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# Contents

# Communication

## Handong Yin, Hongyun Wang, Daqi Wang

J. Organomet. Chem. 693 (2008) 585

Synthesis, characterization and crystal structure of a novel 3D network triorganotin(IV) polymer containing two types of macrocycles A novel triorganotin(IV) complex 1 has been synthesized and structurally characterized by elemental analysis, FT-IR, <sup>1</sup>H NMR spectra and X-ray crystallography. This complex displays a 3D network structure, which contains two types of chair form macrocycles.



# **Regular Papers**

# René Kalio, Peter Lönnecke, Evamarie Hey-Hawkins

J. Organomet. Chem. 693 (2008) 590

New ferrocenylmethylphosphines – Preparation, characterisation and coordination chemistry of PH(CH<sub>2</sub>Fc)<sub>2</sub>, P(CH<sub>2</sub>Fc)<sub>3</sub> [Fc = Fe- $(\eta^5-C_5H_5)(\eta^5-C_5H_4)$ ] and their derivatives New ferrocenylmethylphosphines  $PH(CH_2Fc)_2$ (1) [Fc = Fe( $\eta^5$ -C<sub>5</sub>H<sub>3</sub>)( $\eta^5$ -C<sub>5</sub>H<sub>4</sub>)], P(CH<sub>2</sub>Fc)<sub>3</sub> (2), and phosphonium salts [P(CH<sub>2</sub>Fc)<sub>3</sub>-(CH<sub>2</sub>OH)]I (3), [P(CH<sub>2</sub>Fc)(CH<sub>2</sub>OH)<sub>3</sub>]Cl (4) and [P(CH<sub>2</sub>Fc)<sub>4</sub>]I (8) were prepared. Reactions with transition metal complexes showed that 2 is too bulky to coordinate in octahedral complexes.



# Santiago Gómez-Ruiz, Dorian Polo-Cerón, Sanjiv Prashar, Mariano Fajardo, Ýıctor L. Cruz, Javier Ramos, Evamarie Hey-Hawkins

# J. Organomet. Chem. 693 (2008) 601

Synthesis, characterization and catalytic behaviour of *ansa*-zirconocene complexes containing tetraphenylcyclopentadienyl rings: X-ray crystal structures of [Zr{Me<sub>2</sub>Si( $\eta^{5}$ -C<sub>5</sub>Ph<sub>4</sub>)( $\eta^{5}$ -C<sub>5</sub>Ph<sub>3</sub>R)}Cl<sub>2</sub>] (R = H, Bu')

The synthesis and structural characterization of the *ansa*-zirconocene complexes, [Zr{Me<sub>2</sub>-Si( $\eta^5$ -C<sub>5</sub>Ph<sub>4</sub>)( $\eta^5$ -C<sub>5</sub>H<sub>3</sub>R){Cl<sub>2</sub>] (R = H and Bu'), are reported. They have been tested as catalysts in the polymerization and found to be inactive. In order to explain this, DFT calculations based on the transition states present in the polymerization process have been carried out.



# Mahmoud M. Al-Ktaifani, Peter B. Hitchcock, John F. Nixon

J. Organomet. Chem. 693 (2008) 611

Lithiation and alkylation reactions of the triphosphaferrocenes, [Fe( $\eta^5$ -P<sub>3</sub>C<sub>2</sub><sup>*t*</sup>Bu<sub>2</sub>)( $\eta^5$ -C<sub>5</sub>R<sub>3</sub>)], (R = H and Me): Crystal and molecular structures of the LiFe( $\eta^4$ -P<sub>2</sub>C<sub>2</sub><sup>*t*</sup>Bu<sub>2</sub>P<sup>*n*</sup>Bu)( $\eta^5$ -C<sub>5</sub>Me<sub>5</sub>)<sub>2</sub> dimer, [Fe( $\eta^4$ -P<sub>2</sub>C<sub>2</sub><sup>*t*</sup>Bu<sub>2</sub>P<sup>*n*</sup>BuMe)( $\eta^5$ -C<sub>5</sub>Me<sub>5</sub>)] and *cis*-[PtCl<sub>2</sub>(PMe<sub>3</sub>)Fe( $\eta^4$ -P<sub>2</sub>C<sub>2</sub><sup>*t*</sup>Bu<sub>2</sub>P<sup>*n*</sup>BuMe)-( $\eta^5$ -C<sub>5</sub>H<sub>5</sub>)]

Treatment of the 1,2,4-tri-phosphaferrocenes, [Fe( $\eta^5$ -P<sub>3</sub>C<sub>2</sub>'Bu<sub>2</sub>( $\eta^5$ -C<sub>5</sub>R<sub>5</sub>)], (R = H; Me) with "BuLi leads to alkylation of one of the two

#### Richard S. Herrick, Christopher J. Ziegler, Melissa Precopio, Kerianne Crandall, Janet Shaw, Ronald M. Jarret

J. Organomet. Chem. 693 (2008) 619

Synthesis of tungsten compounds with Schiff base ligands prepared from ferrocenecarboxaldehyde: Observation of the migration of an imine double bond adjacent ring phosphorus atoms to afford the corresponding lithium salts LiFe( $\eta^4$ -P<sub>2</sub>C<sub>2</sub>'Bu<sub>2</sub>-P"Bu)( $\eta^5$ -C<sub>5</sub>R<sub>5</sub>)<sub>2</sub> (R = H; Me). A single crystal X-ray diffraction study reveals that LiFe( $\eta^4$ -P<sub>2</sub>C<sub>2</sub>'Bu<sub>2</sub>P"Bu)( $\eta^5$ -C<sub>5</sub>Me<sub>5</sub>)<sub>2</sub> exhibits an unusual dimeric structure in the solid state. Treatment of the lithium salts with MeI gives the monomeric zwitterion complexes [Fe( $\eta^4$ -P<sub>2</sub>C<sub>2</sub>'Bu<sub>2</sub>P"BuMe)( $\eta^5$ -C<sub>5</sub>R<sub>5</sub>)], (R = H; Me). The molecular structure of [Fe( $\eta^4$ -P<sub>2</sub>C<sub>2</sub>'Bu<sub>2</sub>P"BuMe)( $\eta^5$ -C<sub>5</sub>Me<sub>5</sub>)] and the platinum(II) complex *cis*-[PtCl<sub>2</sub>(PMe<sub>3</sub>)Fe( $\eta^4$ -P<sub>2</sub>C<sub>2</sub>'Bu<sub>2</sub>P" BuMe)( $\eta^5$ -C<sub>5</sub>H<sub>5</sub>)] have also been determined by single crystal X-ray diffraction studies.

The reactions of ferrocenecarboxaldehyde, W(CO)<sub>4</sub>(pip)<sub>2</sub> (pip = piperidine) and either 2-(aminomethyl)pyridine or 2-(2-aminoethyl)pyridine lead to formation of W(CO)<sub>4</sub>( $\eta^2$ -NC<sub>5</sub>H<sub>4</sub>CH=NCH<sub>2</sub>C<sub>5</sub>H<sub>4</sub>FeCp) (1) and W(CO)<sub>4</sub>-( $\eta^2$ -NC<sub>5</sub>H<sub>4</sub>C<sub>2</sub>H<sub>4</sub>N=CHC<sub>5</sub>H<sub>4</sub>FeCp) (2), respectively. Crystal structures show that in 1 the imine double bond has migrated and is conjugated with the pyridine ring. Spectroscopic measurements highlight the differences between the compounds.





#### Noriyoshi Nagahora, Takahiro Sasamori, Yoshinobu Hosoi, Yukio Furukawa, Norihiro Tokitoh

J. Organomet. Chem. 693 (2008) 625

Generation, isolation, and reactivity of a kinetically stabilized diphosphene anion radical The stable lithium diphosphene anion radical,  $[Li(dme)_3]^+[TbtPPTbt]^-$  (dme; 1,2-dimethoxyethane, Tbt; 2,4,6-tris[bis(trimethylsilyl)methyl]phenyl), was readily synthesized by the oneelectron reduction of the corresponding neutral diphosphene (TbtP = PTbt). The diphosphene anion radical was found to undergo ready chalcogenation reactions using elemental sulfur and selenium to afford the corresponding thiadiphosphirane and selenadiphosphirane, respectively.



[Li(dme)<sub>3</sub>]+[TbtPPTbt]<sup>-</sup>

Tbt; 2,4,6-tris[bis(trimethylsilyl)methyl]phenyl DME; 1,2-dimethoxyethane

# Siwei Bi, Qingming Xie, Xiaoran Zhao, Yanyun Zhao, Xiaojian Kong

J. Organomet. Chem. 693 (2008) 633

Theoretical investigation on the mechanisms of transfer hydrogenation of ketones catalyzed by iridium complexes

The detailed catalytic mechanisms on transfer hydrogenation of ketones are explored by employing the representative reaction of 3-pentanone and 2-propanol catalyzed by the model complex  $IrH_3[(Me_2PC_2H_4)_2NH]$ , derived from the catalyst  $IrH_3[(Pr_2PC_2H_4)_2NH]$ , with the aid of the density functional theory calculations.



### Siwei Bi, Yanyun Zhao, Xiaojian Kong, Xiaoran Zhao, Qingming Xie

J. Organomet. Chem. 693 (2008) 639

Bonding analysis and the mechanisms on the ring-opening of alkoxy-bridged bis(silylene) transition-metal complexes toward MeOH The mechanistic study on the ring-opening of alkoxy-bridged bis(silylene) transition-metal complexes toward MeOH is performed by using density functional theory.



#### Zilu Chen, Yunsheng Ma, Fupei Liang, Zhaohui Zhou

J. Organomet. Chem. 693 (2008) 646

Synthesis, crystal structure and magnetic properties of three polynuclear manganese compounds bearing ferrocenecarboxylato ligands Three discrete polynuclear Mn-ferrocenecarboxylate complexes were obtained by using both different ancillary ligands and ratios of the starting materials to tune the nuclearities and structures. Magnetic susceptibility measurements of 1 and 2 revealed that both of them mediate a weak antiferromagnetic coupling.

	+ phen (1:1:1)	$IMn_{2}(EeCO2)_{2}(nhen)_{2}^{+}(1)$
$\text{Mn}(\text{ClO}_4)_2$	+ 2,2'-bpy (1:2:1)	[Mn_(FeCO_) (2.21 hrst) 1 (2)
+		linear skeleton
recO <sub>2</sub> ina	+ 2,2-bpy (1:1:1)	$- [Mn_4O_2(FcCO_2)_7(2,2'-bpy)_2]^+ (3)$
		butterfly-like skeleton

#### Do Nam Lee, Bong Kwan Soh, Shin Han Kim, Young Moo Jun, Sook Hyun Yoon, Won-Yong Lee, Byeong Hyo Kim

J. Organomet. Chem. 693 (2008) 655

Star-shaped electrochemiluminescent metallodendrimers with central polypyridyl Ru(II) complexes: Synthesis and their photophysical and electrochemical properties Star-shaped metallodendrimers of polynuclear ruthenium complexes were synthesized and their photophysical and electrochemical properties were studied.





# Bin Li, Xing Tan, Shansheng Xu, Haibin Song, Baiquan Wang

J. Organomet. Chem. 693 (2008) 667

Unexpected reactions of  $(Me_2C)(Me_2Si)[(\eta^5-C_5H_3)Mo(CO)_3]_2$  with diazoalkane and carbon disulfide: Activation and cleavage of the N=N bond and disproportionation of carbon disulfide

The thermal reactions of  $(Me_2C)(Me_2Si)[(\eta^5-C_5H_3)Mo(CO)_3]_2$  (1) with diazoalkane  $Ar_2CN_2$  led to the N=N bond cleavage and an orthometalation of the aryl products. The reaction of complex 1 with CS<sub>2</sub> afforded two products with the disproportionation of carbon disulfide.



Željko Petrovski, Marta R.P. Norton de Matos, Susana S. Braga, Cláudia C.L. Pereira, Márcia L. Matos, Isabel S. Gonçalves, Martyn Pillinger, Paula M. Alves, Carlos C. Romão

J. Organomet. Chem. 693 (2008) 675

Synthesis, characterization and antitumor activity of 1,2-disubstituted ferrocenes and cyclodextrin inclusion complexes

The cytotoxic activity of several 1,2-disubstituted ferrocene derivatives tested in vitro against Ehrlich ascites tumor cells was found to vary from  $IC_{50} > 1000 \ \mu\text{M}$  for 1,2-bis(hydroxymethyl)ferrocene to  $IC_{50}$  71.2  $\mu\text{M}$  for 2-(N,N-dimethylaminomethyl)ferrocenecarboxamide. An inclusion compound comprising the latter derivative and 2-hydroxypropyl- $\beta$ cyclodextrin exhibited an improved  $IC_{50}$  value of 20.0  $\mu\text{M}$ .



#### Leticia Naya, Digna Vázquez-García, Margarita López-Torres, Alberto Fernández, José M. Vila, Nina Gómez-Blanco, Jesús J. Fernández

J. Organomet. Chem. 693 (2008) 685

Activation of C–H and C–Br bonds in cyclopalladation reactions of Schiff base ligands: Influence of the benzylidene ring substituents Cyclometallated compounds may be synthesized by activation of C–H or C–Br bonds as determined by the differing palladium reagents, to give acetato- or bromo-bridged dinuclear species.



# Tebogo V. Segapelo, Ilia A. Guzei, James Darkwa

J. Organomet. Chem. 693 (2008) 701

Synthesis, characterization and bromination of bis(phosphinoferrocenyl) gold(I) compounds

Reaction of  $[(dppf)Au_2Br_2]$  (3),  $[(dippf)-Au_2Br_2]$  (4), dppf or dippf with excess bromine results in the bromination of the cyclopentadienyl rings of the phosphinoferrocene instead of oxidation of the gold in the case of the gold complexes.



#### Harry Adams, Peter Blenkiron, Louise J. Gill, Raoul Hervé, Anne-Gönke Huesmann, Michael J. Morris

J. Organomet. Chem. 693 (2008) 709

Reaction of metal carbonyl anions with electrophilic alkynes: Synthesis of isomeric  $\eta^3\text{-}acryloyl$  and  $\sigma\text{-}vinyl$  complexes

Treatment of the metal carbonylate anions  $[CpMo(CO)_2(L)]^-$  (L = PPh<sub>2</sub>Me, PPh<sub>2</sub>Et) with RC=CCO<sub>2</sub>Me (R = H or CO<sub>2</sub>Me) followed by protonation affords mainly the acryloyl complexes [CpMo( $\eta^3$ -COCR=CHCO<sub>2</sub>Me)-(CO)(L)], with small amounts of the isomeric vinyl complexes *trans*-[CpMo(CR=CHCO<sub>2</sub>-Me)(CO)<sub>2</sub>(L)].



## Contents

J. Organomet. Chem. 693 (2008) 717

Transition-metal complexes of phenoxy-imine ligands modified with pendant imidazolium salts: Synthesis, characterisation and testing as ethylene polymerisation catalysts A series of zirconium, vanadium, chromium and iron complexes with modified phenoxyimine chiral ligands containing pendant imidazolium bromide salts, have been synthesised and characterised. The zirconium, vanadium and chromium complexes are active as precatalysts for ethylene polymerisation using methylaluminoxane (MAO) cocatalyst.



R = R = BI; M = Zr; x = 2 (2)  $R^{1}=H; R^{2}=NO_{2}; M = Zr; x = 2 (3)$   $R^{1}=R^{2}={}^{t}BI; M = V; x = 1 (4)$  $R^{1}=R^{2}={}^{t}BI; M = Cr; x = 1 (5)$ 

# Mahmoud M. Al-Ktaifani, Peter B. Hitchcock, John F. Nixon

J. Organomet. Chem. 693 (2008) 725

Protonation of the lithio derivatives of the 1,2,4-tri-phosphaferrocenes, [LiFe( $\eta^4$ -P<sub>2</sub>C<sub>2</sub><sup>'</sup>-Bu<sub>2</sub>PBu)( $\eta^5$ -C<sub>5</sub>R<sub>5</sub>)] (R = H, Me): Crystal and molecular structure of [Fe( $\eta^4$ -P<sub>3</sub>C<sub>2</sub><sup>'</sup>Bu<sub>2</sub>BuH)-( $\eta^5$ -C<sub>5</sub>Me<sub>5</sub>)]

A new synthetic route is described to generate the 4-centre-5 electron donor ring system (P<sub>3</sub>C<sub>2</sub>'Bu<sub>2</sub>BuH), *via* protonation of the lithium salts [LiFe( $\eta^4$ -P<sub>2</sub>C<sub>2</sub>'Bu<sub>2</sub>PBu)( $\eta^5$ -C<sub>5</sub>R<sub>5</sub>)] (R = H, Me). The molecular structure of [Fe( $\eta^4$ -P<sub>3</sub>C<sub>2</sub>'Bu<sub>2</sub>BuH) ( $\eta^5$ -C<sub>5</sub>R<sub>5</sub>)] (R = Me) has been determined by a single crystal X-ray study.



R = H 5; R = Me 6

#### Naresh H. Tarte, Seong Ihl Woo, Liqiang Cui, Young-Dae Gong, Young Ho Hwang

J. Organomet. Chem. 693 (2008) 729

Novel non-chelated cobalt(II) benzimidazole complex catalysts: Synthesis, crystal structures and cocatalyst effect in vinyl polymerization of norbornene The novel non-chelated monodentate benzimidazole (BI) complexes  $CoCl_2(BI)_2$  (1)–(3), show similar coordination behavior to their analogue nickel(II) benzimidazole complexes. But unlike nickel(II) complexes, these catalysts show very low activity for vinyl polymerization of norbornene upon activation with MAO; however, the activity abruptly increased by a factor of  $10^3$  in MMAO.



# Robin Haunschild, Gernot Frenking

J. Organomet. Chem. 693 (2008) 737

Ethylene addition to group-6 transition metal oxo complexes – A theoretical study

The  $[2+2]_{M,C}$  addition across the Mo=CH<sub>2</sub> double bond of M(=O)(=CH<sub>2</sub>)(CH<sub>3</sub>)<sub>2</sub> is kinetically favored over the  $[3+2]_{C,O}$  cycloaddition and the  $[2+2]_{M,O}$  addition across the M=O double bond for M = Cr, Mo, W. The chromium system exhibits a complex reactivity pattern where the rearrangement of the molecule to a Cr(IV) species with subsequent ethylene addition to the metal is predicted as the most favorable pathway.



### Yanjun Chen, Weiwei Zuo, Peng Hao, Shu Zhang, Kun Gao, Wen-Hua Sun

J. Organomet. Chem. 693 (2008) 750

Chromium(III) complexes ligated by 2-(1isopropyl-2-benzimidazolyl)-6-(1-(arylimino)ethyl)pyridines: Synthesis, characterization and their ethylene oligomerization and polymerization A series of chromium(III) complexes bearing 2-(1-isopropyl-2-benzimidazole)-6-(1-(arylimino)ethyl)pyridines were synthesized and characterized. These chromium complexes exhibited good to high catalytic activities for ethylene oligomerization and polymerization in the presence of MMAO.



#### Jairo Bordinhão, Nadia M. Comerlato, Laila de Castro Cortás, Glaucio Braga Ferreira, R. Alan Howie, James L. Wardell

J. Organomet. Chem. 693 (2008) 763

Studies of stannylated-1,2-dithiolato compounds: Synthesis and crystal structure of cocrystalline 4,5-bis[(triphenylstannyl)methylthiolato]-1,2-dithiole-3-thione (Ph<sub>3</sub>SnCH<sub>2</sub>)<sub>2</sub>-(dmt) and 5-[(triphenylstannyl)methylthiolato]-4-[(triphenylstannyl)thiolato]-1,2-dithiole-3-thione (Ph<sub>3</sub>SnCH<sub>2</sub>)(Ph<sub>3</sub>Sn)(dmt) [72:28] Co-crystalline 4,5-bis[(triphenylstannyl)methylthiolato]-1,2-dithiole-3-thione (Ph3SnCH2)2-(dmt) and 5-[(triphenylstannyl)methylthiolato]-4-[(triphenylstannyl)thiolato]-1,2-dithiole-3thione (Ph3SnCH2)(Ph3Sn)(dmt).



Vitor Rosa, Sónia A. Carabineiro, Teresa Avilés, Pedro T. Gomes, Richard Welter, João M. Campos, M. Rosário Ribeiro

J. Organomet. Chem. 693 (2008) 769

Synthesis, characterisation and solid state structures of  $\alpha$ -diimine cobalt(II) complexes: Ethylene polymerisation tests

Compounds of Co(II) of general formulation  $[CoX_2(\alpha-diimine)]$  ( $\alpha$ -diimine = bis(aryl)acenaphthenequinonediimine or 1,4-diaryl-2,3-dimethyl-1,4-diaza-1,3-butadiene; X = Cl or I) were synthesised, characterised, and tested as ethylene polymerisation catalysts in the presence of methylaluminoxane (MAO).



#### Notes

#### Anthony C. Benjamin, Alistair S.P. Frey, Michael G. Gardiner, Colin L. Raston, Brian W. Skelton, Allan H. White

J. Organomet. Chem. 693 (2008) 776

Reactivity variations within Group 4 complexes of 1,4-di-*tert*-butyl-1,4-diazabuta-1,3diene: Structures of  $[(C_5H_5)TiCl{(t-BuN CH)_2}]$  and  $[(C_5H_5)_2Zr{(t-BuNCH)_2}]$  The metathetical exchange reactions employed in the syntheses of the Ti and Zr 1,4-diazabuta-1,3-diene complexes follow different pathways, with elimination of Cl<sup>-</sup> and/or (C<sub>5</sub>H<sub>5</sub>)<sup>-</sup>. <sup>1</sup>H NMR spectroscopy shows the complexes to be fluxional in solution, which is likely to involve a ring flipping process of the non-planar chelating reduced 1,4-diazabuta-1,3-diene.



#### Byung Soo Kang, Dae Sung Lim, Woo Sung Ahn, Ho-jae Lee, Jahyo Kang

J. Organomet. Chem. 693 (2008) 781

Synthesis of chiral highly hindered cyclopentadienylruthenium compounds Optically active highly hindered half-sandwich ruthenium(II) compounds with C<sub>2</sub>-symmetric cyclopentadienyl ligands were synthesized from the ligand precursors, which were derived from (-)- $\beta$ -pinene. Thus, the reaction of the ligands with triruthenium dodecacarbonyl produced ruthenium compounds, after oxidative treatment. These compounds were characterized by single crystal X-ray crystallography.



#### Hongwei Zhou, Guoliang Liu, Changying Zeng

J. Organomet. Chem. 693 (2008) 787

Bismetalated carbon for tandem Wittig-type reaction via allylgallation of magnesium acetylides: A convenient and efficient method to allyl allenes A tandem Wittig-type reaction of 1,1-bismetalated olefins from allylgallation of magnesium acetylides with aldehydes affords allyl allenes.





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