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# Contents

# Papers

# Shu-Lan Ma, Wen-Xiang Zhu Miao-Qiong Xu, Ying-Li Wang, Qian-Ling Guo, Ying-Chun Liu

Polyhedron 22 (2003) 3249

Syntheses and crystal structures of copper complexes of 7,16-bis (5-*t*-butyl-2-hydroxy-benzyl)-1,4,10,13-tetraoxa-7,16-diazacyclo-octadecane

Two copper complexes of a double-armed crown ether were synthesized. Structural characterization shows that the side-arm *ptert*-butylphenols of the original crown ether unexpectedly were nitrated in the complex prepared from Cu(NO<sub>3</sub>)<sub>2</sub>. Electrochemical studies indicate that the two complexes undergo irreversible reduction in DMF solution.



# Ángel García-Raso, Juan J. Fiol, Bartomeu Adrover, Pere Tauler, Antoni Pons, Ignasi Mata, Enrique Espinosa, Elies Molins

Polyhedron 22 (2003) 3255

Reactivity of copper(II) peptide complexes with bioligands (benzimidazole and creatinine)

In the ternary benzimidazole complexes the lateral chain of the peptide moiety play an important role on the relative orientation of the ligand. In contrast, in the creatinine complexes the presence of two important intramolecular hydrogen bonds yield a nearly co-planar system which is independent of the nature of the peptidic lateral chain.



### Urszula Rychlewska, Miloš I. Djuran, Beata Warżajtis, Dusanka D. Radanović, Miorad M. Vasojević, Dušan J. Radanović

Polyhedron 22 (2003) 3265

Crystal structure of cis-polar, trans(Cl,O<sub>5</sub>)-Na<sub>2</sub>[Rh(1,3-pddadp)Cl] $\cdot$ 7H<sub>2</sub>O and structural correlations between octahedral pentadentate metal(III) complexes with diaminopolycarboxylato-type ligands

The structural characteristics of a new pentadentate rhodium(III) complex, the *cis*-polar,*trans*(Cl,O<sub>5</sub>)-isomer of Na<sub>2</sub>[Rh(1,3pddadp)Cl]  $\cdot$ 7H<sub>2</sub>O, obtained in the reaction of RhCl<sub>3</sub> $\cdot$  3H<sub>2</sub>O with the 1,3-pddadp ligand (1,3-pddadp is the 1,3-propanediamine-*N*,*N'*diacetate-*N*,*N'*-di-3-propionate ion) have been reported. The electronic absorption spectrum of this complex is also given and compared with those of hexadentate *trans* (O<sub>5</sub>O<sub>6</sub>)-[Rh(1,3-pddadp)]<sup>-</sup> and *trans*(O<sub>5</sub>)-[Rh(1,3-pddadp)]<sup>-</sup> complexes.



# William T.A. Harrison, R. Alan Howie, Marcel Jaspars, Solange M.S.V. Wardell, James L. Wardell

Polyhedron 22 (2003) 3277

Further studies of  $[\omega$ -(haloalkylstannyl)alkyl] phosphine oxides. Structures of bis[2-(bromodimethylstannyl)ethyl] phenylphosphine oxide and *t*-butyl [3-(iododimethylstannyl)propyl] phenylphosphine oxide Structures of  $(BrMe_2SnCH_2CH_2)_2P(O)Ph$ and  $IMe_2SnCH_2CH_2CH_2P(O)PhBu^t$  are reported and compared with those of related compounds.



### Eduardo R. Pérez, Rogerio M. Carvalho, Regina H. A. Santos, Maria T. P. Gambardella, Benedito S. Lima-Neto

Polyhedron 22 (2003) 3289

Synthesis of *trans*-[RuCl<sub>2</sub>(dppe)<sub>2</sub>] using the tetraalkylammonium chloride under transfer phase catalysis conditions. Crystal structure of the novel *trans*-[RuBrCl(dppe)<sub>2</sub>]

The complex *trans*-[RuCl<sub>2</sub>(dppe)<sub>2</sub>] was synthesized by solid state reaction of RuCl<sub>3</sub>·3H<sub>2</sub>O with Bu<sub>4</sub>NCl as catalyst and subsequent coordination with dppe in dichloromethane. The complex *trans*-[RuBrCl(dppe)<sub>2</sub>] was obtained when the TBAB was used. The crystal structure of the later complex was determined.

 $\operatorname{RuCl}_{3} \operatorname{3H}_{2}O \xrightarrow[\text{solid state}]{dppe} trans-[\operatorname{RuCl}_{2}(\operatorname{dppe})_{2}]$ 

### Viorel Cîrcu, Manuel A. Fernandes, Laurence Carlton

Polyhedron 22 (2003) 3293

Reactions of  $[Rh(Tp^*)(PPh_3)_2]$   $(Tp^* = hy$ drotris(3,5-dimethylpyrazolyl)-borate) involving fragmentation or loss of Tp\*. $Structures of <math>[Rh(Cl)_2(H)(PPh_3)_2(pz^*)]$ ,  $[(PPh_3)_2Rh(\mu-SC_6F_5)_2Rh(SC_6F_5)(H)(PPh_3)$  $(pz^*)]$   $(pz^* = 3, 5-dimethylpyrazole)$  and  $[{Rh(Cl)_2(PPh_3)_2}_2 Hg]$  In the reaction of  $[Rh(Tp^*)(PPh_3)_2]$  with  $Ph_3SiH/CH_2Cl_2$ , and  $C_6F_5SH$  the  $Tp^*$  ligand is broken up; with  $HgCl_2$  it is lost altogether. Structures of  $[Rh(Cl)_2(H)(PPh_3)_2$  (pz\*)],  $[(PPh_3)_2Rh(\mu-SC_6F_5)_2Rh(SC_6F_5)(H)$  (PPh\_3)\_2 (pz\*)] and  $[{Rh(Cl)_2(PPh_3)_2}_2Hg]$  are reported.



# Julita Eilmes, Marcin Ptaszek, Łukasz Dobrzycki, Krzysztof Woźniak

Polyhedron 22 (2003) 3299

New alkoxycarbonyl derivatives of dibenzotetraaza[14]annulene. Crystal and molecular structure of [5,14-dihydro-7,16-diisopropoxy-carbonyl-8,15-dimethyl-6,17-diphenyldi benzo [b,i][1,4,8,11]tetraazacyclotetradecinato(2-)- $\kappa^4$ N]nickel(II) New supramolecular receptors equipped with two extended concave surfaces have been synthesized based on dibenzotetraaza[14]annulene framework. The X-ray diffraction data of diisopropoxycarbonyl derivative of dibenzotetraaza[14]annulene Ni(II) complex revealed its potential to associate with the molecules of appropriate guests.



### Jan O. Dzięgielewski, S. Michalik, R. Kruszynski', T.J. Bartczak, J. Kusz

Polyhedron 22 (2003) 3307

The syntheses, crystal, molecular and electronic structures of two polymorphs of [Re- $Cl_2(N_2COPh)(C_3N_2H_4)(PPh_3)_2$  and [Re Cl<sub>2</sub>(N<sub>2</sub>COPh)(py)(PPh<sub>3</sub>)<sub>2</sub>] complexes

The  $[\text{ReCl}_2(\eta^2-N_2\text{COPh-N}',O)(\text{PPh}_3)_2]$  complex is a precursor of a variety organodiazenido complexes. [ReCl2(n2-N2COPh-N',O) (PPh<sub>3</sub>)<sub>2</sub>] reacts with neutral donor ligands L, such as pyrazole and pyridine, giving organodiazenido species [ReCl2(N2COPh)L(P  $Ph_{3})_{2}].$ 



### Wen Dong, Qing-Lun Wang, Zhan-Quan Liu, Dai-Zheng Liao, Zong-Hui Jiang, Shi-Ping Yan, Peng Cheng

Polyhedron 22 (2003) 3315

Syntheses, structures and magnetic properties of 1-D complex {[Ni( $\mu_{1:5}$ -dca)(pn)<sub>2</sub>] 2-D complex[Mn( $\mu_{1:5}$ -dca)<sub>2</sub>  $(ClO_4)$ <sub>n</sub>, (phen)]<sub>n</sub> and 3-D complex  $[Mn(\mu_{1;5}-dca)_2L]_n$  $(dca = dicyanamide, N(CN)_{2}; pn = 1,3-pro$ pane diamine;phen = phenanthroline; L = 4,4'-ditriazole methane)

Anantharam Sreekanth, Maliyeckal

Structural and spectral studies on four

coordinate copper(II) complexes of 2-ben-

zoylpyridine N(4), N(4)-(butane-1,4-diyl)thi-

Michael A. Beckett, Martin P. Rugen-

Hankey, K. Sukumar Varma

Polyhedron 22 (2003) 3333

Ar), derivatives

**R.** Prathapachandra Kurup

Polyhedron 22 (2003) 3321

osemicarbazone

### Three novel dicyanamide complexes {[Ni- $(\mu_{1,5}-dca)(pn)](ClO_4)_n$ (I), $[Mn(\mu_{1,5}-dca)_2]$ $(phen)]_n$ (II) and $[Mn(\mu_{1,5}-dca)_2L]_n$ (III) have been synthesized and structurally characterized. Complex I forms 1-D chain and II forms 2-D layer structure, whereas complex III contains 3-D networks bridging via $\mu_{1.5}$ -dca and 4,4'-ditriazole methane ligands. The magnetic measurements indicate that all these complexes exhibit weak antiferromagnetic interaction through the dicyanamide ligands.

Eight new copper(II) complexes of 2-benzoylpyridine N(4),N(4)-(butane-1,4-diyl)thiosemicarbazone (HBpypTsc) with general stoichiometry CuBpypTscX [X=N3, Cl, NO3, NCS, ClO<sub>4</sub>, Br, SH and CN] were synthesized and characterized by IR and UV/Vis spectroscopies. The terdentate nature of the ligand is inferred from the IR spectra. Spin Hamiltonian parameters of the compounds were calculated from the EPR spectra. The structures of the compounds CuBpypTscCl (2), CuBpypTscBr (bf 6) and CuBpypTscSH (7) were solved by single crystal X-ray diffraction. CuBpypTscCl (2) is a centrosymmetric dimer with chloro bridges. The geometry around copper in other

# Synthesis and characterisation of cyclo-boraexcess of Et<sub>3</sub>N. The cyclo-boratetrasiloxanes tetrasiloxane, (RBO)(Me<sub>2</sub>SiO)<sub>3</sub> ( $R = {}^{n}Bu$ , are weakly Lewis acidic, with acceptor number (AN) values of $\sim$ 30, but do not form

adducts with amines.







The dependence of the Curie temperature

 $T_c$  on hydrostatic pressure was determined

to 6 kbar for the quasi-1D molecular mag-

nets [MnR<sub>4</sub>TPP][TCNE] for  $R = OC_{10}H_{21}$ ,

 $OC_{14}H_{29}$  and F. In all three  $T_c$  decreases initially with pressure but passes through

a sharp minimum near 2 kbar (see fig-

ure) indicative of a pressure-induced lattice

distortion.

# C.W. Looney, K. Falk, James J. Hamlin, Takahiro Tomita, James S. Schilling, W. Haase, Z. Tomkowicz

Polyhedron 22 (2003) 3339

Hydrostatic pressure dependence of the Curie temperature of  $[MnR_4TPP][TCNE]$  for  $R = OC_{10}H_{21}$ ,  $OC_{14}H_{29}$ , and F (TPP, tetraphenylporhyrin; TCNE, tetracyanoeth-ylene)

David G. Morris, Kenneth W. Muir, Cindy Ong Woei Chii

Polyhedron 22 (2003) 3345

Silver(I) and mercury(II) complexes of  $Me_3N(+)-\ N(-)X$  ylides: synthesis and structure

The ligating abilities of nitrogen ylides,  $L=Me_3N(+)-N(-)X$ , are displayed in the coordination polymer LAgNO<sub>3</sub>, the discrete complex L<sub>2</sub>AgNO<sub>3</sub> and the *catena*-[LHgCl<sub>2</sub>] ylide adduct. In the salt [LH][Hg<sub>2</sub>Cl<sub>5</sub>] protonated ylide cations are anchored by hydrogen bonds to a novel [Hg<sub>2</sub>Cl<sub>5</sub><sup>-</sup>]<sub>∞</sub> sheet structure built from both octahedrally and tetrahedrally coordinated Hg(II) cations.

![](_page_3_Figure_9.jpeg)

### Genivaldo J. Perpétuo, Marcelo R.L. Oliveira, Jan Janczak, Heulla P. Vieira, Fabiana F. Amaral, Vito M. De Bellis

Polyhedron 22 (2003) 3355

Syntheses, crystal structure and spectroscopic characterization of novel *N*-R-sulfonyl-dithiocarbimate zinc(II) complexes Two new *N*-R-sulfonyldithiocarbimate zinc(II) complexes with the formula of  $(Ph_4P)_2[Zn(RSO_2NCS_2)_2]$ , where  $R = C_6H_5$ (1) and 4-CH<sub>3</sub>C<sub>6</sub>H<sub>4</sub> (2) have been obtained in crystalline form by the reaction of the appropriate potassium *N*-R-sulfonyldithiocarbimate salt and zinc(II) acetate. The compounds are characterized by single crystal X-ray diffraction technique and by IR and NMR spectroscopy.

![](_page_3_Figure_14.jpeg)

![](_page_3_Figure_15.jpeg)

![](_page_3_Figure_16.jpeg)

### Margarita Crespo, Emilia Evangelio, Mercè Font-Bardía, Sonia Pérez, Xavier Solans

Polyhedron 22 (2003) 3363

Oxidative addition of methyl iodide to dimethylplatinum (II) compounds containing bulky ligands gave platinum (IV) compounds for which isomers such as rotamers, E–Z conformers, or diastereomers have been detected.

![](_page_3_Figure_21.jpeg)

### Peter J. Heard, Paul M. King, Phunrawie Sroisuwan, Nikolas Kaltsoyannis

Polyhedron 22 (2003) 3371

Tricarbonylrhenium(I) halide complexes of chiral non-racemic 2-(dioxolanyl)-6-(dioxanyl) pyridine ligands: synthesis, NMR and DFT calculations DFT calculations on the  $[ReX(CO)_3]$  complexes of chiral non-racemic 2-(dioxolanyl)-6-(dioxanyl)pyridines, in which the ligands coordinate in a bidentate N/O fashion, indicate that binding of the five-membered dioxolanyl ring is strongly favoured over that of the six-membered dioxanyl ring. In solution 3 of the 8 possible diastereoisomers are observed, two of which undergo exchange above ambient temperature.

![](_page_4_Figure_6.jpeg)

# F.J. Ramos-Lima, A.G. Quiroga, Jose M. Pérez, Carmen Navarro-Ranninger

Polyhedron 22 (2003) 3379

Preparation, characterization and cytotoxic activity of new compounds *trans*-[PtCl<sub>2</sub>NH<sub>3</sub> (3-(hydroxymethyl)-pyridine)] and *trans*-[PtCl<sub>2</sub>NH<sub>3</sub>(4-(hydroxymethyl)-pyridine)]

We report the synthesis, characterization and cytotoxic assays of new *trans*-platinum compounds, *trans*-[PtCl<sub>2</sub>NH<sub>3</sub>(3-(hydroxymethyl)-pyridine)] and *trans*-[PtCl<sub>2</sub>NH<sub>3</sub>(4-(hydroxymethyl)-pyridine)].

![](_page_4_Figure_11.jpeg)

### Konstantin A. Brylev, Nikolai G. Naumov, Gabriel Peris, Rosa Llusar, Vladimir E. Fedorov

Polyhedron 22 (2003) 3383

Novel inorganic ionic compounds based on Re<sub>6</sub> chalcocyanide cluster complexes: synthesis and crystal structures of  $[CuNH_3$  (trien)]<sub>2</sub>[Re<sub>6</sub>S<sub>8</sub>(CN)<sub>6</sub>]·7H<sub>2</sub>O,  $[CuNH_3$ (trien)]<sub>2</sub> [Re<sub>6</sub>Se<sub>8</sub>(CN)<sub>6</sub>] and  $[CuNH_3$ (trien)]<sub>2</sub>[Re<sub>6</sub>Te<sub>8</sub> (CN)<sub>6</sub>]·H<sub>2</sub>O Three new octahedral rhenium chalcocyanide cluster compounds [CuNH<sub>3</sub>(trien)]<sub>2</sub>[Re<sub>6</sub> $Q_8$  (CN)<sub>6</sub>]-*n*H<sub>2</sub>O (Q=S, Se and Te) exhibiting ionic structures have been obtained. The compounds have been characterized by single-crystal X-ray diffraction. All three compounds contain a cationic complex [CuNH<sub>3</sub>(trien)]<sup>2+</sup> which was not described previously.

![](_page_4_Figure_16.jpeg)

# Edward Szłyk, Robert Kucharek, Iwona Szymańska, Leszek Pazderski

Polyhedron 22 (2003) 3389

Synthesis and characterization of Cu(I) chelate complexes with 1,3-bis(diphenylphosphino)propane, 1,2-bis(diphenylphosph ino) benzene and perfluorinated carboxylates Cu(I) complexes with 1,3-bis(diphenylphosphino)propane, 1,2-bis(diphenylphosphino)benzene and perfluorinated carboxylates consist of distinct bis-chelated [Cu(diphosphine)<sub>2</sub>]<sup>+</sup> cations and uncoordinated carboxylates.

![](_page_4_Picture_21.jpeg)

### Ioan Ghesner, Albert Soran, Cristian Silvestru, John E. Drake

Polyhedron 22 (2003) 3395

 $\label{eq:composition} Trimethylantimony(V) tetraphenyldichal$ cog-enoimidodiphosphinates: crystal struc $ture of Me_3Sb[O-PPh_2=N-PPh_2=S]_2, a$ compound containing true O-monometallicmono-connective phosphorus ligands withXPNPY skeleton Me-S-PPh<sub>2</sub>=N-PPh<sub>2</sub>=S (1) was obtained from Me<sub>3</sub>SbCl<sub>2</sub> and K[(SPPh<sub>2</sub>)<sub>2</sub>N] as a result of the migration of a methyl group from antimony to sulfur. Reaction of Me<sub>3</sub>SbCl<sub>2</sub> and K[(OPPh<sub>2</sub>)(SPPh<sub>2</sub>)N] gave Me<sub>3</sub>Sb[O-PPh<sub>2</sub>=N-PPh<sub>2</sub>=S]<sub>2</sub> (2) which exhibits a trigonal bipyramidal coordination around antimony, with two *O*-monometallic monoconnective phosphorus ligands and a planar SbC<sub>3</sub> system.

![](_page_5_Figure_6.jpeg)

### M. Gabriela Ballinas-López, Efrén V. García-Báez, María J. Rosales-Hoz

Polyhedron 22 (2003) 3403

Solid state structure and fluxionality in solution of  $[H_4Ru_4(CO)_{11}L]$   $(L = P(C_6F_5)_3, PMe_2Ph, P(OMe)_3 and P(OEt)_3)$ : two different structures

The spectroscopy and structure of compounds  $[H_4Ru_4(CO)_{11}L]$   $(L=P(C_6F_5)_3,$ PMe<sub>2</sub>Ph, P(OMe)<sub>3</sub> and P(OEt)<sub>3</sub>) were obtained including multinuclear VT NMR studies. The effect of the substituents in the phosphorus ligand, in the structure and dynamical behaviour of the compounds, was analysed. The phosphite and P(C\_6F\_5)\_3 derivatives showed the same *D2d* structure in the solid state but in the compound containing PMe<sub>2</sub>Ph, a geometry with *Cs* symmetry can be appreciated. Both types of structures are proposed to participate in the dynamical equilibriums showed by all four compounds.

![](_page_5_Figure_11.jpeg)

Masahiro Ebihara, Masami Iiba, Satohisa Higashi, Naoki Tsuzuki, Takashi Kawamura, Tsunenori Morioka, Shinji Ozawa, Tokio Yamabe, Hideki Masuda

Polyhedron 22 (2003) 3413

Benzylidyne-capped group 9 trinuclear clusters: synthesis, structure and properties of trirhodium and cobalt–rhodium mixed-metal clusters  $[Co_{3-n}Rh_nCp_3(\mu_3-CPh)_2]$  (*n* = 1; 2; 3)

A series of benzylidyne-capped clusters  $[M_3Cp_3(\mu_3-CPh)_2]$   $(M_3=Rh_3, CoRh_2$  and  $Co_2Rh)$  were synthesized and characterized (X-ray structure analyses, cyclic voltammetry, UV–Vis, ESR of their anionic radicals), and their electronic structures were examined by DFT calculations of their model complexes.

![](_page_5_Picture_16.jpeg)

Contents

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![](_page_6_Picture_5.jpeg)

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![](_page_6_Picture_7.jpeg)

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