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Papers

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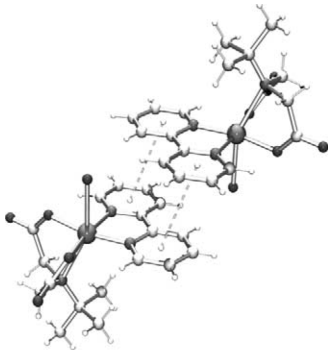
Polyhedron 22 (2003) 1027

Synthesis, crystal structure and properties of *N*-*tert*-butyliminodiacetic acid (H_2TEBIDA), [Cu(TEBIDA)$(H_2O)_2$], {[Cu(TEBIDA)(Him)]$\cdot 2H_2O\}_n$, {Cu(TEBIDA) (5MeHim)$\cdot H_2O\}_n$, and [Cu(TEBIDA)(2,2′-bipy)$(H_2O)]\cdot 4.5H_2O$, (Him = imidazole, 5MeImH = 5-methylimidazole and 2,2′-bipy = 2,2′-bipyridine)

In addition to the *fac*-NO+O(apical) conformation previously reported for the chromium(III) bis-chelate, the structural study of *N*-*tert*-butyliminodiacetic acid (H_2TEBIDA) and ternary complexes of copper(II), TEBIDA and aqua, imidazole, 5-methylimidazole or 2,2′-bipyridine revealed the *mer*-NO_2 or *fac*-O_2+N(apical) conformations for TEBIDA, which are explained on the basis of interligand interactions.



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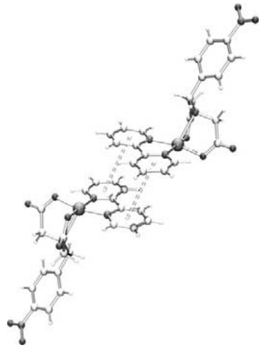
Polyhedron 22 (2003) 1039

Ring–ring or nitro-ring π,π-interactions in *N*-(*p*-nitrobenzyl)iminodiacetic acid (H_2NBIDA) and mixed-ligand copper(II) complexes of NBIDA and imidazole (Him), 2,2′-bipyridine (bipy) or 1,10-phenanthroline (phen). Crystal structures of H_2NBIDA, [Cu(NBIDA)(Him)(H_2O)], [Cu(NBIDA)(bipy)]$\cdot 3H_2O$ and [Cu(NBIDA)(phen)]$\cdot 2H_2O$

Inter-molecular interligand π,π-interactions of the type 'benzyl–benzyl stacking' in *N*-(*p*-nitrobenzyl)iminodiacetic acid (H_2NBIDA) and [Cu(NBIDA(Him)(H_2O))] (Him = imidazole) and of the type 'nitro-benzyl' in [Cu(NBIDA)(bipy)]$\cdot 3H_2O$ and [Cu(NBIDA)(phen)]$\cdot 2H_2O$ are discussed on structural basis. Their significance for molecular recognition processes to build these and closely related crystals is emphasised.



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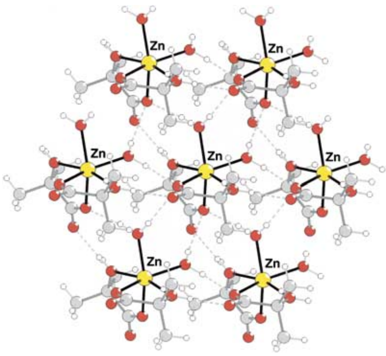
Polyhedron 22 (2003) 1051

The interaction of 2-methyllactic acid (H_2mL) with divalent metal cations. The structures of [M$(HmL)_2(H_2O)_2$], M = Mn(II), Zn(II)

The mononuclear complexes [M$(HmL)_2$-$(H_2O)_2$], M = Mn(II) (**1**), Ni(II) (**2**) or Zn(II) (**3**) and HmL = 2-methyllactato, were prepared and characterised and their thermal behaviour was investigated. The crystal structures of **1** and **3** were established by single-crystal X-ray diffraction. Both compounds consist of the metal ion octahedrically coordinated by two (O,O′)-bidentate monoanionic 2-methyllactato ligands and two aqua ligands.

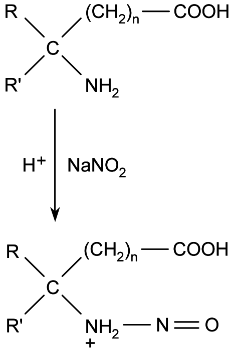


María del Pilar García Santos, Emilio Calle, Julio Casado

Polyhedron 22 (2003) 1059

A method for the kinetic study of amino acid nitrosation reactions

A method for the kinetic study of amino acid nitrosation reactions whose products are unstable is described. The reactions of $NaNO_2$ with α-, β-, and γ-amino acids with a primary amino group in acidic media were studied spectrophotometrically. The experimental rate equation $r = k_{3exp}$[amino acid][nitrite]^2 was found.

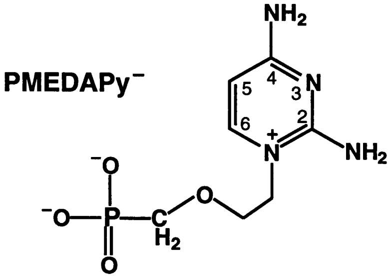


Alfonso Fernández-Botello, Antonín Holý, Virtudes Moreno, Helmut Sigel

Polyhedron 22 (2003) 1067

Stability and structure of binary and ternary metal ion complexes in aqueous solution of the quaternary 1-[2-(phosphonomethoxy)ethyl] derivative of 2,4-diaminopyrimidine ($PMEDAPy^-$). Properties of an acyclic nucleotide analogue

The acidity constants of $H_2(PMEDAPy)^+$ and the stability constants of the $M(PMEDAPy)^+$ complexes [$M^{2+} = Mg^{2+}$, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+} or Cd^{2+}, and also Cu(2,2′-bipyridine)$^{2+}$ or Cu(1,10-phenanthroline)$^{2+}$] were determined in aqueous solution. Comparison with previous results shows that for all binary M^{2+} complexes inhibition due to charge repulsion of the pyrimidinium residue occurs ($\Delta \log \Delta_{M/PMEDAPy} = 0.42 \pm 0.04$) indicating also that no M^{2+}–ether oxygen interaction takes place. The mixed ligand $Cu(Bpy/Phen)(PMEDAPy)^+$ complexes have an increased stability due to intramolecular aromatic-ring stacking.

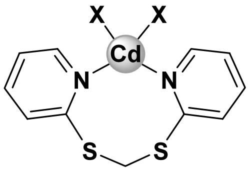


Almudena Amoedo-Portela, Rosa Carballo, José S. Casas, Emilia García-Martínez, Angeles Sánchez-González, José Sordo, Ezequiel M. Vázquez-López

Polyhedron 22 (2003) 1077

Bis(2-pyridylthio)methane complexes of cadmium(II) halides

Cadmium complexes of the type [Cd_2X_4(bpytm)] and [CdX_2(bpytm)] [bpytm = bis(2-pyridylthio)methane] were prepared and characterized. In the complexes of the type [CdX_2(bpytm)] the ligand is *N*,*N*′-bidentate, forming an eight-membered chelate ring.

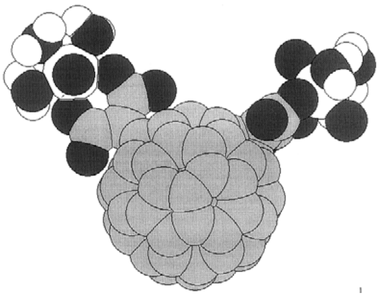


Julio Soto-Guerrero, Josef Havel

Polyhedron 22 (2003) 1085

Dimalonate[C_{60}]fullerene protonation and complexation with uranyl in aqueous solution. Spectrophotometric study

Protonation of water-soluble *e*-dimalonate[C_{60}]fullerene and uranyl complexation with this ligand in aqueous solution were investigated using UV spectrophotometry.

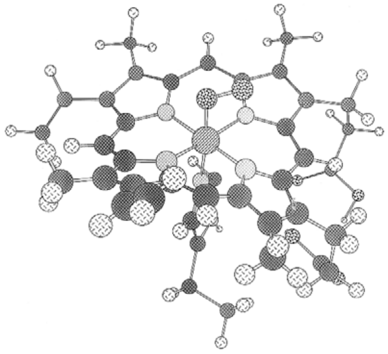


Francisco Torrens

Polyhedron 22 (2003) 1091

Nature of Fe^{III}–O_2, Fe^{II}–CO and Fe^{III}–CN complexes of hemoprotein models

Parametrization of a molecular-mechanics program to include terms specific for 5- and 6-coordinate transition metal complexes results in computer-simulated structures of hemo complexes. The calculations show clearly that certain conformations are much more favourable that others for fixing O_2. From the O_2 binding in haemoglobin and myoglobin and in simple Fe porphyrin models it is concluded that the bent O_2 ligand is best viewed as bound superoxide, O_2^-.

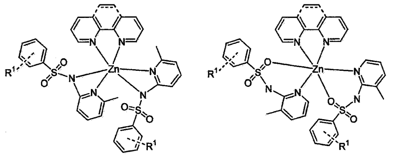


Inmaculada Beloso, Jesús Castro, José A. García-Vázquez, Paulo Pérez-Lourido, Jaime Romero, Antonio Sousa

Polyhedron 22 (2003) 1099

Different coordinative behaviour of methyl-substituted 2-pyridylsulfonamide derivatives as ligands in zinc complexes

Neutral zinc complexes [ZnL_2L'] of a series of methyl substituted *N*-2-pyridylsulfonamide ligands, HL, and 1,10-phenanthroline or 2,2′-bipyridine, L′, have been synthesized by electrochemical oxidation of anodic zinc metal. The crystal structures show different octahedral environments around the metal, N6 or N4O2, depending on the position of the substituent on the pyridine ring.



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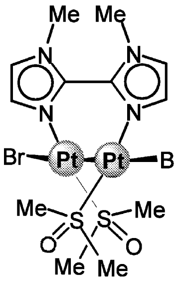
Polyhedron 22 (2003) 1113

Pd(II) and Pt(II) complexes of 2,2′-biimidazole and its *N,N′*-dimethyl derivative. The crystal structure of [{PtBr(DMSO)}$_2$(Me$_2$bim)] (Me$_2$bim = *N,N′*-dimethyl-2,2′-biimidazole)

Compounds of type [MX_2(LL)] [M = Pd, Pt; LL = 2,2′-biimidazole (H$_2$bim) or its *N,N′*-dimethyl derivative (Me$_2$bim)] were prepared and characterized. DMSO solvolyses both the Pt–Cl and Pt–N bonds of [$PtCl_2$(H$_2$bim)], giving several polynuclear species. The structure of [{PtBr(DMSO)}$_2$(Me$_2$bim)], a dinuclear compound containing a Pt(I)–Pt(I) bond, was determined by X-ray crystallography.

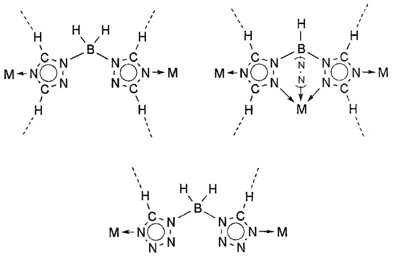


Christoph Janiak, Tobias G. Scharmann

Polyhedron 22 (2003) 1123

Supramolecular C–H···O, C–H···N and C–H···Cl interactions in metal compounds with multi-topic poly(pyrazolyl)borate ligands

Supramolecular C–H···O and C–H···N hydrogen bonding interactions in metal complexes with dihydrobis(1,2,4-triazolyl)borate (**3**), hydrotris(1,2,4-triazolyl)borate (**4**) and dihydrobis(tetrazolyl)borate ligands (**5**) have been analyzed statistically and with respect to their role in determining the crystal packing arrangement.

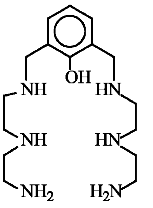


Gianluca Ambrosi, Mauro Formica, Vieri Fusi, Luca Giorgi, Annalisa Guerri, Mauro Micheloni, Roberto Pontellini, Patrizia Rossi

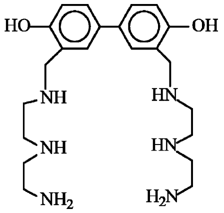
Polyhedron 22 (2003) 1135

Synthesis, acid–base and coordination properties towards Cu(II), Zn(II), and Cd(II) ions of two new polyamino-phenolic ligands, including the crystal structure of a fully protonated ligand

The synthesis of the two new flexible ligands bearing two triaza-polyamine units linked together by phenol or by 4,4′-bis(1-phenol) as spacers is reported. The formation constants of both ligands with Cu(II), Zn(II), and Cd(II) complexes were determined. The role in metal ion coordination of the two topologies obtained is discussed.



L1



L2

Elena Bermejo, Alfonso Castiñeiras, Isabel García, Douglas X. West

Polyhedron 22 (2003) 1147

Spectral and structural studies of mercury(II) complexes of 2-pyridineformamide N(4)-dimethylthiosemicarbazone

Complexes of formula [Hg(HAm4DM)X_2] (X = Cl, Br, I) were synthesized by reaction of 2-pyridineformamide N(4)-dimethylthiosemicarbazone (HAm4DM) with halides of mercury(II) in ethanolic solution, and were characterized by spectroscopic techniques. From solutions of these compounds, crystals of [Hg(Am4DM)Cl]$_2$, [Hg(Am4DM)Br]$_2$ and [Hg(HAm4DM)Br_2]·DMSO were obtained. Single-crystal X-ray structure analysis shows that in all three the ligand coordinates through the sulfur and pyridine and azomethine nitrogen atoms and that the mercury is penta-coordinate.