

## Contents

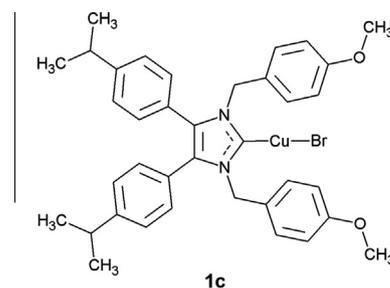
Preface..... 1

**Wojciech Streciwilk, Frauke Hackenberg, Helge Müller-Bunz and Matthias Tacke**

*Polyhedron 80 (2014) 3*

Synthesis and cytotoxicity studies of *p*-benzyl substituted NHC–copper(I) bromide derivatives

Ten novel *N*-heterocyclic carbene–copper(I) bromide derivatives were synthesised, chemically characterised and biologically evaluated against two human cancer cell lines, where the best compound showed nanomolar activity.



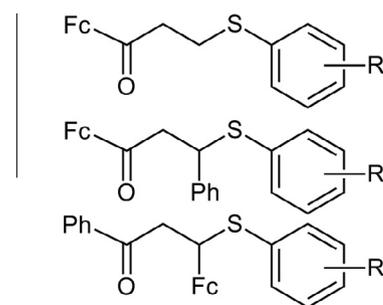
**IC<sub>50</sub> MCF-7: 0.60 (+/- 0.09) 10<sup>-6</sup> M**  
**IC<sub>50</sub> Caki-1: 0.65 (+/- 0.08) 10<sup>-6</sup> M**

**Dragana Stevanović, Goran A. Bogdanović and Rastko D. Vukićević**

*Polyhedron 80 (2014) 10*

New ferrocene containing 3-(arylthio)propan-1-ones: Synthesis, spectral characterization and crystal structure of 3-[(4-chlorophenyl)thio]-1-ferrocenylpropan-1-one, 3-[(4-chlorophenyl)thio]-1-ferrocenyl-3-phenylpropan-1-one and 3-[(4-chlorophenyl)thio]-3-ferrocenyl-1-phenylpropan-1-one

Three series of ferrocene containing 3-(arylthio)propan-1-ones (24 in total, 16 being new ones) have been synthesized by thia-Michael addition of 8 thiophenols to the corresponding enones promoted by the catalyst generated from a sacrificial zirconium anode. The single crystal X-ray structure analysis was performed for three of the synthesized compounds.



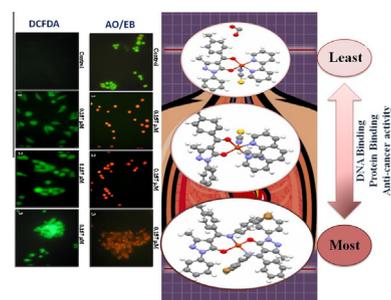
Fc = ferrocenyl, R= H, CH<sub>3</sub>, C(CH<sub>3</sub>)<sub>3</sub>, Cl

**Komal M. Vyas, R.N. Jadeja, Dipak Patel, R.V. Devkar and Vivek K. Gupta**

*Polyhedron 80 (2014) 20*

Effect of ligand substitution in pyrazolone based binary and ternary Cu(II) complexes on DNA binding, protein binding and anti-cancer activity on A549 lung carcinoma cell lines

A new set of pyrazolone based Cu(II) complexes has been reported with single crystal structures. DNA/protein binding and anti-cancer activity against A549 lung cancer cells suggested strong influence of ligand substitution on pharmacological activities.

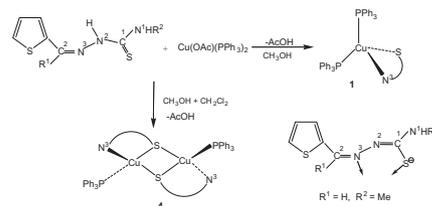


**Tarlok S. Lobana, Shikha Indoria,  
Manvi Sharma, Jyoti Nandi,  
Amanpreet K. Jassal, Maninder S. Hundal  
and Alfonso Castineiras**

*Polyhedron* 80 (2014) 34

Synthesis, structure and spectroscopy of mono- and di-nuclear copper(I) complexes incorporating anionic thiophene based thiosemicarbazones—first examples

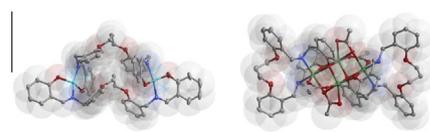
Six new copper(I) complexes with thiophene based anionic thiosemicarbazones are reported: three mononuclear (**1–3**) with N<sup>3</sup>,S-chelation and three dinuclear (**4–6**) with N<sup>3</sup>,S-chelation-S-bridging. It was found that for R<sup>1</sup> = H and R<sup>2</sup> = Me, the thio-ligand HttscN–Me yielded a mononuclear complex **1** in methanol solvent and a dinuclear complex **4** in methanol–dichloromethane mixture. For R<sup>1</sup> = Me, there is preference for the formation of dinuclear complexes (**5, 6**).



**Seyed A. Hosseini-Yazdi,  
Parvin Samadzadeh-Aghdam,  
Azadeh Mirzaahmadi, Ali Akbar Khandar,  
Chodrat Mahmoudi, Michael Ruck,  
Thomas Doert, Salet S. Balula and  
Luís Cunha-Silva**

*Polyhedron* 80 (2014) 41

Synthesis, crystal structures, spectroscopic and electrochemical studies on Cu(II) and Ni(II) complexes with compartmental nitrogen–oxygen mixed donor ligands

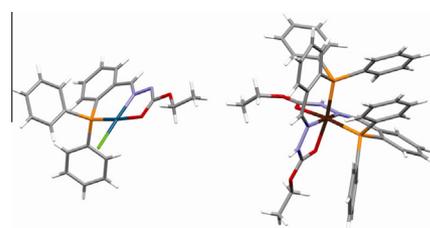


**Milica Milenković, Giulia Cantoni,  
Alessia Bacchi, Vojislav Spasojević,  
Marina Milenković, Dušan Sladić,  
Natalija Krstić and Katarina Andelković**

*Polyhedron* 80 (2014) 47

Synthesis, characterization and antimicrobial activity of Pd(II) and Fe(III) complexes with ethyl (2*E*)-2-[2-(diphenylphosphino)benzylidene]hydrazinecarboxylate

Complexes of Pd(II) and Fe(III) with the condensation derivative of 2-(diphenylphosphino)benzaldehyde and ethyl carbamate were synthesized, characterized, and their antimicrobial activity was evaluated.

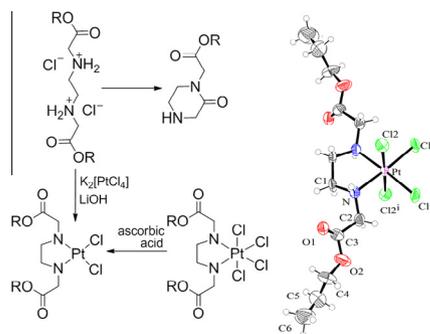


**Goran N. Kaluderović, Nebojša Pantelić,  
Thomas Eichhorn, Martin Bette,  
Christoph Wagner, Bojana B. Zmejkovski  
and Harry Schmidt**

*Polyhedron* 80 (2014) 53

Platinum(II) complexes with R<sub>2</sub>edda ligands (R = Me, Et, *n*-Pr; edda = ethylenediamine-*N,N'*-diacetate): Synthesis and characterization

Three novel [PtCl<sub>2</sub>(R<sub>2</sub>edda)] complexes (R = Me, Et, *n*-Pr; edda = ethylenediamine-*N,N'*-diacetate; **1–3**) are synthesized and characterized. Hydrolytic stability of ligand precursors, crystal structure of [PtCl<sub>4</sub>((*n*-Pr)<sub>2</sub>edda)] and reduction of *rac*-[PtCl<sub>4</sub>(Et<sub>2</sub>edda)] are presented. The *in vitro* cytotoxic activity of complexes **1–3** was studied on 11 tumor cell lines.

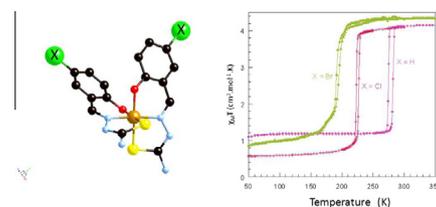


**Sébastien Floquet, Eric Rivière,  
Kamel Boukheddaden, Denis Morineau  
and Marie-Laure Boillot**

*Polyhedron* 80 (2014) 60

Neutral ferric complexes of salicylaldehyde thiosemicarbazone ligands: An exceptional family of complexes exhibiting discontinuous spin transition behavior

Three neutral thiosemicarbazone ferric complexes  $[\text{Fe}(\text{H5XThsa})(\text{5XThsa})]\cdot\text{H}_2\text{O}$  ( $\text{X} = \text{H}, \text{Cl}, \text{Br}$ ) are studied by magnetic susceptibility, DSC and Mössbauer measurements. The three compounds display abrupt spin transition with thermal hysteresis, which highlights the fascinating magnetic behavior of this class of ferric complexes.

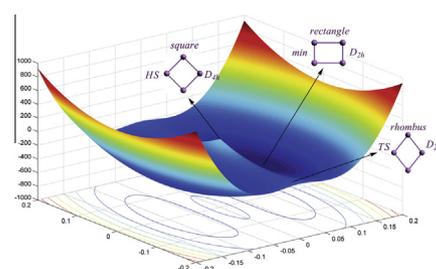


**Marko Perić, Ljubica Andjelković,  
Matija Zlatar, Claude Daul and  
Maja Gruden-Pavlović**

*Polyhedron* 80 (2014) 69

DFT investigation of the influence of Jahn–Teller distortion on the aromaticity in square-planar arsenic and antimony clusters

We report detailed analysis and explanation of antiaromaticity in  $\text{As}_4^{2-}$  and  $\text{Sb}_4^{2-}$  rectangular metalloid clusters. In addition, the influence of Jahn–Teller distortion on aromatic behavior in  $\text{As}_4^-$  and  $\text{Sb}_4^-$  was explored. NICS values were scanned along the Intrinsic Distortion Path (IDP).

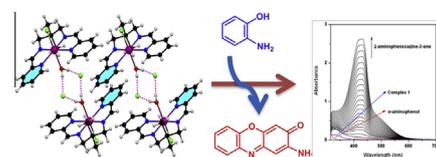


**Anangamohan Panja**

*Polyhedron* 80 (2014) 81

Syntheses and structural characterizations of cobalt(II) complexes with  $\text{N}_4$ -donor Schiff base ligands: Influence of methyl substitution on structural parameters and on phenoxazinone synthase activity

Syntheses and crystal structures of mononuclear cobalt(II) complexes with  $\text{N}_4$ -donor Schiff base ligands are reported. All the complexes are moderately reactive towards the oxidative coupling of *o*-aminophenol in aerobic condition similar to the function of phenoxazinone synthase. Effect of methyl substitution in pyridyl ring on the geometrical parameter and on the phenoxazinone synthase mimicking activity is noticed.

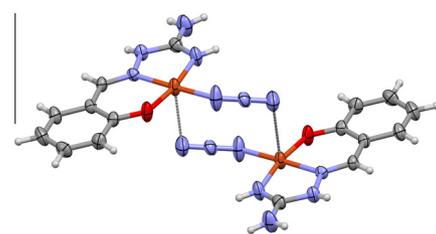


**Ljiljana S. Vojinović-Ješić,  
Mirjana M. Radanović, Marko V. Rodić,  
Ljiljana S. Jovanović, Valerija I. Češljević  
and Milan D. Joksović**

*Polyhedron* 80 (2014) 90

Syntheses, structures and spectral characterization of copper(II) and dioxidovanadium(V) complexes with salicylidene-aminoguanidine

Syntheses and characterization of the complexes  $[\text{Cu}(\text{SalAG-H})\text{NCS}]$ ,  $[\text{Cu}_2(\text{SalAG-H})_2(\text{N}_3)_2]$  and  $[\text{VO}_2(\text{SalAG-H})]$  with salicylidene-aminoguanidine (SalAG) are presented. Monoanionic SalAG-H is coordinated as a tridentate ONN ligand. Electrochemical characterization showed that the copper(II) complexes in DMF are present in two complex forms which may be reduced in separate electrode processes.

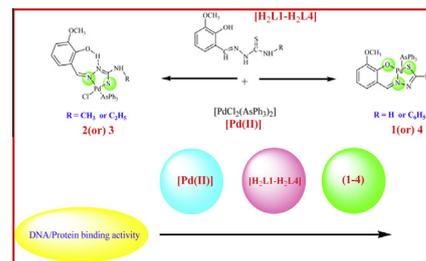


**P. Kalaivani, C. Umadevi, R. Prabhakaran, F. Dallemer, P.S. Mohan and K. Natarajan**

*Polyhedron* 80 (2014) 97

New palladium(II) complexes of 3-methoxysalicylaldehyde-4(*N*)-substituted thiosemicarbazones: Synthesis, spectroscopy, X-ray crystallography and DNA/protein binding study

A series of new palladium complexes containing 4(*N*)-substituted 3-methoxysalicylaldehyde thiosemicarbazone were prepared and structurally characterized. The new complexes were subjected to test their DNA/Protein binding studies.

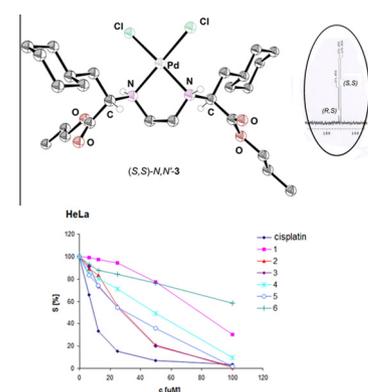


**Bojana B. Zmejovski, Aleksandar Savić, Jelena Poljarević, Nebojša Pantelić, Sandra Arandelović, Siniša Radulović, Sanja Grgurić-Šipka, Goran N. Kaluderović and Tibor J. Sabo**

*Polyhedron* 80 (2014) 106

Synthesis, characterization and *in vitro* antitumor activity of new palladium(II) complexes with (*S,S*)-*R*<sub>2</sub>edda-type esters

Six new palladium(II) complexes: [PdCl<sub>2</sub>{(*S,S*)-*R*<sub>2</sub>eddh}], R = Me, Et, *n*-Pr, **1–3**; [PdCl<sub>2</sub>{(*S,S*)-*R*<sub>2</sub>pddch}], R = Et, *n*-Pr, **4, 5**; [PdCl<sub>2</sub>{(*S,S*)-*R*<sub>2</sub>eddip}], R = *i*-Am, **6**; were synthesized and characterized. Two diastereoisomers were observed in NMR spectra of **1–4** and **6**, but only one for **5**. DFT calculations are in agreement with NMR findings. Cytotoxicity of **1–6** was studied on 3 cell lines.

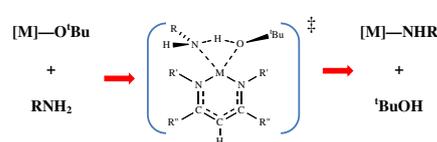


**Cody R. Freitag, Francisco J. Birk, William C. Ou and Thomas R. Cundari**

*Polyhedron* 80 (2014) 112

Modeling of late 3d transition metal metathesis of *tert*-butoxide complexes with amines

A DFT study of the alkoxide/amide metathesis reaction for late 3d transition metal  $\beta$ -diketiminato (nacnac) *tert*-butoxide and amide (N(H)R) complexes was performed: [M]-O<sup>t</sup>Bu + RNH<sub>2</sub> → [M]-NHR + <sup>t</sup>BuOH (M = Co, Ni, Cu, Zn; R = H, Ph, Ad (Ad = 1-adamantyl), [M] = nacnac complex).

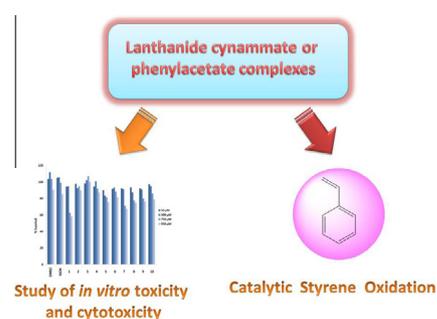


**Alberto Aragón-Muriel, María Camprubí-Robles, Elena González-Rey, Alfonso Salinas-Castillo, Antonio Rodríguez-Diéguez, Santiago Gómez-Ruiz and Dorian Polo-Cerón**

*Polyhedron* 80 (2014) 117

Dual investigation of lanthanide complexes with cinnamate and phenylacetate ligands: Study of the cytotoxic properties and the catalytic oxidation of styrene

Eleven lanthanide compounds with phenylacetate or cinnamate ligands have been synthesized and structurally characterized. The toxicity of these complexes towards macrophages and erythrocytes, as well as the cytotoxicity against human cancer cell lines has been reported. In addition, the catalytic properties of these compounds in the oxidation of styrene have also been studied.

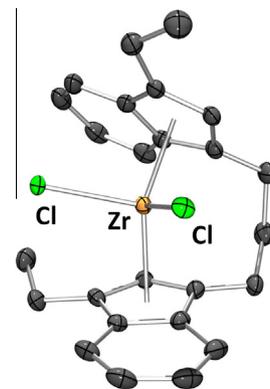


**Dorian Polo-Cerón,  
Santiago Gómez-Ruiz,  
Jesús Ceballos-Torres, Sanjiv Prashar,  
Mariano Fajardo and Manuel L. Reyes**

*Polyhedron* 80 (2014) 129

Synthesis and structural characterization of novel three carbon atom bridged *ansa*-bis(indenyl)zirconocene complexes: Applications in ethylene polymerization

The synthesis and characterization of *ansa*-indenyl zirconocene complexes containing a three carbon atom bridge is described. In addition, their molecular structures have been determined by single crystal X-ray diffraction studies. The catalytic activity of the zirconocene derivatives in the polymerization of ethylene is reported.

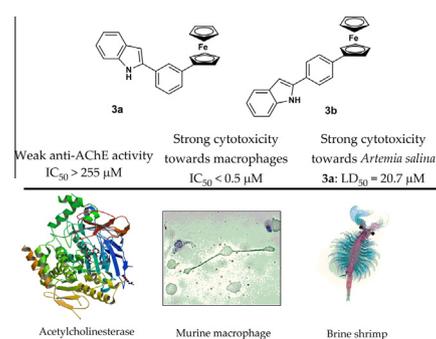


**Niko S. Radulović, Dragan B. Zlatković,  
Katarina V. Mitić, Pavle J. Randjelović  
and Nikola M. Stojanović**

*Polyhedron* 80 (2014) 134

Synthesis, spectral characterization, cytotoxicity and enzyme-inhibiting activity of new ferrocene-indole hybrids

Two new ferrocene-indole hybrids were designed, synthesized and characterized by extensive 2D NMR studies. Although the compounds exerted weak inhibition of acetylcholinesterase, they demonstrated significant cytotoxic activities against *Artemia salina* (24 h LD<sub>50</sub> 20.7 and 120.4 μM) and rat macrophages (IC<sub>50</sub> ca. 0.5 μM for both compounds).

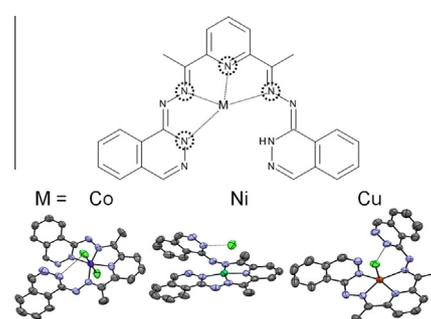


**Berta Holló, József Magyarai,  
Vukosava Živković-Radovanović,  
Gordana Vučković, Zoran D. Tomić,  
Imre Miklós Szilágyi, György Pokol and  
Katalin Mészáros Szécsényi**

*Polyhedron* 80 (2014) 142

Synthesis, characterisation and antimicrobial activity of bis(phthalazine-1-hydrazone)-2,6-diacetylpyridine and its complexes with Co<sup>III</sup>, Ni<sup>II</sup>, Cu<sup>II</sup> and Zn<sup>II</sup>

Complex compounds of Ni<sup>II</sup>, Co<sup>III</sup>, Cu<sup>II</sup> with bis(phthalazine-1-hydrazone)-2,6-diacetylpyridine (Hz<sub>2</sub>DAP) ligand were synthesised. The coordination sphere of the metals is different in spite of the same synthetic procedure and same degree of protonation of the ligand, Hz<sub>2</sub>DAP-H. With Zn<sup>II</sup> a neutral complex [Zn(Hz<sub>2</sub>DAP-2H)]·H<sub>2</sub>O is obtained with double deprotonated ligand molecule.

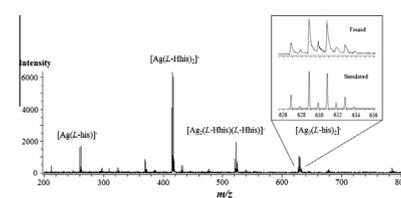


**Akihiko Takayama, Yoshitaka Takagi,  
Kousuke Yanagita, Chisato Inoue,  
Rie Yoshikawa,  
Noriko Chikaraishi Kasuga and  
Kenji Nomiya**

*Polyhedron* 80 (2014) 151

Synthesis, characterization and antimicrobial activities of sodium salt of *L*-histidinatoargentate(I) derived from the pH 11 solution

Novel anionic silver(I) complex with solely coordinated by dianion of histidine, a sodium salt of *L*-histidinatoargentate(I) (**L-4**), was prepared by a reaction of Ag<sub>2</sub>O with *L*-histidine (*L*-H<sub>2</sub>his) in water at pH 11. ESI-MS and elemental analysis showed that the composition and formula of **L-4** was ∞{Na[Ag<sub>3</sub>(*L*-his)<sub>2</sub>]*n*H<sub>2</sub>O} (*n* = 1–5). Complex **L-4** inhibited growth of four bacteria, two yeasts and a mold.

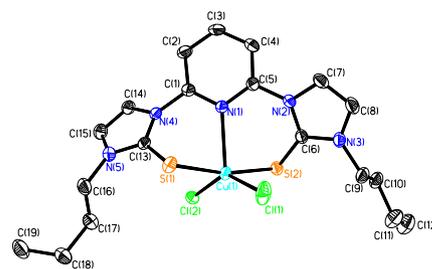


**John R. Miecznikowski, Matthew A. Lynn, Jerry P. Jasinski, Wayne Lo, Daniel W. Bak, Mekhala Pati, Elizabeth E. Butrick, Anne Elise R. Drozdowski, Kerry A. Archer, Christine E. Villa, Elise G. Lemons, Erin Powers, Margaret Siu, Camile D. Gomes, Nicholas A. Bernier and Kaitlyn N. Morio**

*Polyhedron 80 (2014) 157*

Syntheses and characterization of five-coordinate copper(II) complexes based on tridentate SNS pincer ligand precursors

A series of tridentate pincer ligands, each possessing two sulfur- and one nitrogen-donor functionalities (SNS), based on a bis-imidazolyl precursor were metallated with  $\text{CuCl}_2$  to give new tridentate SNS pincer copper(II) complexes  $[(\text{SNS})\text{CuCl}_2]$ , which were purple in color. The  $[(\text{SNS})\text{CuCl}_2]$  complexes were characterized with single crystal X-ray diffraction, electro-spray mass spectrometry, EPR spectroscopy, attenuated total reflectance infrared spectroscopy, UV-Vis spectroscopy, cyclic voltammetry, and elemental analysis. We performed computational studies to learn which oxidation state of copper ion is best situated to bind to our tridentate SNS ligand precursors.

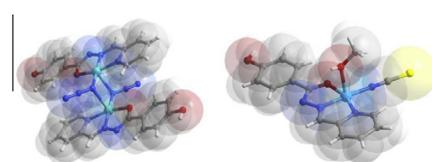


**Behrouz Shaabani, Ali Akbar Khandar, Haedeh Mobaiyen, Nahid Ramazani, Salet S. Balula and Luís Cunha-Silva**

*Polyhedron 80 (2014) 166*

Novel pseudohalide-bridged Cu(II) complexes with a hydrazone ligand: Evaluation of antimicrobial activity

Two unprecedented Cu(II) complexes with a hydrazone based ligand have been prepared, characterized and their antimicrobial activity was also evaluated.

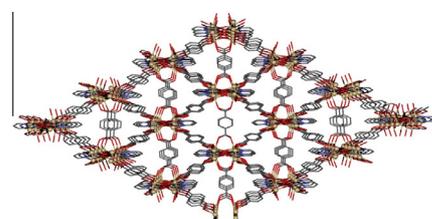


**Enrique Colacio and Antonio Rodríguez-Diéguez**

*Polyhedron 80 (2014) 173*

Possibilities with 2-pyrimidinecarbonitrile to design MOFs

Ten years ago, our research group synthesized for the first time the 2-pyrimidine-carboxylate anionic ligand by hydrothermal routes. In these years, a lot of researches have used this ligand to construct MOFs with interesting properties. We show the great variety of structures that can be synthesized with this ligand and cadmium chloride by solvothermal routes.

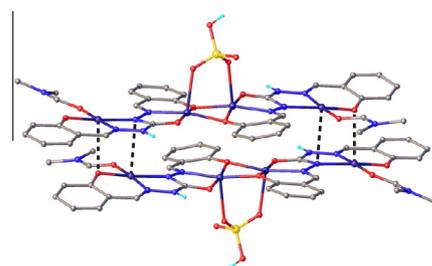


**Diana Dragancea, Sergiu Shova, Éva A. Enyedy, Martin Breza, Peter Rapta, Luca M. Carrella, Eva Rentschler, Anatolie Dobrov and Vladimir B. Arion**

*Polyhedron 80 (2014) 180*

Copper(II) complexes with 1,5-bis(2-hydroxybenzaldehyde)carbohydrazone

The acid-base properties of 1,5-bis(2-hydroxybenzaldehyde)carbohydrazone and its thioanalogue have been studied experimentally and by DFT methods. Five copper(II) complexes with 1,5-bis(2-hydroxybenzaldehyde)carbohydrazone have been synthesised and characterised by X-ray crystallography. The ditopic ligand possesses two binding sites able to accommodate transition metal ions. Magnetic measurements showed antiferromagnetic interactions between copper(II) centres.

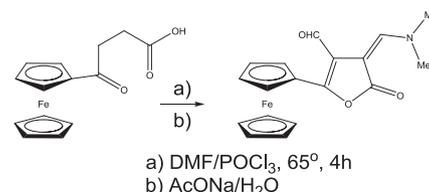


**Zoran Ratković, Jovana Muškinja, Sladjana B. Novaković, Goran A. Bogdanović, Karoly Micskei and Rastko D. Vukićević**

*Polyhedron* 80 (2014) 193

4-[(Dimethylamino)methylene]-2-ferrocenyl-5-oxo-4,5-dihydrofuran-3-carboxaldehyde: Synthesis, spectral characterization and single crystal X-ray analysis

From 3-ferrocenylpropanoic acid and Vilsmeier reagent compound 4-[(dimethylamino)methylene]-2-ferrocenyl-5-oxo-4,5-dihydrofuran-3-carboxaldehyde was synthesized. Under the same conditions electron-rich 3-arylpropanoic acids, 3-thenylpropanoic and 3-(4-methoxybenzoyl)propanoic acid gave similar products. This result is rather unexpected, since 3-arylpropanoic acids under these conditions usually give the corresponding 2-aryl-4-chloro-3-formylfurans. Single crystal X-ray analysis was successfully performed for 4-[(dimethylamino)methylene]-2-ferrocenyl-5-oxo-4,5-dihydrofuran-3-carboxaldehyde and 4-[(dimethylamino)methylene]-2-(2-thienyl)-5-oxo-4,5-dihydrofuran-3-carboxaldehyde.



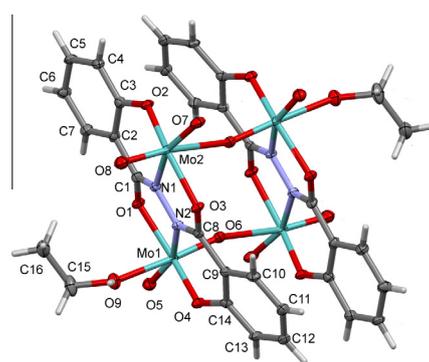
Reaction of 3-ferrocenylpropanoic acids with Vilsmeier reagent

**Sagarika Pasayat, Subhashree P. Dash, Sudarshana Majumder, Rupam Dinda, Ekkehard Sinn, Helen Stoeckli-Evans, Subhadip Mukhopadhyay, Sujit K. Bhutia and Partha Mitra**

*Polyhedron* 80 (2014) 198

Synthesis, structure, characterization and study of antiproliferative activity of dimeric and tetrameric oxidomolybdenum(VI) complexes of *N,N'*-disalicyloylhydrazine

The *in situ* reaction of salicyloylhydrazide and its corresponding hydrazone with  $[\text{MoO}_2(\text{acac})_2]$  afforded two novel and unusual dimeric  $[(\text{Mo}^{\text{VI}}\text{O}_2)_2\text{L}]$  (**1**) and tetrameric  $[\{(\text{C}_2\text{H}_5\text{OH})\text{LO}_3\text{Mo}_2^{\text{VI}}\}_2(\mu\text{-O})_2]\text{C}_2\text{H}_5\text{OH}$  (**2**) oxidomolybdenum(VI) complexes with *N,N'*-disalicyloylhydrazine ( $\text{H}_2\text{L}$ ). The complexes have been characterized by various spectroscopic techniques (IR, UV and NMR), and structural studies by X-ray crystallography. The *in vitro* antiproliferative activity of complexes **1** and **2** was assayed against HeLa cell line.

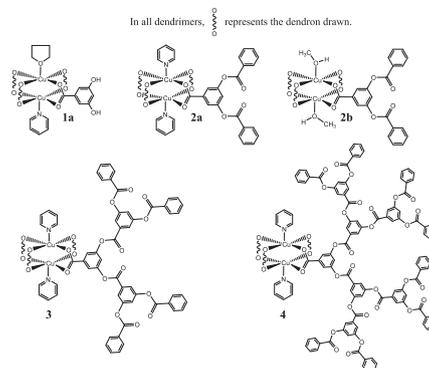


**Linsheng Feng, Zhichao Chen, Matthias Zeller and Rudy L. Luck**

*Polyhedron* 80 (2014) 206

Dicopper moieties stabilized by Fréchet-type dendrons: Syntheses and structural characterizations

Paddlewheel shaped dicopper dendrimers, **1–4**, were prepared from the reaction of copper acetate and the corresponding dendrons. Crystals of **1**, **2a** and **2b** were obtained and characterized crystallographically. A 3D network formed via H-bonds in **1** and  $\pi$ - $\pi$  interactions were evident between phenyl rings on adjacent molecules in **2b**. All compounds were characterized by FT-IR, UV-Vis spectroscopy, TGA and DSC.

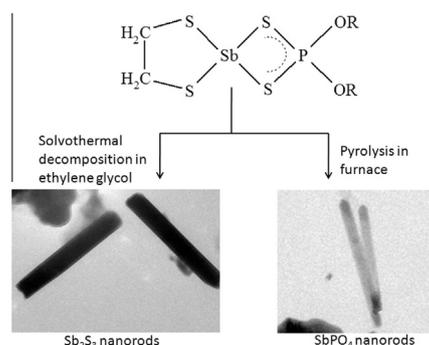


**Jasmine B. Biswal, Shivram S. Garje and Neerish Revaprasadu**

*Polyhedron* 80 (2014) 216

A convenient synthesis of antimony sulfide and antimony phosphate nanorods using single source dithiolatoantimony(III) dialkyldithiophosphate precursors

The solvothermal decomposition of ethane-1,2-dithiolatoantimony dialkyldithiophosphates complexes in ethylene glycol afforded  $\text{Sb}_2\text{S}_3$  nanorods whereas their pyrolysis in a furnace resulted into the formation of  $\text{SbPO}_4$  nanorods.

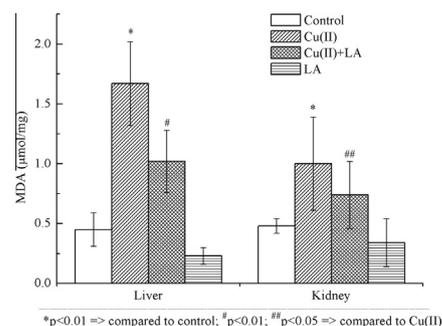


**Ružica S. Nikolić, Nenad S. Krstić,  
Goran M. Nikolić, Gordana M. Kocić,  
Milorad D. Cakić and  
Darko H. Andelković**

*Polyhedron 80 (2014) 223*

Molecular mechanisms of beneficial effects of lipoic acid in copper intoxicated rats assessment by FTIR and ESI-MS

Lipoic acid was shown to largely decrease the production of malondialdehyde in copper intoxicated rats. FTIR spectroscopy and ESI-MS were used to clarify the mechanisms of this beneficial effect by investigating Cu(II) ion-lipoic acid interactions in model systems.

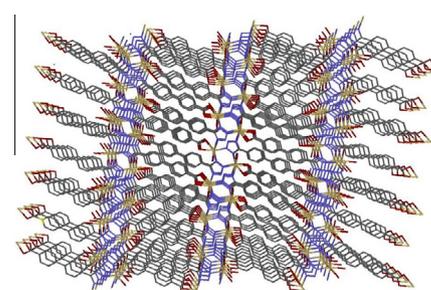


**Antonio J. Calahorra,  
Guillermo Zaragoza,  
Alfonso Salinas-Castillo, José M. Seco  
and Antonio Rodríguez-Diéguez**

*Polyhedron 80 (2014) 228*

Unique Metal–Organic-Framework with based on 4'-tetrazolate-4-biphenyl carboxylate spacer: Blue-green photoluminescence

The first Metal–Organic-Frameworks with the novel 4'-tetrazolate-4-biphenyl carboxylate spacer is presented. We report the formation *in situ* of cadmium MOF by hydrothermal routes. The compound is a three-dimensional structure with small channels that shows an intense blue-green photoluminescence emission at room temperature in the solid state.



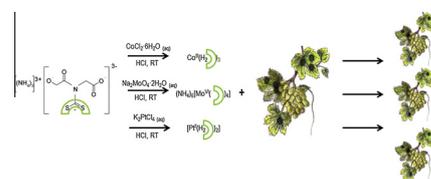
**Zorica Leka, Danijela Vojta,  
Milica Kosović, Nedeljko Latinović,  
Marijana Daković and  
Aleksandar Višnjjevac**

*Polyhedron 80 (2014) 233*

Syntheses, structures and antifungal activities of novel Co, Mo and Pt complexes with triammonium *N,N*-diacetatodithiocarbamate

Complexes of Co(II), Co(III), Mo(VI) and Pt(II) with our, previously reported, biologically active ligand, triammonium *N,N*-diacetatodithiocarbamate, (NH<sub>4</sub>)<sub>3</sub>dadtc were prepared with the aim of enhancing the antifungal activity of the free ligand. Anionic Co(II)

complex [Co<sub>2</sub>(H<sub>2</sub>dadtc)<sub>5</sub>]<sup>−</sup> (**2**), undergoes spontaneous oxidation of Co(II) to Co(III), followed by an overall chemical rearrangement, resulting with formation of molecular complex **3**. In the [Mo<sup>VI</sup>(dadtc)<sub>4</sub>]<sup>6−</sup> anion of the complex **4**, the Mo(VI) centre is located at the fourfold rotoinversion axis and coordinated by eight approximately equidistant sulfur atoms from four bidentate dithiocarbamate ligands in the centre of a slightly distorted triangular dodecahedron. Pt(II) complex **5**, [Pt(H<sub>2</sub>dadtc)<sub>2</sub>] reveals a distorted square planar coordination of the Pt(II) ion. Complexes were characterised by classical chemical methods and X-ray diffraction studies and tested for their antifungal activities. All complexes revealed encouraging levels of antifungal activity when subjected to the tests of mycelia growth inhibition of *Botryosphaeria dothidea*.

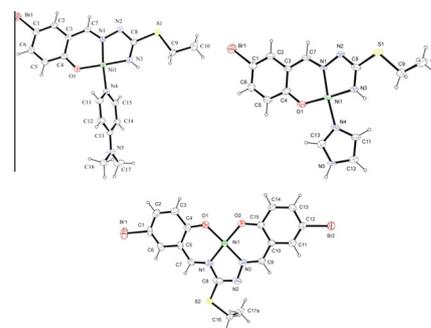


**Reza Takjoo, Roberto Centore,  
Alireza Akbari and Mehdi Ahmadi**

*Polyhedron 80 (2014) 243*

Square planar nickel(II) complexes derived from 5-bromo-2-hydroxybenzaldehyde *S*-ethylisothiosemicarbazone: Preparation, characterization and structural studies

5-Bromo-2-hydroxybenzaldehyde *S*-ethylisothiosemicarbazone (H<sub>2</sub>L) utilized as ligand. Ni(II) complexes were prepared and characterized by spectral and single crystal X-ray crystallography. These complexes reveal a have distorted square pyramidal geometries. Furthermore the electronic structures of complexes were also elucidated by DFT calculations.

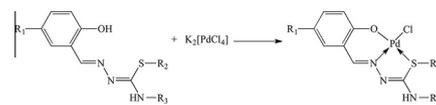


**Mihail Revenco, Petru Bulmaga,  
Elena Jora, Oleg Palamarciuc,  
Victor Kravtsov and Paulina Bourosh**

*Polyhedron* 80 (2014) 250

Specificity of salicylaldehyde S-alkylisothiosemicarbazones coordination in palladium(II) complexes

Salicylaldehyde S-alkylisothiosemicarbazones (HL) are coordinated as tridentate monodeprotonated ONS ligands in the palladium complexes of the general formula  $[Pd(L)Cl]$ .

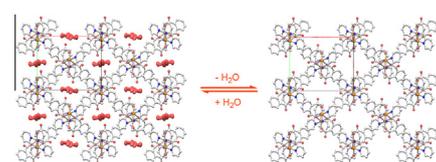


**Jelena Zdravković, Dejan Poleti,  
Jelena Rogan and Dragica M. Minić**

*Polyhedron* 80 (2014) 256

Bis(2,2'-bipyridine)-bis( $\mu_3$ -phthalato)-dicopper(II) tetrahydrate as molecular sieve with zero-dimensional structure

Copper(II) complex with 2,2'-bipyridine (bipy) and dianion of phthalic acid (pht) consists of binuclear  $[Cu_2(bipy)_2(pht)_2]$  units with water molecules located in channels parallel to the  $[0 0 1]$  direction. This flexible MOF shows a complete reversibility of dehydration and rehydration.  $[Cu_2(bipy)_2(pht)_2] \cdot 4H_2O$  is the first reported 0D molecular sieve retaining the structure upon dehydration–rehydration cycles.

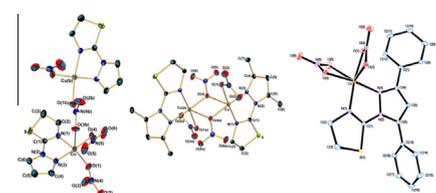


**R. Pedrero-Marín, A.V. Sánchez-Huertas,  
F. Luna-Giles, F. De la Cruz-Martínez and  
E. Viñuelas-Zahínos**

*Polyhedron* 80 (2014) 265

Substituent's size in pyrazole derivative ligands as determining factor on nuclearity in Cu(II) complexes

Three copper(II) nitrate complexes with pyrazole/thiazoline derivative ligands with different steric features have been prepared and structurally characterized. The role played by ligands substituents size on nuclearity of complexes has been analyzed.

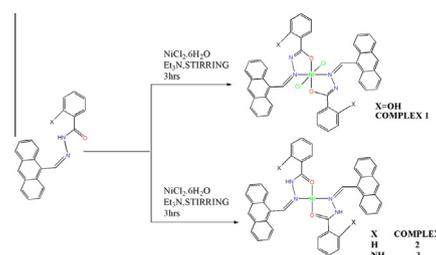


**Satyajit Mondal, Chandrima Das,  
Bipinbhari Ghosh, Bholanath Pakhira,  
Alexander J. Blake, Mike G.B. Drew and  
Shyamal Kumar Chattopadhyay**

*Polyhedron* 80 (2014) 272

Synthesis, spectroscopic studies, X-ray crystal structures, electrochemical properties and DFT calculations of three Ni(II) complexes of aryl hydrazone ligands bearing anthracene moiety

Three new mononuclear Ni(II) complexes with N,O-donor hydrazone ligands, are reported. The molecular and supramolecular structures of the complexes are controlled by H-bonding ability of the hydrazone ligand. The fluorescence of the ligands are quenched by the  $Ni^{2+}$ .

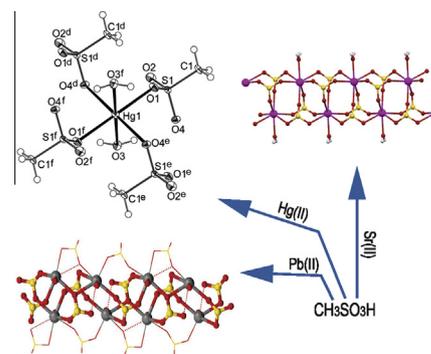


**Milena Dorđević, Dejan Jeremić,  
Goran N. Kaluderović,  
Santiago Gómez-Ruiz, Boban Andelković,  
Dušanka Radanović and Ilija Brčeski**

*Polyhedron 80 (2014) 282*

Synthesis and spectroscopic properties of large single-crystals of Pb(II), Hg(II) and Sr(II) methanesulfonato 1D coordination polymers

Three new 1D coordination polymers,  $[\text{Pb}_2(\text{CH}_3\text{SO}_3)_4(\text{H}_2\text{O})_2]_n$ ,  $[\text{Hg}(\text{CH}_3\text{SO}_3)_2(\text{H}_2\text{O})_2]_n$  and  $[\text{Sr}(\text{CH}_3\text{SO}_3)_2(\text{H}_2\text{O})]_n$ , were synthesized as large single crystals. The low price of starting materials and the facile methods used for the preparation of title compounds and their UV-Vis and broad range IR spectrums imply the studied compounds could potentially be used as optical materials.

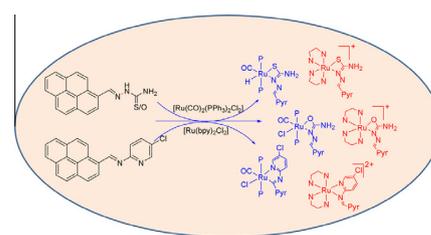


**Soumik Mandal, Varun Kundi,  
Dipravath K. Seth, K. Srikanth and  
Parna Gupta**

*Polyhedron 80 (2014) 290*

Studies on ruthenium complexes of pyrene-appended Schiff base ligands

The synthesis of six new ruthenium(II) complexes with pyrene-appended Schiff bases were done and their coordination behavior and photophysical properties were studied. Two different sets of Lewis base ligands (i) 2,2'-bipyridine and (ii) triphenyl phosphine and carbonyl together were chosen to generate two well known ruthenium(II) precursor. Schiff base ligands were reacted with these ruthenium(II) precursor to generate six ruthenium(II) complexes. The molecular structures of two of the complexes were studied by X-ray crystallography. The effect of these two different set of ligands as well as the Schiff base ligands on the fluorescence spectra of the complexes were studied in details.



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