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POLYHEDRON

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Contents

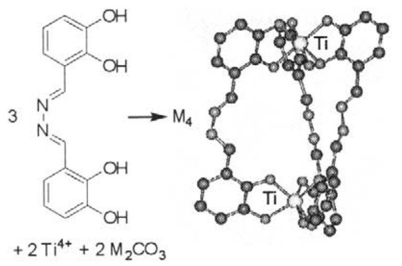
Papers

Markus Albrecht, Susanne Kamptmann, Roland Fröhlich

Polyhedron 22 (2003) 643

3,3′-{(1*E*,2*E*)-Hydrazine-1,2-diylidene-di[(*E*)methylylidene]}dibenzene-1,2-diol ($BCAz\text{-}H_4$): an easy to prepare but very useful building block for the self-assembly of triple-stranded helicates; the X-ray crystal structure of $Na_4[(BCAz)_3Ti_2]\cdot 7$ dmf$\cdot H_2O$

An azine-bridged ligand (**$BCAz\text{-}H_4$**) is prepared by simple condensation of one equivalent of hydrazine with two equivalents of 2,3-dihydroxybenzaldehyde. The ligand forms triple-stranded dinuclear helicates with titanium(IV) ions. X-ray crystallography of the sodium salt reveals that one of the counterions in the solid state is encapsulated in the interior of the helicate.

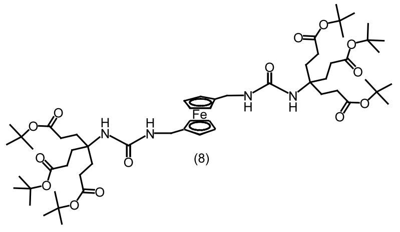


Michelle D. Pratt, Paul D. Beer

Polyhedron 22 (2003) 649

Anion recognition and sensing by mono- and bis-urea substituted ferrocene receptors

New mono- and bis-urea substituted ferrocene receptors have been synthesised. Proton NMR anion coordination studies with chloride and dihydrogen phosphate reveal the presence of bulky *tert*-butyl ester group urea substitiuents disfavours $H_2PO_4^-$ complexation and amplifies the recognition of Cl^-.

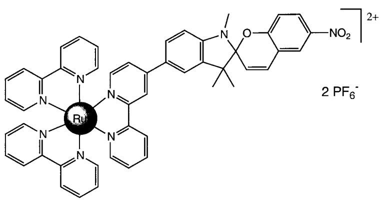


Manel Querol, Biljana Bozic, Nunzio Salluce, Peter Belser

Polyhedron 22 (2003) 655

Synthesis, metal complex formation, and switching properties of spiropyrans linked to chelating sites

The synthesis of a new series of photoactive spiropyran compounds containing covalently bounded bipyridine and phenanthroline ligands is described. Incorporated in a ‘wire’ type bridging ligand such spiropyran switches can play an important role in the modulation of light-induced energy or electron transfer processes. The excited ruthenium complex does not influence the state (open or closed) of the attached spiropyran.



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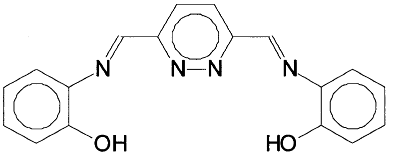
Sally Brooker, Simon S. Iremonger,
Paul G. Plieger

Polyhedron 22 (2003) 665

A new bis(phenol-armed) pyridazine-containing Schiff base ligand: synthesis, complexation and reduction to the amine ligand analogue

A structure determination shows that H_2L is close to planar. Hydrogen-bonding and $\pi-\pi$ stacking interactions are instrumental in H_2L stacking into columns of a stepped criss-cross array. H_2L is redox active (cyclic voltammetry). Chemical reduction of H_2L gives the diamine analogue H_6L'. Three complexes, $Co_2L(CH_3COO)_2$, $Ni_2L(CH_3COO)_2(H_2O)$ and $Cu_2L(CH_3COO)_2(H_2O)_2(CH_3CN)$, are described.



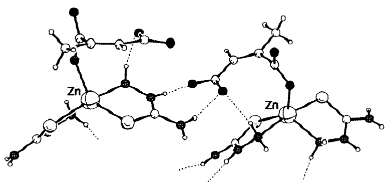
H_2L

Jennifer E.V. Babb, Andrew D. Burrows,
Ross W. Harrington, Mary F. Mahon

Polyhedron 22 (2003) 673

Zinc thiosemicarbazide dicarboxylates: the influence of the anion shape on supramolecular structure

The reactions of bis(thiosemicarbazide)zinc complexes with a range of dicarboxylates are reported and eight products crystallographically characterised. Linear dicarboxylates give products containing chains of cations and anions with the ions linked together by hydrogen bonding, as typified by $[Zn(tsc)_2(OH_2)_2]$[fumarate]. In contrast, non-linear dicarboxylates give products in which carboxylate groups are co-ordinated to the zinc, such as $[Zn(tsc)_2$(citraconate]$\cdot H_2O$ and $[Zn(Metsc)_2$(Hphthalate)][Hphthalate]$\cdot H_2O$.

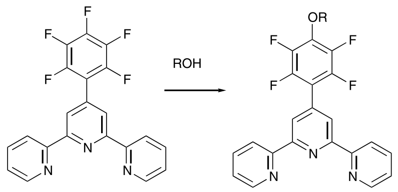


Edwin C. Constable, Benson Kariuki,
Azad Mahmood

Polyhedron 22 (2003) 687

New approaches to sugar-functionalised 2,2′:6′,2″-terpyridines based upon tetrafluorophenoxy spacers; crystal and molecular structures of 4′-(tetrafluoro-4-hydroxyphenyl)-2,2′:6′,2″-terpyridine and 4′-(4-methoxytetrafluorophenyl)-2,2′:6′,2″-terpyridine

4′-Pentafluorophenyl-2,2′:6′,2″-terpyridine reacts with alcohols to give 4′-(4-alkoxytetrafluorophenyl)-2,2′:6′,2″-terpyridines which may be converted to 4′-(tetrafluoro-4-hydroxyphenyl)-2,2′:6′,2″-terpyridine. Reaction of the phenol with electrophilic sugar derivatives allows the preparation of new biofunctionalised ligands. Iron(II) complexes have been prepared and show the new compounds behave as typical tpy ligands with strongly electron-withdrawing substituents.

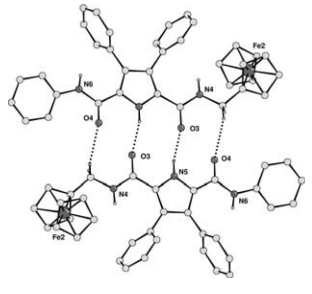


Simon J. Coles, Guy Denuault,
Philip A. Gale, Peter N. Horton,
Michael B. Hursthouse, Mark E. Light,
Colin N. Warriner

Polyhedron 22 (2003) 699

Mono- and bis-ferrocene 2,5-diamidopyrrole clefts: solid-state assembly, anion binding and electrochemical properties

The solid-state self-assembly, anion binding and electrochemical properties of four ferrocene functionalized 2,5-diamidopyrrole cleft species have been studied. The compounds containing a ferrocene directly conjugated to the amidopyrrole hydrogen bond donor group have higher affinities for anions than the compounds containing a methylene spacer group. Significant shifts in the ferrocene/ferrocenium redox couple are observed upon addition of benzoate to these former systems.

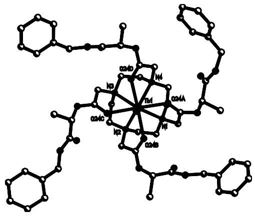


**Thorfinnur Gunnlaugsson,
R. Jeremy H. Davies, Mark Nieuwenhuyzen,
John E. O'Brien, Clarke S. Stevenson,
Sinéad Mulready**

Polyhedron 22 (2003) 711

Synthesis, structural and biological evaluation of GlyAla based lanthanide macrocyclic conjugates as supramolecular ribonuclease mimics

The synthesis of several lanthanide ion complexes of the glycine–alanine based ligands **1** and **2** is described. These supramolecular complexes were designed to mimic the nature of the hydrophobic active site of ribonucleases. All the complexes gave rise to enhancement in the hydrolysis of HPNP a RNA mimic compound at pH 7.4.

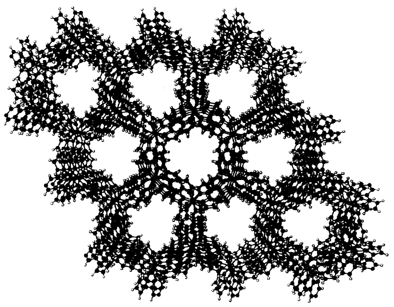


**Robert J. Smithson, Colin A. Kilner,
Adrian R. Brough, Malcolm A. Halcrow**

Polyhedron 22 (2003) 725

Iron(II) complexes of (pyrazol-3-yl)pyrazine. Anion-dependent formation of a hydrogen-bonded, chiral nanoporous lattice

The complex *fac*-$[Fe(L^1)_3](BF_4)_2 \cdot 2H_2O$ (L^1 = {pyrazol-3-yl}pyrazine) has a chiral honeycomb structure, held together by inter-cation hydrogen bonding. The pores in the structure are 5.3 Å across, and contain a mixture of BF_4^- anions and water. In contrast, *mer*-$[Fe(L^1)_3](ClO_4)_2 \cdot H_2O$ forms a more conventional 3D hydrogen-bonded lattice.

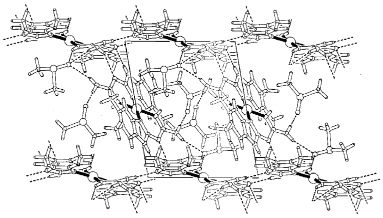


**Michael M. Bishop, Andrew H.W. Lee,
Leonard F. Lindoy, Peter Turner**

Polyhedron 22 (2003) 735

A comparative study of supramolecular assemblies containing N''-(5,6-dimethyl-1*H*-benzimidazol-2-yl)guanidine, 2-guanidinobenzimidazole and their Ni(II) complexes

The synthesis and X-ray structures of simple supramolecular assemblies based on N''-(5,6-dimethyl-1*H*-benzimidazol-2-yl)guanidine and incorporating (i) the free ligand, (ii) the complex formed by this ligand and phthalimide and (iii) the structure of the corresponding neutral bis-ligand Ni(II) complex are presented. The role of the methyl substituents in inhibiting the ligand from being incorporated into the same supramolecular structures as found for the related (unsubstituted) ligand assemblies based on 2-guanidinobenzimidazole is discussed.

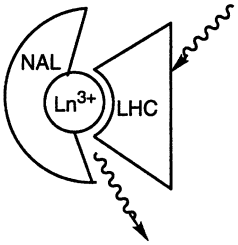


**Steven W. Magennis, J. Craig, A. Gardner,
Flavia Fucassi, Peter J. Cragg,
Neil Robertson, Simon Parsons,
Zoe Pikramenou**

Polyhedron 22 (2003) 745

Crown ether lanthanide complexes as building blocks for luminescent ternary complexes

Crown ethers have been used as non-absorbing ligands to control the triggering of lanthanide emission from light-harvesting centres by formation of ternary complexes.

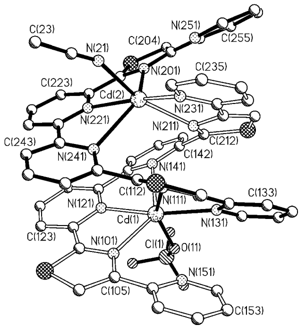


Craig R. Rice, Christian J. Baylies, Lindsay P. Harding, John C. Jeffery, Rowena L. Paul, Michael D. Ward

Polyhedron 22 (2003) 755

Cadmium-containing pyridyl–thiazole complexes: crystal structures and solution behaviour of mononuclear, dinuclear double helicate and dinuclear triple helicate complexes

Reaction of $Cd(ClO_4)_2$ with the potentially tetra-, penta- and hexadentate pyridine–thiazole-containing ligands gives $[Cd_2(L^1)_3(H_2O)][ClO_4]_4$ (a dinuclear triple helicate), mononuclear $[Cd(L^2)(ClO_4)_2]$, and $[Cd_2(L^3)_2(ClO_4)(CH_3CN)][ClO_4]_3$ (a dinuclear double helicate), respectively. Each of these complexes have been characterised by crystallography. Furthermore ^1H NMR shows that these structures are retained in solution.

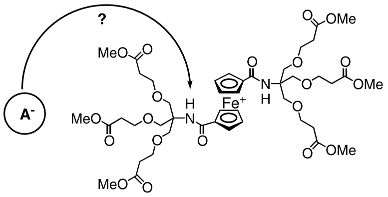


Diane L. Stone, David K. Smith

Polyhedron 22 (2003) 763

Anion binding at the core of branched ferrocene derivatives

This paper investigates the effect of dendritic functionalisation on the anion binding ability at the core of a ferrocenoyl dendrimer. It is argued that the dendritic shielding hinders the ability of these receptors to bind and sense the target halide anions.

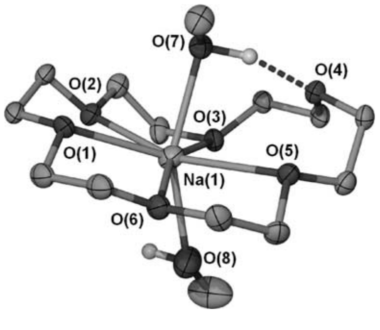


Jonathan W. Steed, Karin Johnson, Christina Legido, Peter C. Junk

Polyhedron 22 (2003) 769

Influence of hydrogen bonding on 'soft' coordination geometries: further examples

The effects of hydrogen bonding interactions on the conformations of metal crown ether compounds are examined as part of a wide study on the subject. An interesting example of an intermolecular *pseudo*-agostic interaction to Ag^+ is also reported.

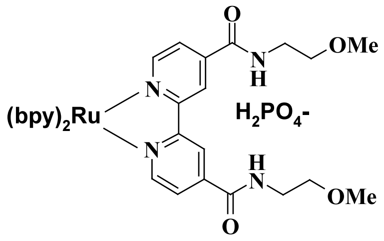


Thomas Duff, André Grüßing, Jean-Luc Thomas, Marco Duati, Johannes G. Vos

Polyhedron 22 (2003) 775

Luminescent anion recognition: probing the interaction between dihydrogenphosphate anions and Ru(II) polypyridyl complexes in organic and aqueous media

An emission study of the interaction between dihydrogen phosphate and a series of ruthenium polypyridyl complexes containing the anion receptor 4,4′-bis[(2-methoxyethyl)carbamoyl]-2,2′-bipyridine is reported. An increase of the emission intensity and lifetime are observed in the range 0–2.5 molar equivalents of $H_2PO_4^-$. The effect of the addition of trace amounts of water is also examined.

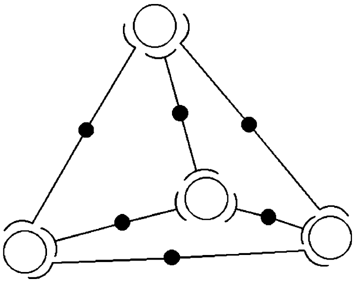


Rowena L. Paul, Zöe R. Bell,
John C. Jeffery, Lindsay P. Harding,
Jon A. McCleverty, Michael D. Ward

Polyhedron 22 (2003) 781

Complexes of a bis-bidentate ligand with d^{10} ions: a mononuclear complex with Ag(I), and a tetrahedral cage complex with Zn(II) which encapsulates a fluoroborate anion

A bridging ligand in which two bidendate pyrazolyl–pyridine units are separated by a 2,3-naphthyl spacer has been used to prepare complexes with the d^{10} ions Ag(I) and Zn(II). Whereas $[Ag(L^2)][ClO_4]$ is mononuclear with two short and two long Ag–N bonds in a near-planar arrangement, $[Zn_4(L^2)_6(BF_4)][BF_4]_7$ has a tetrahedral cage structure (shown) in which bridging ligand spans each edge of the Zn_4^{II} tetrahedron and a $[BF_4]^-$ anion is bound in the central cavity. This encapsulated anion dose not exchange with the external anions on the NMR timescale.

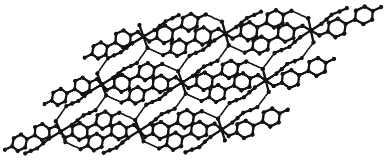


Aneta Nedelcu, Zdirad Žak,
Augustin M. Madalan, Jiri Pinkas,
Marius Andruh

Polyhedron 22 (2003) 789

Supramolecular solid-state architectures constructed from 4,4′-bipyridine-N,N′-dioxide and dicyanamido tectons. Synthesis and crystal structures of $[M(bpno)_2\{N(CN)_2\}_2(H_2O)_2]$ (M = Co, Mn) and $[Cu(bpno)\{N(CN)_2\}_2(H_2O)]$

The convolution of coordinative, hydrogen bonding and π–π stacking interactions leads to new solid-state architectures, which have been constructed by using 4,4′-bipyridine-N,N′-dioxide and the dicyanamido ion as tectons.



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Paul D. Beer, Andrew R. Cowley,
John C. Jeffery, Rowena L. Paul,
Wallace W.H. Wong

Polyhedron 22 (2003) 795

Self-assembled xanthate-transition metal polyether macrocycles and cryptands

The synthesis of novel dinuclear nickel(II)–xanthate polyether macrocycles and dinuclear cobalt(III)–xanthate polyether cryptands is reported. The assemblies have been characterised by a range of spectroscopic techniques and in one case by X-ray crystal structure determination. The ability of these compounds to bind various cations was also examined.