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Volume 690, issue 19, 1 October 2005



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# Contents

# **Regular** papers

## Alexey N. Ryabov, Alexander Z. Voskoboynikov

J. Organomet. Chem. 690 (2005) 4213

Constrained geometry complexes of titanium (IV) and zirconium (IV) involving cyclopentadienyl fused to thiophene ring

Constrained geometry complexes (CGCs) of Ti(IV) and Zr(IV) containing isomeric cyclopentadienyls fused to thiophene fragment, i.e., 4,5-dimethylcyclopenta[b]thienyl and 5,6-dimethylcyclopenta[b]thienyl, have been prepared and unambiguously characterized. Preliminary studies showed that the studied CGCs/MAO are active olefin polymerization catalysts.



## Keisham Sarjit Singh, Carsten Thöne, Mohan Rao Kollipara

J. Organomet. Chem. 690 (2005) 4222

Part 1: 1,3-Dipolar addition of activated alkyne towards coordinated azido group in ruthenium(II) complexes containing  $\eta^5$ -cyclichydrocarbons

The indenyl and pentamethyl-cyclopentadienyl ruthenium(II) triazole complexes can be prepared by 3 + 2 cycloaddition reaction of activated alkyne to azido ruthenium complexes of indenyland pentamethylcyclopentadienyl systems.



## Tushar S. Basu Baul, Keisham Surjit Singh, Michal Holčapek, Robert Jirásko, Eleonora Rivarola, Anthony Linden

J. Organomet. Chem. 690 (2005) 4232

Synthesis, characterization and crystal structures of polymeric and dimeric triphenyltin(IV) complexes of  $4-[((E)-1-{2-hydroxy-5-[(E)-2-(2-carboxyphenyl)-1-diazenyl] phenyl}methylidene)amino]aryls$ 

The triphenyltin(IV) complexes of 4-[((*E*)-1-{2-hydroxy-5-[(*E*)-2-(2-carboxyphenyl)-1-diazenyl]phenyl}methylidene)amino]aryls (aryls = 4-CH<sub>3</sub> (1), 4-Br (2), 4-Cl (3) 4-OCH<sub>3</sub> (4)) have been synthesized and characterized by <sup>1</sup>H-, <sup>13</sup>C-, <sup>119</sup>Sn-NMR, ESI-mass spectrometry, IR and <sup>119m</sup>Sn Mössbauer spectroscopic techniques in combination with elemental analysis. X-ray crystallography reveals that complexe 1 and 2 adopt a polymeric form, while complex 4 is a cyclic dinuclear complex. The coordination environment in each complex is trigonal bipyramidal *trans*-Ph<sub>3</sub>SnO<sub>2</sub>. A single zwitterionic carboxylate ligand bridges adjacent Sn atoms via the carboxylate and phenoxide O atoms.



## Anupam Singh, Sanjay K. Singh, Manoj Trivedi, Daya S. Pandey

J. Organomet. Chem. 690 (2005) 4243

Synthetic, spectral and structural studies of some homo and hetero binuclear arene ruthenium (II) polypyridyl complexes Homo-hetero binuclear cationic complexes with the general formulation  $[(\eta^6\text{-arene})\text{-}RuCl(\mu\text{-}bppz)(L)]^*$   $(\eta^6\text{-}arene = benzene; L = PdCl_2, 1a; PtCl_2, 1b, and <math>\eta^6\text{-}arene = p\text{-}cymene; L = PdCl_2, 2a; PtCl_2, 2b), [(\eta^6\text{-}arene)RuCl(\mu\text{-}bppz)(L)]^{2+} (\eta^6\text{-}arene = p\text{-}cymene; L = [(\eta^6\text{-}C_6H_6)RuCl], 2c, and [(\eta^6\text{-}C_{10}H_{14})\text{-}RuCl], 2d)$  have been isolated and the complex 2d has been structurally characterized.



# Zhong-Xia Wang, Zuo-Yun Chai, Ye-Xin Li

J. Organomet. Chem. 690 (2005) 4252

Reaction of aryl azides with tris-(trimethylsilyl)silyllithium: Synthesis of tmeda or thf adducts of  $[Li{N(Ar)Si-(SiMe_3)_3}]$  and 1,4-trimethylsilyl migra- tion from oxygen to nitrogen Aryl azides (ArN<sub>3</sub>, Ar = Ph, *p*-MeC<sub>6</sub>H<sub>4</sub> or 1naphthyl) or *o*-phenylene diazide react with [Li{Si(SiMe<sub>3</sub>)<sub>3</sub>}(thf)<sub>3</sub>] to give lithium amides [Li{N(Ar)Si(SiMe<sub>3</sub>)<sub>3</sub>}L] [L = tmeda or (thf)<sub>2</sub>] or dilithium diamide [{Li(thf)}<sub>2</sub>{1,2-( $\mu$ -NSi(SiMe<sub>3</sub>)<sub>3</sub>)<sub>2</sub>}C<sub>6</sub>H<sub>4</sub>]. Reaction of *o*-Me<sub>3</sub>-SiOC<sub>6</sub>H<sub>4</sub>N<sub>3</sub> with [Li{Si(SiMe<sub>3</sub>)<sub>3</sub>}(thf)<sub>3</sub>] affords, via 1,4-trimethylsilyl migration from oxygen to nitrogen [Li{OC<sub>6</sub>H<sub>4</sub>{N(SiMe<sub>3</sub>)Si-(SiMe<sub>3</sub>)<sub>3</sub>}-2}]<sub>2</sub>.



Svetlana I. Pomogailo, Gennady V. Shilov, Victoria A. Ershova, Alexander V. Virovets, Vladimir M. Pogrebnyak, Nina V. Podberezskaya, Anatoly V. Golovin, Gulzhian I. Dzhardimalieva, Anatolii D. Pomogailo

J. Organomet. Chem. 690 (2005) 4258

Preparation, X-ray structure, copolymerization with styrene of  $[(\mu-H)Os_3(\mu-OCNMe_2)(CO)_9{P(CH_2CH=CH_2)Ph_2}]$  and catalytic properties of the cluster/styrene copolymer The complex  $[(\mu-H)Os_3(\mu-OCNMe_2)(CO)_9-\{P(CH_2CH=CH_2)Ph_2\}]$  derived from the replacement of a lightly-stabilizing NMe\_3 ligand in  $[(\mu-H)Os_3(\mu-OCNMe_2)CO)_9(N-Me_3)]$  by allyldiphenylphosphine molecule was physico-chemically and X-ray structurally characterized and served further as a metal cluster monomer to be immobilized on a polymer surface.



## Jun Yin, Guang-Ao Yu, Jintao Guan, Fusheng Mei, Sheng Hua Liu

J. Organomet. Chem. 690 (2005) 4265

Synthesis and properties of conjugated bimetallic ruthenium complexes with  $\sigma$ , $\sigma$ -bridging azobenzene chains

Several conjugated bimetallic ruthenium complexes with  $\sigma$ , $\sigma$ -bridging azobenzene chains were synthesized and characterized. These bimetallic complexes showed a remarkable absorption in the visible region, and undergo *trans*-to-*cis* isomerization under UV light irradiation for short time. Electrochemical study showed that the metals linked through the CH=CH-C<sub>6</sub>H<sub>4</sub>N=NC<sub>6</sub>H<sub>4</sub>-CH=CH bridge interact with each other.



#### v

## Take-aki Koizumi, Takashi Tomon, Koji Tanaka

J. Organomet. Chem. 690 (2005) 4272

Synthesis, structures and electrochemical properties of ruthenium (II) complexes bearing bidentate 1,8-naphthyridine and terpyridine analogous (N,N,C)-tridentate ligands 1,8-Naphthyridine (napy) and (N,N,C) tridentate ligands coordinated ruthenium (II) complexes, [RuL(napy- $\kappa^2 N,N'$ )(dmso)]-(PF<sub>6</sub>)<sub>2</sub> (1: L = N''-methyl-4'-methylthio-2,2': 6',4''-terpyridinium, 2: L = N''-methyl-4'-methylthio-2,2':6',3''-terpyridinium) were prepared and their electrochemical properties were characterized. The generation of CO from CO<sub>2</sub> was observed by IR spectra of 1 in CO<sub>2</sub>-saturated CH<sub>3</sub>CN solution under controlled potential reduction conditions.



## A.F.M. Mustafizur Rahman, Toshihiro Murafuji, Motoko Ishibashi, Youhei Miyoshi, Yoshikazu Sugihara

J. Organomet. Chem. 690 (2005) 4280

Chlorination of *p*-substituted triarylpnictogens by sulfuryl chloride: Difference in the reactivity and spectroscopic characteristics between bismuth and antimony Oxidative chlorination of *p*-substituted triarylstibines was carried out and the effect of the *p*-substituents on the chlorination was compared with that of the bismuth congeners. The spectroscopic characteristics of the stibines and their dichlorides were studied by  $^{13}$ C NMR spectrum.

Ar<sub>3</sub>Sb  $\xrightarrow{SO_2Cl_2}$  Ar<sub>3</sub>SbCl<sub>2</sub>

 $\begin{array}{l} \mbox{Ar}=\mbox{$\rho$-XC_6H_4$; $X=OMe, $H$, $Cl$,}\\ \mbox{CO}_2\mbox{Et}, \mbox{CF}_3, \mbox{CN}, \mbox{NO}_2 \end{array}$ 

## Martin Lamač, Ivana Císařová, Petr Štěpnička

J. Organomet. Chem. 690 (2005) 4285

Synthesis and structural characterization of *rac*-2-[(diphenylphosphino)methyl]ferrocenecarboxylic acid, its selected derivatives and some rhodium complexes A novel ferrocene carboxyphosphine, *rac*-2-[(diphenylphosphino)methyl]ferrocenecarboxylic acid (1), has been synthesized and further converted to the respective methyl ester, phosphine oxide and phosphine sulfide. The acid and the corresponding methyl ester were studied as ligands in rhodium complexes.



## Damian Plażuk, Janusz Zakrzewski, Agnieszka Rybarczyk-Pirek, Sławomir Domagała

J. Organomet. Chem. 690 (2005) 4302

Ferrocenecarbothioamide and *N*-ethoxycarbonylferrocenecarbothioamide: Synthesis, structure and application in synthesis of 2,4-diferrocenylthiazole The complexes 1 and 2 were synthesized by a Friedel–Crafts type reaction of ferrocene with potassium thiocyanide and ethoxycarbonyl isothiocyanate. 1 reacts with chloroacetylferrocene to afford 3. X-ray structures of 1 and 3 were determined. Redox properties of 3 were studied by means of cyclic voltammetry.



## Alejandro Capapé, Margarita Crespo, Jaume Granell, Mercè Font-Bardía, Xavier Solans

J. Organomet. Chem. 690 (2005) 4309

Synthesis and reactivity of cyclometallated platinum (II) compounds containing [C,N,N'] terdentate ligands: Crystal structures of  $[PtCl{(CH_3)_2N(CH_2)_3NCH(4-ClC_6H_3)}]$ , [Pt-Cl{(CH\_3)\_2N(CH\_2)\_3NCH(2-ClC\_6H\_3)}] and [Pt-Cl{(CH\_3)\_2N(CH\_2)\_3NCH(3-(CH\_3)C\_6H\_3)}]

## Kunhye Lee, Yong-Joo Kim, Kyoung Koo Baeck

J. Organomet. Chem. 690 (2005) 4319

A quantum chemical study on the mechanism of S-coordinated tetrazolethiolato formation by the reaction of organic isothiocyanates with metal azido complexes of Pt(II), Pd(II), and Sn The reaction of compound *cis*-[PtCl<sub>2</sub>(dmso)<sub>2</sub>] with ligands RCHN(CH<sub>2</sub>)<sub>3</sub>NMe<sub>2</sub> produced compounds [PtCl<sub>2</sub>{(CH<sub>3</sub>)<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>NCHR}], which are precursors of cyclometallated platinum compounds containing a terdentate [C,N,N'] ligand.

The mechanism of the reaction of isothiocyanates with metal-azido complexes of Pt(II), Pd(II), and Sn is studied using the density functional theory method. The first step is the approach of the S-atom of the organic isothiocyanate to the central metal atom followed by the nucleophilic attack of the coordinated N-atom of the azido group to the C-atom of the isothiocyanate. The activation barrier of this step is 22-24 kcal mol<sup>-1</sup>, and the resulting intermediate has the imidoyl azide form. The electrophilic attack of the terminal N-atom of the azide to the N-atom of the isothiocyanate transforms the intermediate to the S-coordinated tetrazole-thiolato product in the second step with a barrier of about 11 kcal mol<sup>-1</sup>.





## Vasily V. Bashilov, Feodor M. Dolgushin, Pavel V. Petrovskii, Viatcheslav I. Sokolov, Mara Sada, Tiziana Benincori, Gianni Zotti

J. Organomet. Chem. 690 (2005) 4330

Synthesis and structure of the chiral palladium–fullerene  $C_{60}$  and  $C_{70}$  complexes with enantiomeric ligand 2,2',5,5'-tetramethyl-4,4'-bis(diphenylphosphino)-3,3'-bithiophene [(–)tetraMe-BITIOP]  $\eta^2$ -Fullerene (C\_{60} and C\_{70}) palladium optically active complexes with the axially chiral enantiomeric ligand of bithienyl series, tetraMe-BITIOP, have been synthesized and investigated by  $^{31}P-\{^1H\}$  NMR, electronic spectroscopy, CD spectroscopy, cyclic voltammetry and by single crystal X-ray diffraction.

## Stefanus Otto, Adriana Ionescu, Andreas Roodt

J. Organomet. Chem. 690 (2005) 4337

Tertiary phosphine abstraction from a platinum(II) coordination complex with SeCN<sup>-</sup>: Crystal and molecular structures of Se=PTA and [Se=PTA-Me]I · CH<sub>3</sub>OH

Reacting [PtCl(PTA)<sub>3</sub>]Cl (PTA = 1,3,5-triaza-7-phosphatricyclo[ $3.3.1.1^{3.7}$ ]decane) with KSeCN in water or MeOH results in abstraction of PTA to yield Se=PTA. The reaction also proceeds by reaction of PTA or the methylated PTA ligand, [PTA-Me]I with KSeCN in water or methanol. The crystal structures of Se=PTA and [Se=PTA-Me]I · CH<sub>3</sub>OH are reported.



## Philip C. Andrews, Simone M. Calleja, Melissa Maguire

J. Organomet. Chem. 690 (2005) 4343

 $\pi$ (Arene) versus donor ligand complexation in the formation of the heterobimetallic lithium–potassium dianion of (*S*)-*N*-( $\alpha$ methylbenzyl)allylamine Reaction of the chiral amine (*S*)-*N*-( $\alpha$ -methylbenzyl)allylamine with *n*-BuLi and *n*-BuK in the presence of thf produces crystals of the N and C metallated heterobimetallic tetramer, {[(*S*)- $\alpha$ -(PhC(H)Me)(CH<sub>2</sub>CH)= CHK)N]Li · (thf)}<sub>4</sub>. The three different K<sup>+</sup> cations in the asymmetric unit show differing coordination environments dependent on preferential binding with either thf molecules or available  $\pi$  electron density.





## Goran Stojcevic, Ernest M. Prokopchuk, Michael C. Baird

J. Organomet. Chem. 690 (2005) 4349

Coordination insertion reactions of acrylonitrile into Pd–H and Pd–methyl bonds in a diimine-palladium(II) system

Acrylonitrile (AN) coordinates to a cationic diiminemethylpalladium(II) complex to form the N-bonded complex  $[Pd(N-N)Me(AN)]^+$  which on standing or heating undergoes 2,1-insertion to give the complex  $[Pd(N-N)(CH(CN)CH_2Me)(AN)]^+$ ; the latter also undergoes  $\beta$ -hydrogen elimination to give a hydride,  $[Pd(N-N)H(AN)]^+$ , which reacts further with AN to give the cyanoethyl complex  $[Pd(N-N)(CH(CN)Me)]^+$ .

## Shamindri M. Arachchige, Mary Jane Heeg, Charles H. Winter

J. Organomet. Chem. 690 (2005) 4356

Synthesis and structural characterization of unsymmetrical osmocenes containing the pentamethylcyclopentadienyl ligand Treatment of dibromo(pentamethylcyclopentadienyl)osmium(III) dimer with alkali metal salts of a variety of cyclopentadienyl derivatives provides a simple approach to pentamethylosmocene, ( $\eta^5$ -pentamethylcyclopentadienyl)( $\eta^5$ -indenyl)osmium, ( $\eta^5$ -pentamethylcyclopentadienyl)( $\eta^5$ -fluorenyl)osmium, ( $\eta^5$ -pyrrolyl)( $\eta^5$ -fluorenyl)ospium, and ( $\eta^5$ -3,5-di-*tert*-butylpyrazolato)( $\eta^5$ -pentamethylcyclopentadienyl)osmium. The molecular structures have been determined by X-ray crystal structure analyses.



#### Notes

## Rufen Zhang, Jiafeng Sun, Chunlin Ma

J. Organomet. Chem. 690 (2005) 4366

Structural chemistry of mononuclear, tetranuclear and hexanuclear organotin(IV) carboxylates from the reaction of di-*n*-butyltin oxide or diphenyltin oxide with rhodanine-*N*-acetic acid

Three new organotin(IV) carboxylates, {[*n*-Bu<sub>2</sub>-Sn(O<sub>2</sub>CC<sub>4</sub>H<sub>4</sub>NOS<sub>2</sub>)]<sub>2</sub>O}<sub>2</sub> (1), *n*-Bu<sub>2</sub>Sn(O<sub>2</sub>CC<sub>4</sub>-H<sub>4</sub>NOS<sub>2</sub>)]<sub>2</sub>O}<sub>3</sub> (2) and [PhSn(O)O<sub>2</sub>CC<sub>4</sub>H<sub>4</sub>NOS<sub>2</sub>]<sub>6</sub> · 3H<sub>2</sub>O (3) were synthesized by the reaction of di-*n*-butyltin/diphenyltin oxide and rhodanine-*N*-acetic acid. The complexs 1–3 are characterized by elemental, IR, <sup>1</sup>H, <sup>13</sup>C and <sup>119</sup>Sn NMR and X-ray crystallography diffraction analyses. The complex 1 has a tetranuclear structure based on a planar four-membered Sn<sub>2</sub>O<sub>2</sub> ring, while complex 2 is a hexa-coordinated monomer. As for complex 3, it adopts the hexameric drum-shaped structure.



# Akira Nakamura, Takashi Ohshima, Kazushi Mashima

J. Organomet. Chem. 690 (2005) 4373

A topological isomer of ferrocene: Theoretical approach for transition metal complexes with conjugated all *trans* cyclodecapentaene We demonstrate the ability of all-*trans* DPEN as a suitable ligand for transition metals by DFT computation [B3LYP/6-311+G(2d,p) and BP86 level]. The iron complex schematically shown below is a unique topological isomer of ferrocene.



#### Jin An, Luis Urrieta, Rayshonda Williams, Wayne Tikkanen, Robert Bau, Muhammed Yousufuddin

J. Organomet. Chem. 690 (2005) 4376

Piano stool complexes containing the bulky pentaphenylcyclopentadienyl( $C_5Ph_5$ ) ligand: Preparation, characterization and X-ray structure of  $C_5Ph_5Zr(N(CH_3)_2)_3$  (I) Tris(dimethylamido) pentaphenylcyclopentadienyl zirconium (I) has been prepared and its structure reflects strong amido  $\pi$ donation. I reacts rapidly with (*R*)-(+)-secphenethyl alcohol to give the trisubstituted complex.



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