situ

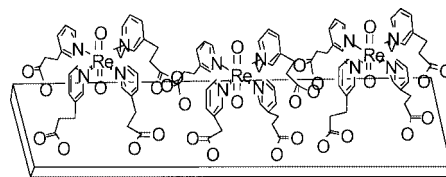
Keywords: Germanium / Helical structures / Hydrothermal synthesis / Isomers



4550 H. Sugimoto,* H. Tsukube, K. Tanaka

Immobilization of a High-Valent Rhenium Complex on an Indium-Doped Tin-Oxide Electrode: Enhanced Catalytic Activity of a *trans*-Dioxorhenium(V) Complex in Electrochemical Oxidation of Alcohols

Keywords: Surface analysis / Cyclic voltammetry / Immobilization / Rhenium / Oxidation

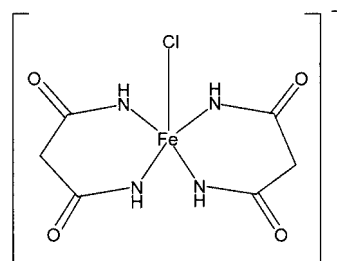


FULL PAPERS

**4555 A. Ghosh,* E. Tangen, H. Ryeng
P. R. Taylor***

Electronic Structure of High-Spin Iron(IV) Complexes

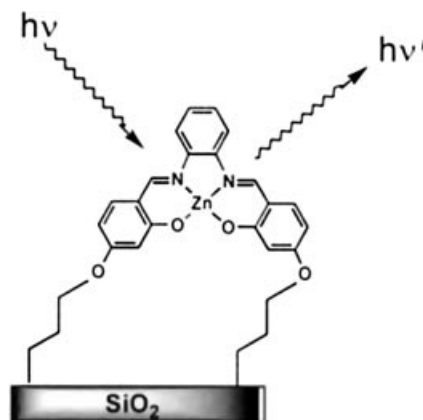
Keywords: High-spin species / Nonheme / Iron / Oxo ligand / Diamond core / Quantum chemistry



**4561 S. Di Bella,* N. Leonardi, G. Consiglio,
S. Sortino,* I. Fragalà**

Fluorescent Self-Assembled Monolayers of Bis-(salicylaldiminato)zinc(II) Schiff-Base Complexes

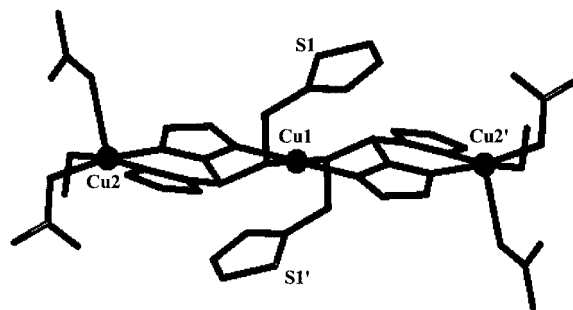
Keywords: Fluorescence / Monolayers / Schiff bases / Zinc



**4566 Y. F. Song, C. Massera, M. Quesada,
I. A. Koval, P. Gamez,
A. M. Manotti Lanfredi, J. Reedijk***

A New Trinuclear Linear Copper(II) Complex: Unusual Crystal Structure with Semi-Coordinated Thiophene Moieties and Weak Antiferromagnetic Coupling Through the Bridging Imidazole Rings

Keywords: Copper / Trinuclear complexes / EPR / Thiophene / N,S ligands / Imidazole

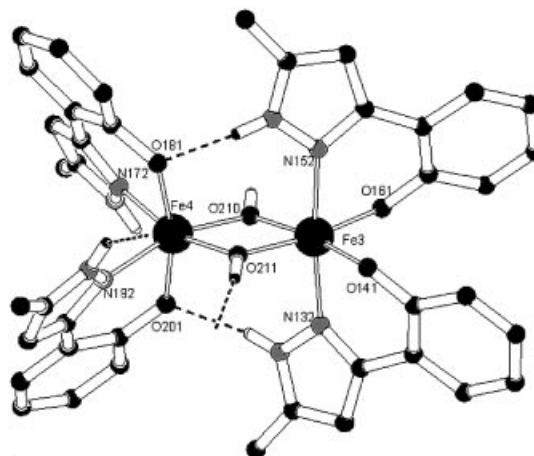


- 4572** S. Tanase, E. Bouwman, G. J. Long,
A. M. Shahin, A. M. Mills, A. L. Spek,
J. Reedijk*



Acid-Base Self-Assembly Chemistry and Hydrogen Bonding Interactions Resulting in the Formation of a Tetranuclear Aggregate Containing Four Crystallographically Non-Equivalent Fe^{III} Centers

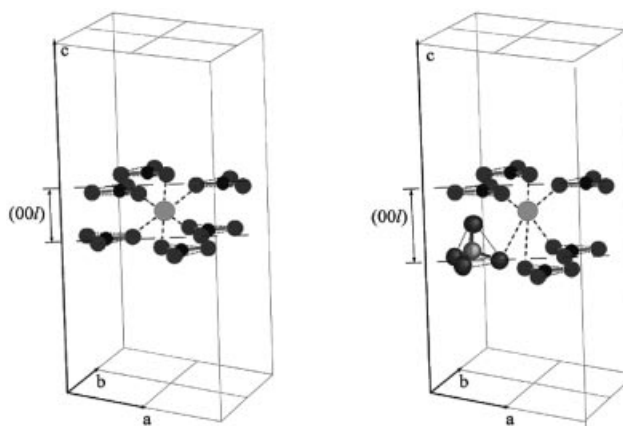
Keywords: Iron / Pyrazole ligands / Hydroxo-bridge / Mössbauer



- 4579** J. Kontrec, D. Kralj,* L. Brečević,
G. Falini, S. Fermani, V. Noethig-Laslo,
K. Miroslavljević

Incorporation of Inorganic Anions in Calcite

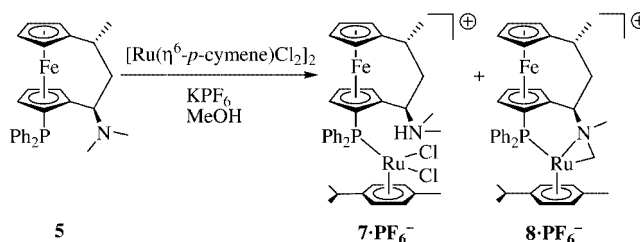
Keywords: Anions / Calcite / Calcium carbonate / Crystal growth / EPR spectroscopy



- 4586** P. Liptau, D. Carmona,* L. A. Oro,*
F. J. Lahoz, G. Kehr, G. Erker*

Facile [N]C–H Activation by a (*P,N*)-Chelate [3]Ferrocenophane–Ruthenium System

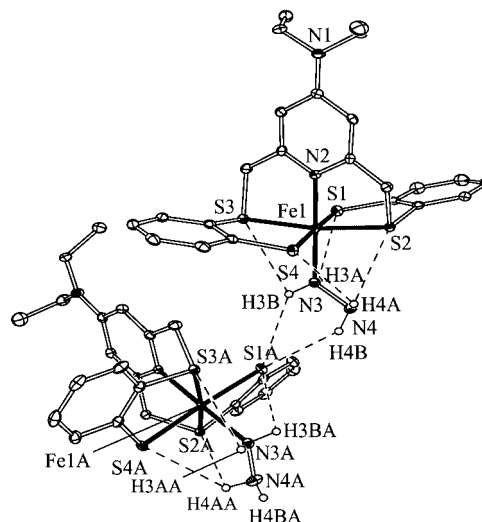
Keywords: (*P,N*)-Chelate ligands / Ruthenium / Ferrocenophane / C–H activation



- 4591** D. Sellmann, S. Y. Shaban,*
F. W. Heinemann

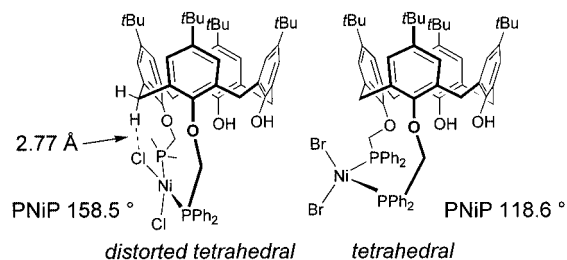
Syntheses, Structures and Reactivity of Electron-Rich Fe and Ru Complexes with the New Pentadentate Ligand Et₂NpyS₄–H₂ {4-(Diethylamino)-2,6-bis[(2-mercaptophenyl)thiomethyl]pyridine}

Keywords: Electron density / Iron / Nitrogenase / Ruthenium / S ligand



4602 P. Kuhn, C. Jeunesse, D. Sémeril, D. Matt,*
P. Lutz, R. Welter

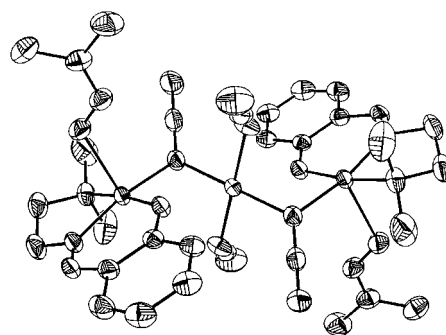
Coordination Chemistry of Large Diphosphanes – Directional Properties of a Calix[4]-arene Proximally Substituted by Two –OCH₂PPh₂ Podand Arms



Keywords: Calixarenes / Large diphosphanes / Nickel complexes / Ethylene oligomerisation

4608 Y.-B. Jiang, H.-Z. Kou,* R.-J. Wang,
A.-L. Cui

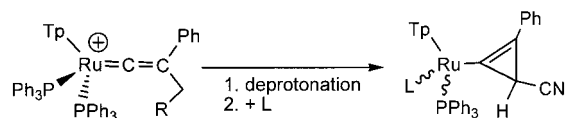
(Schiff-base)Cu^{II} Complexes with Phenolate-Oxygen/Chloro or -Oxygen/Azido Mixed Bridges – Syntheses, Crystal Structures and Magnetic Properties



Keywords: Chloro bridges / Azido bridges / Magnetic properties / Cu^{II} ions / Crystal structures

4616 Y.-H. Lo, Y.-C. Lin,* G.-H. Lee, Y. Wang

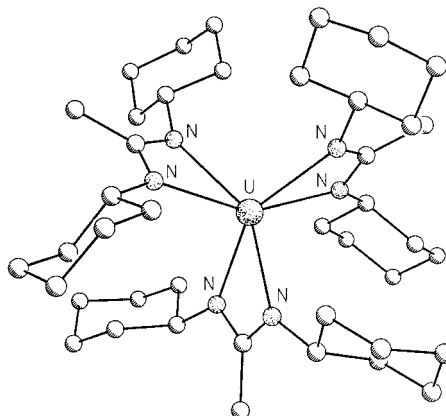
Synthesis of (Vinylidene)- and (Cyclopropenyl)-ruthenium Complexes Containing a Tris-(pyrazolyl)borato (Tp) Ligand



Keywords: Cyclopropenyl / N ligands / Ruthenium / Vinylidene ligands

4624 C. Villiers,* P. Thuéry, M. Ephritikhine*

A Comparison of Analogous 4f- and 5f-Element Compounds: Syntheses, X-ray Crystal Structures and Catalytic Activity of the Homoleptic Amidinate Complexes [M{MeC(NCy)₂}₃] (M = La, Nd or U)



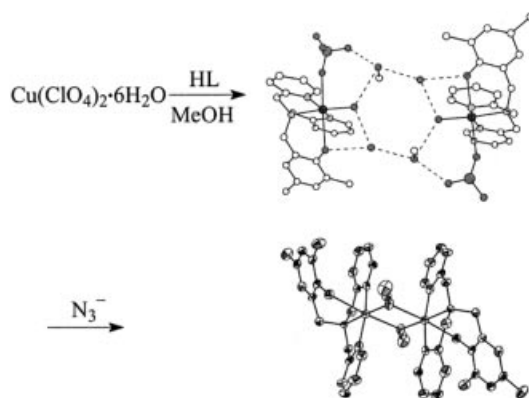
Keywords: ε-Caprolactone / Lanthanides / N ligands / Polymerization / Uranium

4633

S. Sarkar, A. Mondal, J. Ribas,
M. G. B. Drew, K. Pramanik, K. K. Rajak*

Synthesis, Structure and Properties of a Mononuclear and an End-On Double Azido-Bridged Copper(II) Complex Incorporating an N,N,N,O-Coordinating Tripodal Ligand

Keywords: Azide ligands / Copper / Hydrogen bonds / Magnetic properties / Tripodal ligands



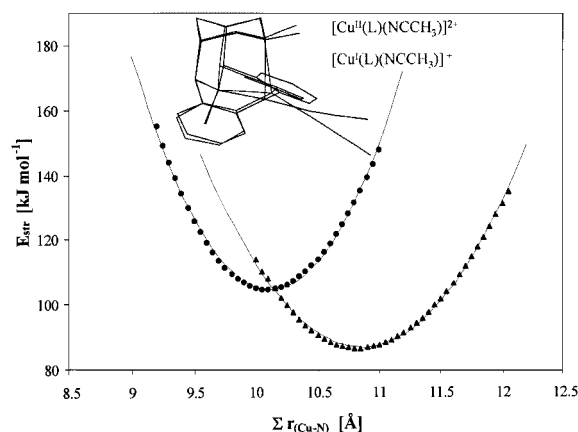
4640

P. Comba,* M. Kerscher, A. Roodt



Slow Electron Self-Exchange in Spite of a Small Inner-Sphere Reorganisation Energy – The Electron-Transfer Properties of a Copper Complex with a Tetradentate Bispidine Ligand

Keywords: Marcus theory / Kinetics / Molecular mechanics / Outer-sphere electron transfer / Cross reaction



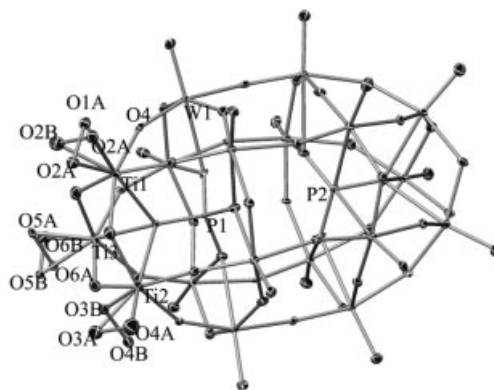
4646

Y. Sakai, Y. Kitakoga, K. Hayashi, K. Yoza,
K. Nomiya*



Isolation and Molecular Structure of a Monomeric, Tris[peroxotitanium(IV)]-Substituted α -Dawson Polyoxometalate Derived from the Tetrameric Anhydride Form Composed of Four Tris[titanium(IV)]-Substituted α -Dawson Substructures and Four Bridging Titanium(IV) Octahedral Groups

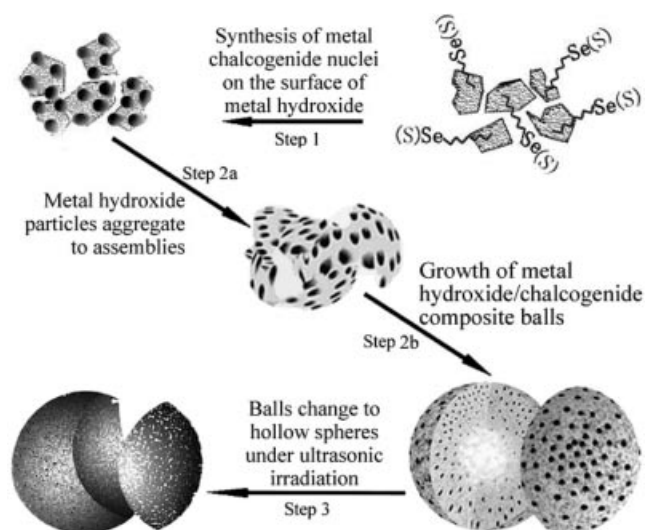
Keywords: Titanium(IV) / Peroxo complexes / Polyoxometalates



4653 S. Xu, H. Wang, J.-J. Zhu,* X.-Q. Xin,
H.-Y. Chen

An in situ Template Route for Fabricating Metal Chalcogenide Hollow Spherical Assemblies Sonochemically

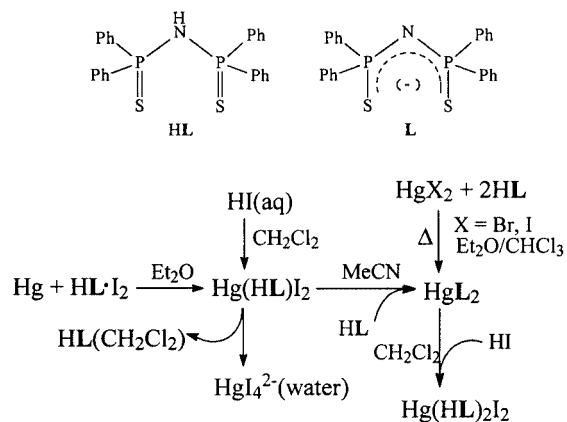
Keywords: Sonochemistry / Nanostructures / Self-assembly / Metal chalcogenides / Hollow spheres



4660 M. C. Aragoni, M. Arca, M. B. Carrea,
F. Demartin, F. A. Devillanova, A. Garau,
F. Isaia,* V. Lippolis, G. Verani

Reaction of Mercury(0) with the I_2 Adduct of Tetraphenyldithioimidodiphosphinic Acid ($SPh_2)_2NH$ (HL) – Crystal Structures of $[Hg(HL)I_2]$ and HgL_2

Keywords: Bridging ligands / Coordination chemistry / Density functional calculations / Iodine / Mercury / S ligands

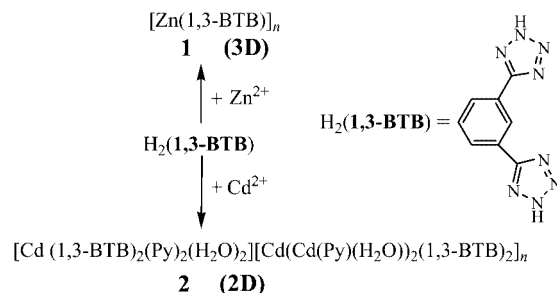


4669 C. Jiang, Z. Yu, C. Jiao, S. Wang, J. Li,
Z. Wang,* Y. Cui*



Luminescent Zn and Cd Coordination Polymers

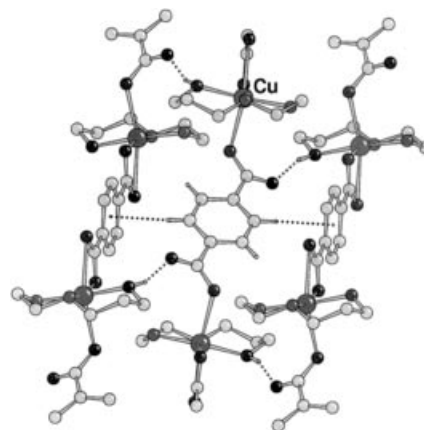
Keywords: N ligands / Coordination polymers / Hydrothermal synthesis / Tubular structures / Fluorescence



4675 P. S. Mukherjee, D. Ghoshal,
E. Zangrando,* T. Mallah,
N. Ray Chaudhuri*

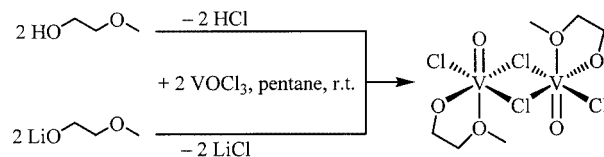
Use of Different Unsaturated Dicarboxylates Toward the Design of New 3D and 2D Networks of Copper(II)

Keywords: Coordination polymers / Copper / Magnetic properties / Weak interaction / Dicarboxylate ligands



4681 E. C. E. Rosenthal,* H. Cui,
K. C. H. Lange, S. Dechert

Synthesis, Molecular Structure, and Olefin Polymerisation Activity of an Oxovanadium(V) Alkoxide with Unprecedented Chloride Bridging Ligands

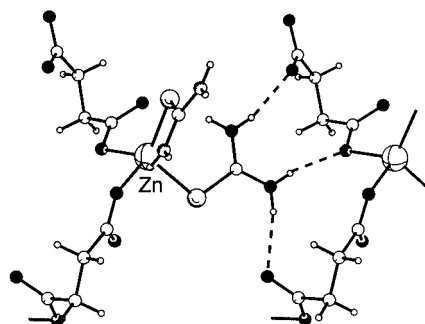


Keywords: Chelates / O ligands / Oxo ligands / Polymerisation / Vanadium

4686 A. D. Burrows,* A. S. Donovan,
R. W. Harrington, M. F. Mahon



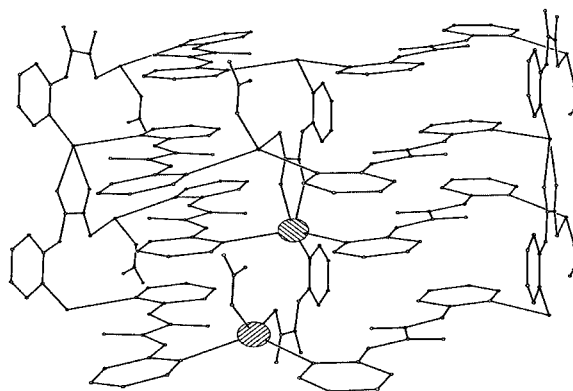
Backbone Flexibility and Counterion Effects on the Structure and Thermal Properties of Di(thiourea)zinc Dicarboxylate Coordination Polymers



Keywords: Crystal engineering / Coordination polymers / Helical structures / Hydrogen bonds / Zinc

4696 H.-L. Hu, C.-W. Yeh, J.-D. Chen*

Synthesis and Structural Characterisation of Ag^I Complexes with *N,N'*-Bis(2-pyridyl)oxalamide and the Anion of *N*-(2-Pyridyl)oxalamic Acid

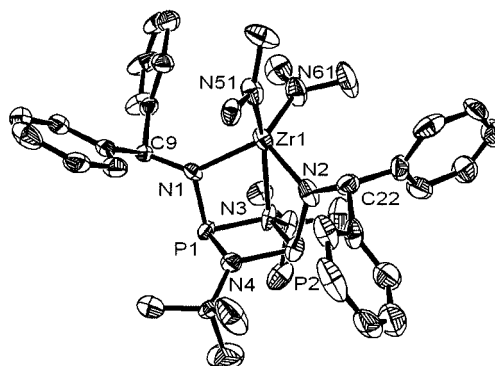


Keywords: Silver / Coordination polymer / *N*-(2-Pyridyl)oxalamic acid / *N,N*-Bis(2-pyridyl)-oxalamide

4702 K. V. Axenov, M. Klinga, M. Leskelä,
V. Kotov, T. Repo*



[Bis(amido)cyclodiphosph(III)azane]dichlorozirconium Complexes for Ethene Polymerization

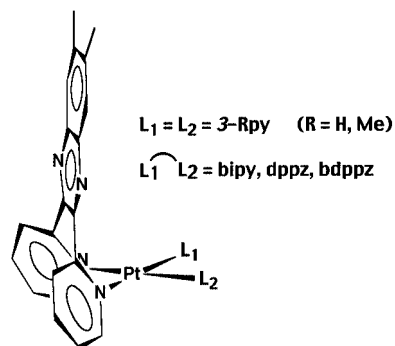


Keywords: Zirconium / Polymerization / Homogeneous catalysis

4710 E. Rotondo,* A. Rotondo, F. Nicoló,
M. L. Di Pietro, M. A. Messina,
M. Cusumano

NMR Study of L-Shaped (Quinoxaline)-
platinum(II) Complexes – Crystal Structure of
[Pt(DMeDPQ)(bipy)](PF₆)₂

Keywords: DNA recognition / N ligands / Nitrogen
heterocycles / NMR spectroscopy / Platinum



4718 S. G. Sreerama, S. Pal*

A Triiron Complex Containing the Carboxylate-
Free {Fe₃(μ₃-O)}⁷⁺ Core and Distorted Pentag-
onal-Bipyramidal Metal Centres

Keywords: Trinuclear iron(III) complex / Crystal
structure / Magnetic properties / Redox
properties

