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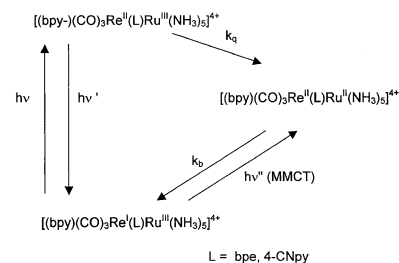
Papers

María G. Mellace, Florencia Fagalde, Néstor E. Katz

Polyhedron 22 (2003) 369

New asymmetric N-heterocyclic-bridged mixed-valent dinuclear complexes of rhenium and ruthenium

Two new mixed-metal mixed-valent complexes, of formulae: $[(\text{CO})_3(\text{bpy})\text{Re}^{\text{I}}(\text{bpe})\text{Ru}^{\text{III}}(\text{NH}_3)_5]^{4+}$ and $[(\text{CO})_3(\text{bpy})\text{Re}^{\text{I}}(4\text{-CNpy})\text{Ru}^{\text{III}}(\text{NH}_3)_5]^{4+}$ were prepared and characterized as solids and in acetonitrile solutions. From their spectroscopic, electrochemical and photophysical properties, the values for the reorganization energies λ and electronic coupling elements H_{AB} for the metal-to-metal intramolecular electron transfers mediated by the N-heterocyclic bridges were calculated, using the Marcus-Hush formalism.

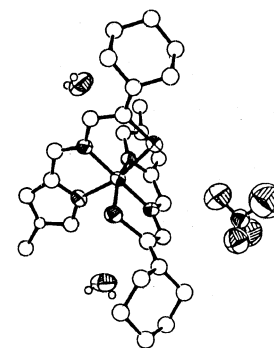


Nitish Chandra Saha, Ray J. Butcher, Siddhartha Chaudhuri, Nityananda Saha

Polyhedron 22 (2003) 375

Synthesis and spectroscopic identification of new iron(III) complexes with 5-methyl-3-formylpyrazole-3-piperidinylthiosemicarbazone ($\text{HMP}_2\text{3Pi}$): X-ray structure of $[\text{Fe}(\text{MP}_2\text{3Pi})_2]\text{ClO}_4 \cdot 2\text{H}_2\text{O}$

$2\text{H}_2\text{O}$ ($\text{X} = \text{Cl}, \text{ClO}_4$ and NO_3) are reported. EPR data (RT and LNT) of the species indicate the presence of spin-paired iron(III) cation with $d_{xz}^2, d_{yz}^2, d_{xy}^1$ configuration. X-ray data on $[\text{Fe}(\text{MP}_2\text{3Pi})_2]\text{ClO}_4 \cdot 2\text{H}_2\text{O}$ have authenticated a FeN_4S_2 octahedral coordination with monoprotic NNS tridentate function of the primary ligand system with two azomethine nitrogen atoms in *trans* positions and the pyrazolyl nitrogen atoms and thiolato sulfurs in *cis* positions.



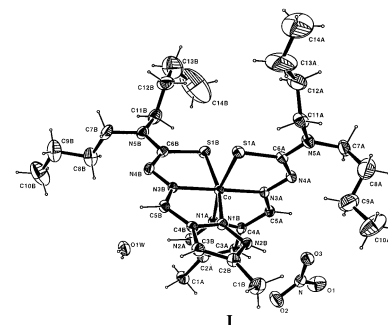
The synthesis and spectroscopic characterization of 5-methyl-3-formylpyrazole-3-piperidinylthiosemicarbazone ($\text{HMP}_2\text{3Pi}$) and its iron(III) complexes, $[\text{Fe}(\text{MP}_2\text{3Pi})_2]\text{X} \cdot$

Nitish Chandra Saha, Ray J. Butcher, Siddhartha Chaudhuri, Nityananda Saha

Polyhedron 22 (2003) 383

Synthesis and spectroscopic characterisation of cobalt(III) and nickel(II) complexes with 5-methyl-3-formylpyrazole-*N*(4)-dibutylthiosemicarbazone (HMP_2NBu_2): X-ray crystallography of $[\text{Co}(\text{MP}_2\text{NBu}_2)_2]\text{NO}_3 \cdot \text{H}_2\text{O}$ (**I**) and $[\text{Ni}(\text{HMP}_2\text{NBu}_2)_2](\text{ClO}_4)_2$ (**II**)

dibutylthiosemicarbazone (HMP_2NBu_2), $[\text{Co}(\text{MP}_2\text{NBu}_2)_2]\text{X} \cdot \text{H}_2\text{O}$ and $[\text{Ni}(\text{HMP}_2\text{NBu}_2)_2]\text{X}_2$ ($\text{X} = \text{Cl}, \text{Br}, \text{ClO}_4, \text{BF}_4$ and NO_3), respectively, are reported. X-ray crystallographic studies on **I** and **II** have authenticated CoN_4S_2 and NiN_4S_2 octahedral coordination, respectively, with the primary ligand behaving as NNS tridentate. In both **I** and **II**, the pair of coordinating ligands are nearly orthogonal to each other, with the difference that while in **I**, the pair of ligands are monodeprotonated, in **II**, the same pair of ligands are neutral.



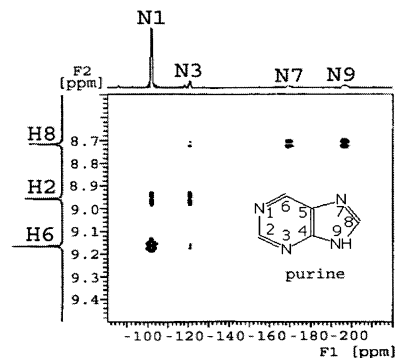
The synthesis and spectroscopic characterisation of cobalt(III) and nickel(II) complexes of 5-methyl-3-formylpyrazole-*N*(4)-

Edward Szlyk, Leszek Pazderski,
Iwona Łakomska, Andrzej Wojtczak,
Lech Kozerski, Jerzy Sitkowski,
Bohdan Kamiński, Harald Günther

Polyhedron 22 (2003) 391

$^1\text{H}\{^{15}\text{N}\}$ heteronuclear correlation and ^{15}N cross-polarized magic angle spinning NMR studies of the coordination modes in Zn(II) chloride complexes with purine and methylpurines

The Zn(II) chloride complexes with purine, 7-methylpurine and 9-methylpurine were studied by NMR methods: $^1\text{H}\{^{15}\text{N}\}$ heteronuclear correlation and ^{15}N cross-polarized magic angle spinning.

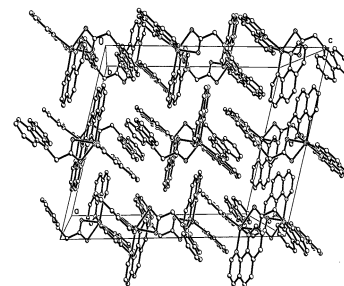


Xuan-Jun Zhang, Yu-Peng Tian,
Sheng-Li Li, Min-hua Jiang, Anwar Usman,
Suchada Chantrapromma, Hoong-Kun Fun

Polyhedron 22 (2003) 397

Zn(II) and Cd(II) *N*-carbazolylacetates with strong fluorescence

Zn(II) and Cd(II) *N*-carbazolylacetates with strong fluorescence *N*-carbazolylacetic acid was synthesized using a new method in high yield and two carbazolylacetato complexes were synthesized and characterized by X-ray determination. Both exhibit strong blue emissions in the solid state as well as high thermal stability and solvent-resistant property.

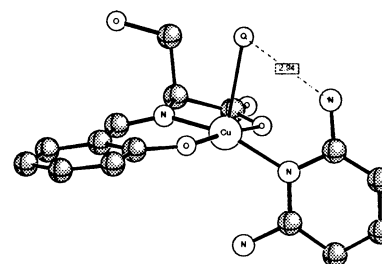


Ángel García-Raso, Juan J. Fiol,
Adela López-Zafra, José A. Castro,
Araceli Cabrero, Ignasi Mata, Elies Molins

Polyhedron 22 (2003) 403

Crystal structure of the copper(II) ternary complex of *N*-salicylidene-L-serinato with 2,6-diaminopyridine. Toxicity studies against *Drosophila melanogaster*

A new ternary [Cu(Sal-(L-Ser))(2,6-diaminopyridine)H₂O] complex has been prepared and the crystal structure determined. Preliminary toxicity studies [larva-to-adult viability (*V*) and developmental time (in days) (DT)] of several copper(II) compounds including the new ternary complex and other related previously described complexes [Cu(Sal-(L-Ser))·H₂O] and [Cu(Sal-Ser)(2-aminopyridine)] against *Drosophila melanogaster* (*Or-R*) show that these copper(II) complexes display less toxicity than simple copper(II) salts.



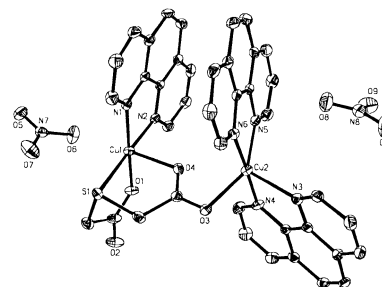
Pavel Kopel, Zdeněk Trávníček,
Jaromír Marek, Maria Korabik,
Jerzy Mrozinski

Polyhedron 22 (2003) 411

Syntheses and properties of binuclear copper(II) mixed-ligand complexes involving thiodiglycolic acid.

The crystal structures of [(phen)₂Cu(μ-tdga)-Cu(phen)](NO₃)₂·5H₂O and [(H₂O)(pmdien)Cu(μ-tdga)Cu(pmdien)(H₂O)](ClO₄)₂

Syntheses and characterization of two binuclear Cu(II) complexes bridged by thiodiglycolate(2-) anion in combination with nitrogen-donor ligands in the coordination sphere is given. The crystal structures of the complexes show well the different coordination possibilities of the dicarboxylate ligand. Magnetochemical study and EPR spectroscopy in relation to the structures is discussed.

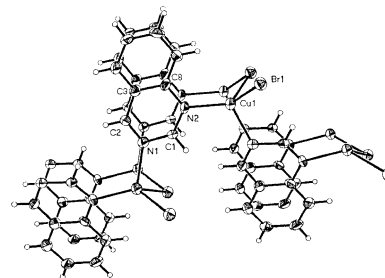


Jonathan T. Maeyer, T. Jason Johnson,
Amy K. Smith, Brian D. Borne,
Robert D. Pike, William T. Pennington,
Mariusz Krawiec, Arnold L. Rheingold

Polyhedron 22 (2003) 419

Pyrimidine, pyridazine, quinazoline, phthalazine, and triazine coordination polymers of copper(I) halides

Self-assembly reactions of $\text{CuX} = \text{CuCl}$, CuBr , and CuI with bridging ligands: B = pyrimidine, quinazoline, pyridazine, phthalazine, and 1,3,5-triazine produced coordination polymers $[\text{CuXB}]$, $[(\text{CuX})_3\text{B}_2]$, $[(\text{CuX})_2\text{B}]$, and $[(\text{CuX})_3\text{B}]$. Ternary reactions with $\text{L} = \text{PPh}_3$ or P(OPh)_3 result in dimeric $[(\text{CuXL})\text{B}]$, polymeric $[(\text{CuXL})_2\text{B}]$, or hexameric $[(\text{CuXL})_3\text{B}]$.

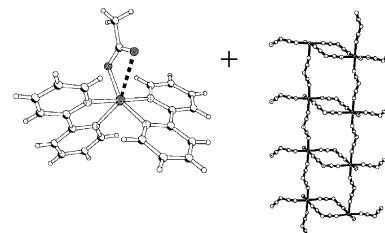


Zhe-Ming Wang, Bai-Wang Sun, Jun Luo,
Song Gao, Chun-Sheng Liao,
Chun-Hua Yan, Yong Li

Polyhedron 22 (2003) 433

Bimetallic sandwiches assembled with chelated Cu/Zn cations and manganese dicyanamide polymeric ladders

Bimetallic sandwich architectures are built by positive layers of Cu- or Zn-bpy-acetate cations and anionic sheets of Mn-dca ladder-like chains, showing very weak antiferromagnetic coupling between Mn-Mn centers in the ladder.

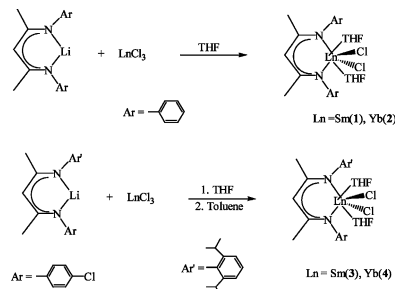


Ying-Ming Yao, Yun-Jie Luo, Rui Jiao,
Qi Shen, Kai-Bei Yu, Ling-Hong Weng

Polyhedron 22 (2003) 441

Synthesis of lanthanide chlorides supported by β -diketiminate ligands and molecular structures of $\text{L}^1\text{LnCl}_2(\text{THF})_2$ ($\text{Ln} = \text{Sm}$ (1), Yb (2)) and $\text{L}^2\text{LnCl}_2(\text{THF})_2$ ($\text{Ln} = \text{Sm}$ (3), Yb (4)), were synthesized in high yield. The substituents on the arene ring have significant effect on the solubility of these complexes. Crystal structure analysis revealed complexes 1 and 3 are both monomeric, and the central metal atom has distorted octahedral geometry.

Four β -diketiminate lanthanide dichlorides, $\text{L}^1\text{LnCl}_2(\text{THF})_2$ ($\text{Ln} = \text{Sm}$ (1), Yb (2)) and $\text{L}^2\text{LnCl}_2(\text{THF})_2$ ($\text{Ln} = \text{Sm}$ (3), Yb (4)), were synthesized in high yield. The substituents on the arene ring have significant effect on the solubility of these complexes. Crystal structure analysis revealed complexes 1 and 3 are both monomeric, and the central metal atom has distorted octahedral geometry.

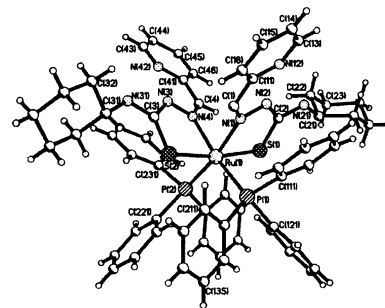


Parbati Sengupta, Rupam Dinda,
Saktiprosad Ghosh, William S. Sheldrick

Polyhedron 22 (2003) 447

Synthesis and characterization of some biologically active ruthenium(II) complexes of thiosemicarbazones of pyridine 2-aldehyde and thiophene 2-aldehyde involving some ring substituted 4-phenylthiosemicarbazides and 4-cyclohexylthiosemicarbazide. Crystal structure of $\text{cis-}[\text{Ru}(\text{PPh}_3)_2(\text{L}^6\text{H})_2](\text{ClO}_4)_2 \cdot 2\text{H}_2\text{O}$ [$\text{L}^6\text{H} = 4$ -(cyclohexyl) thiosemicarbazone of pyridine 2-aldehyde]

A number of ruthenium(II) complexes of a few 4-substituted thiosemicarbazones of pyridine 2-aldehyde and thiophene 2-aldehyde (LH) were isolated and characterized. The complexes are of the general formula $[\text{Ru}(\text{PPh}_3)_2(\text{LH})_2]\text{X}_2$, ($\text{LH} = \text{L}^1\text{H}$, L^2H , $\dots \text{L}^7\text{H}$ and $\text{X} = \text{ClO}_4$, PF_6). One of them, $\text{cis-}[\text{Ru}(\text{PPh}_3)_2(\text{L}^6\text{H})_2](\text{ClO}_4)_2 \cdot 2\text{H}_2\text{O}$, was structurally characterized. All the complexes are found to display biological activity in the form of *E. coli* growth-inhibition and two of them hold the possibility of exhibiting antitumor activity.

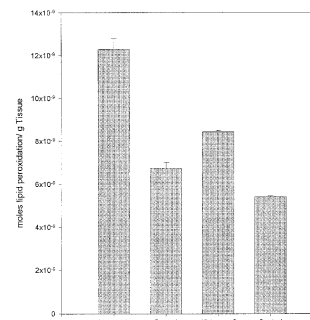


**Dion D.D. Hepburn, J. Marcel Burney,
Stephen A. Woski, John B. Vincent**

Polyhedron 22 (2003) 455

The nutritional supplement chromium picolinate generates oxidative DNA damage and peroxidized lipids in vivo

Chromium picolinate is a popular nutritional supplement. Recently its safety has been questioned. Administration of the supplement to rats has demonstrated for the first time that it can give rise to oxidative DNA damage in whole animals. Further investigation is required to establish the effects of prolonged use by humans.

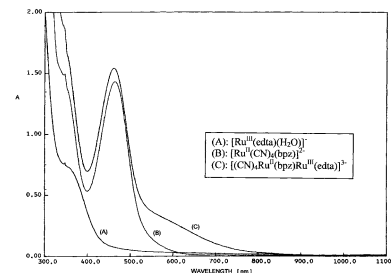


**Mónica E. García Posse,
Mónica M. Vergara, Florencia Fagalde,
Néstor E. Katz**

Polyhedron 22 (2003) 465

Tuning of the reorganization energies by 'innocent' co-ligands in novel mixed-valent dinuclear ruthenium complexes

Two novel mixed-valent ruthenium complexes, of formulae [(tpy)(bpy)-Ru^{II}(pz)Ru^{III}(edta)]⁺ and [(CN)₄Ru^{II}(bpz)-Ru^{III}(edta)]³⁻ were prepared and spectroscopically characterized in aqueous solutions and as solid salts with suitable counterions. From spectral data of metal-to-metal charge transfer (MMCT) absorption bands, a Hush analysis was made, and the reorganization energies for the intramolecular electron transfers were calculated. Tuning is an important factor in devising molecular devices for energy conversion.



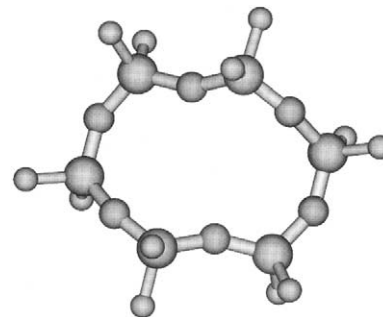
Mark Enlow

Polyhedron 22 (2003) 473

Ab-initio studies of cyclic phosphazine systems (NPX₂)_n.

A study of the structure and bonding in such systems and a search for model systems for the polymer

Ab-initio molecular orbital calculations were carried out for a series of phosphazine compounds, (NPX₂)_n, X = H, F, Cl, and Br, n = 2 through 6, in order to study the electronic structure of such compounds and explore their use as model compounds for the bulk polymer.

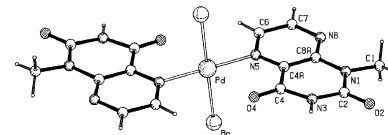


**Esther R. Acuña-Cueva, René Faure,
Nuria A. Illán-Cabeza,
Sonia B. Jiménez-Pulido,
Miguel N. Moreno-Carretero,
Miguel Quirós-Olozábal**

Polyhedron 22 (2003) 483

Synthesis and structural studies on new M^{II}X₂L₂ dihalocomplexes of 1-methylumazine and 1,6,7-trimethylumazine. Crystal structure of copper(II) and palladium(II) complexes

Complexes with general formula MX₂L₂ [M = Cu(II), Pd(II), Pt(II) and L = 1-methylumazine (MLM) or 1,6,7-trimethylumazine (MLMD)] were synthesized and characterized (XRD, IR, NMR, UV-Vis, EPR, magnetic measurements). In Cu/MLM complex, the metal ion involves an octahedral geometry with two *trans* chloride ligands and two lumazine ligands coordinated through O4 and N5 atoms. The molecular unit of the Pd/MLM complex displays a square-planar Pd(II) ion with two bromide anions placed in *trans* position, and two N5 atoms from pteridine moieties.



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