

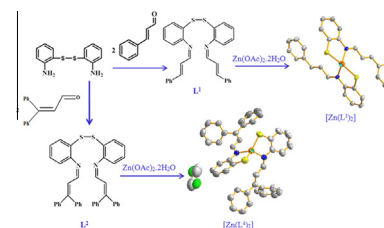
Contents

Mehdi Amirnasr, Maryam Bagheri, Hossein Farrokhpour, Kurt Joß Schenk, Kurt Mereiter and Peter C. Ford

Polyhedron 71 (2014) 1

New Zn(II) complexes with N₂S₂ Schiff base ligands. Experimental and theoretical studies of the role of Zn(II) in disulfide thiolate-exchange

Two potentially tetradentate N₂S₂ Schiff-base ligands **L**¹ and **L**² undergo reductive disulfide bond scission in alcoholic solution in the presence of zinc acetate during the course of Zn(NS)₂ complex formation. The X-ray crystal structures of [Zn(L³)₂] and [Zn(L⁴)₂], and theoretical calculations of the transition state of S–S cleavage are reported.

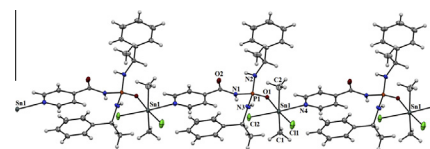


Khodayar Gholivand, Foroogh Molaei, Maryam Rajabi, Mehdi D. Esrafil and Mahdieh Hosseini

Polyhedron 71 (2014) 8

Synthesis, structural characterization and DFT calculations of a new one-dimensional diorganotin(IV) derivative of *N*-isonicotinyl phosphoramidate

A new 1D diorganotin coordination polymer, {SnCl₂(CH₃)₂L}_{*n*} (**1**), **L** = *N*-isonicotinyl, *N,N'*-bis(α-methylbenzyl) phosphoric triamide, was synthesized and characterized. DFT calculations were performed to compare the stability of the complex which showed *trans*–*cis* configuration with its *all-trans* isomer in the gas phase. AIM analysis confirmed the dominant electrostatic nature of Sn–ligand interaction.

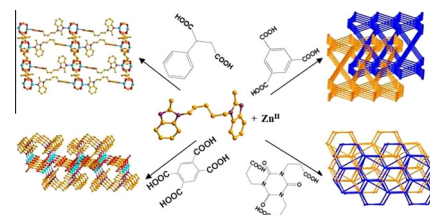


Ang-Ran Li, Qian-Qian Guo, Li Li, Hong-Wei Hou and Yao-Ting Fan

Polyhedron 71 (2014) 17

Synthesis, characterization and properties of four dimeric Zn^{II}–BMP coordination polymers modulated by a series of aromatic polycarboxylate acid

To systematically explore the influence of aromatic polycarboxylate ligands on building Zn^{II}–bmp (1,5-bis(2-methylbenzimidazol) pentane) coordination polymers, four coordination polymers with various dimeric centers have been hydrothermally synthesized.

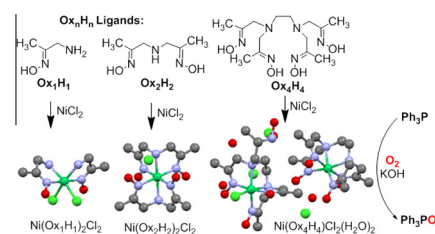


**Yaroslav D. Boyko,
Alexey Yu. Sukhorukov,
Artem N. Semakin, Yulia V. Nelyubina,
Ivan V. Ananyev, K.S. Rangappa and
Sema L. Ioffe**

Polyhedron 71 (2014) 24

Synthesis, structure and dioxygen reactivity of Ni(II) complexes with mono-, bis-, tetra- and hexa-oxime ligands

Four new Ni(II) complexes with β -oximoalkylamines containing one (Ox_1H_1), two (Ox_2H_2), four (Ox_4H_4) and six (Ox_6H_6) oxime groups were synthesized and characterized. Oxidation of Ph_3P with molecular oxygen in presence of these complexes was studied. Bis-oxime complex $Ni(Ox_2H_2)_2Cl_2$ was found to be the most active oxidation promoter among the obtained nickel complexes.

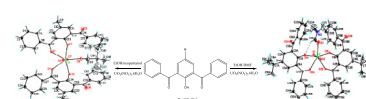


**Sushil K. Gupta, Neha Sen and
Ray J. Butcher**

Polyhedron 71 (2014) 34

Synthesis, X-ray structure, electrochemical behaviour and fluorescence studies of mononuclear dioxouranium complexes with oxygen donor ligands

The reaction of monomeric bidentate ligands [(2,6- $PhCO$)₂(4- R)C₆H₂OH] ($R = Me$ or $t-Bu$) with $[UO_2(NO_3)_2 \cdot 6H_2O]$ gave uranyl complexes with distorted pentagonal bipyramidal geometry at the metal centre. The $U-O_{eq}$ bond lengths increase in the order: phenolic < solvent < carbonyl oxygen. The bidentate OO -donor $mdbpH/bdbpH$ ligands are thus good chelators for the UO_2^{2+} ion. The reduction potential of **2** with a *tert*-butyl substituent on the phenolate ring was shifted to a more negative potential than that of **1** with a methyl substituent, reflecting the stronger electron donating ability of the *tert*-butyl group. The coordinated neopentanol in **1** is readily displaced by DMSO solution. Both complexes exhibit characteristic charge transfer emissions.

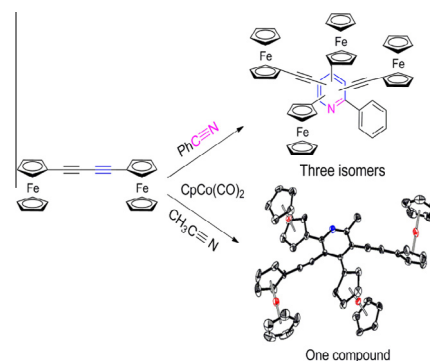


**Ya-Qi Wang, Li-Min Han, Quan-Ling Suo,
Ning Zhu and Fa-Wang Li**

Polyhedron 71 (2014) 42

Synthesis and structural characterization of new multi-ferrocenyl pyridine derivatives

Four new multi-ferrocenyl pyridine derivatives were synthesized via [2 + 2 + 2] cycloaddition reaction using $Fc-C\equiv C-C\equiv C-Fc$ and $CH_3C\equiv N$ or $PhC\equiv N$ as reactants, $CpCo(CO)_2$ as catalyst.



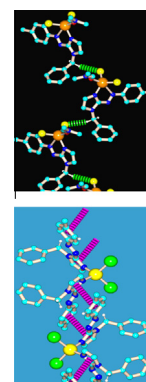
**Paramita Datta, Debashis Mallick,
Tapan Kumar Mondal and
Chittaranjan Sinha**

Polyhedron 71 (2014) 47

Structure and photochromism of zinc(II) complexes with 1-alkyl-2-(aryloxy)imidazole, and the effect of number of coordinated ligands and halide type on the photochromism

$[Zn(RaaiR')(DMF)_2X_2]$ and $[Zn(RaaiR')_2X_2]$ ($RaaiR' = 1$ -alkyl-2-(aryloxy)imidazole and $X = Cl, Br, I$) are structurally characterized and the UV light irradiation in DMF solution of the complexes show *trans*-to-*cis* isomerisation of co-

ordinated azoimidazole. Quantum yields ($\phi_{t \rightarrow c}$) of free ligand are higher than their complexes. The *cis*-to-*trans* transformation is a thermal process and the activation energy (E_a) of the complexes is lower than free ligands. The rate of isomerisation follows $[Zn(RaaiR')_2X_2] < [Zn(RaaiR')(DMF)_2X_2]$ and $[Zn(RaaiR')_nCl_2] < [Zn(RaaiR')_nBr_2] < [Zn(RaaiR')_nI_2]$ ($n = 1$ or 2). It may be related to rotor volume and mass; size and electronegativity of halide which increases the effective molar association in the order of $I < Br < Cl$. DFT and TD-DFT computations of representative complexes are used to explain the difference in the rates and quantum yields of photoisomerisation.



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