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## **Contents**

### Communication

Vitalii S. Tkach, Dmitrii S. Suslov, Gomboo Myagmarsuren, Gennadii V. Ratovskii, Alexander V. Rohin, Tuczek Felix, Fedor K. Shmidt

J. Organomet. Chem. 693 (2008) 2069

An effective route for the synthesis of cationic palladium complexes of general formula [(Acac)PdL<sup>1</sup>L<sup>2</sup>]<sup>+</sup>A<sup>-</sup>

A series of palladium complexes of general formula  $[(Acac)PdL^1L^2]^+A^-$ , where  $L^1$ ,  $L^2$  = phosphines and  $A = BF_4$ ,  $CF_3SO_3$ , were synthesized. Preliminary studies show that the complexes are active in selective dimerization of styrene and addition polymerization of norbornene.

### **Regular Papers**

# Abraham F. Jalbout, Ali Jameel Hameed, Ali Hashem Essa

J. Organomet. Chem. 693 (2008) 2074

Structural isomers of 2-(2,3 and 4-substituted-phenyl)-1,2-benzisoselenazol-3(2H)-one: A Theoretical Study

A series of 2-(2,3 and 4-substituted-phenyl)-1,2-benzisoselenazol-3(2H)-one molecules were investigated theoretically by performing density functional theory calculations at the B3LYP/6-311++G\*\* level of the theory. The substituents investigated are X = H; CH<sub>3</sub>; NH<sub>2</sub>; OH; OCH<sub>3</sub>; F, Cl; Br; NO<sub>2</sub>; CN; COCH<sub>3</sub>; CO<sub>2</sub>H; CO<sub>2</sub>Me; SH; BH<sub>2</sub>. We have selected these substituents to be in 2, 3 and 4 positions in relation to the benzisoselenazol moiety in order to show the effect of such structural change on the electronic properties of the molecules.

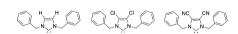
X= H; CH<sub>3</sub>;NH<sub>2</sub>; OH; OCH<sub>3</sub>; F, Cl; Br; NO<sub>2</sub>; CN; COCH<sub>3</sub>;CO<sub>2</sub>H; CO<sub>2</sub>Me: SH: BH<sub>2</sub>

## Agnes Bittermann, Peter Härter, Eberhardt Herdtweck, Stephan D. Hoffmann, Wolfgang A. Herrmann

J. Organomet. Chem. 693 (2008) 2079

Acceptor substituted *N*-heterocyclic carbenes and their Rh(I)complexes: Synthesis, structure and properties

Rhodium(I) complexes of acceptor substituted N-heterocyclic carbenes were obtained either by transmetalation from the corresponding Ag(I) complexes or by thermal decomposition of corresponding pentafluorobenzene carbene adducts. The relative  $\sigma$ -donor/ $\pi$ -acceptor strength of the NHC ligands was determined by means of IR spectroscopy. Dimerisation behaviour of Rh carbonyl complexes was studied.



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#### Thomas E. Bitterwolf

J. Organomet. Chem. 693 (2008) 2091

Frozen matrix photolysis of Group VIII  $M(CO)_2Cl_2L_2$  derivatives: Direct observation of CO-loss species and photochemical isomerization

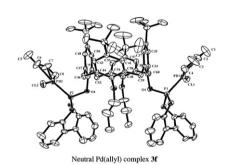
Photolysis of Group VIII complexes of the form  $M(CO)_2X_2L_2$  and chelated ruthenium compounds,  $Ru(CO)_2Cl_2(\kappa^2-L)$  in frozen matrices results in CO-loss. In the case of  $Fe(CO)_2Br_2(PMe_3)_2$  evidence is presented for photochemical bromide ion elimination.

## Arindam Sarkar, Munirathinam Nethaji, Setharampattu S. Krishnamurthy

I. Organomet. Chem. 693 (2008) 2097

Phosphite ligands derived from distally and proximally substituted dipropyloxy calix-[4]arenes and their palladium complexes: Solution dynamics, solid-state structures and catalysis

Phosphorus functionalization in the lower rim of distally and proximally substituted dipropyloxy calix[4]arenes with biphenyl-2,2'-dioxy moiety give two mono- and two bisphosphite ligands. Reactions of these ligands with palladium precursors give either bridged or chelated palladium complexes. The catalytic activity of one of the ligands and its palladium (methyl allyl) complex has been tested in allylic alkylation reaction.

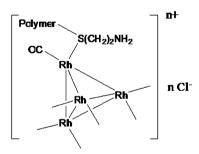


## Wendy J. Shaw, Yongsheng Chen, John Fulton, John Linehan, Anna Gutowska, Tom Bitterwolf

J. Organomet. Chem. 693 (2008) 2111

Structural evolution of a recoverable rhodium hydrogenation catalyst

High pressure XAFS and NMR were used to investigate the structure and kinetics of a recoverable hydrogenation catalyst, (Rh-(CO)<sub>2</sub>Cl(H<sub>2</sub>N-CH<sub>2</sub>CH<sub>2</sub>-S-pNIPAAm)). Upon dissolution in water, a tetrameric rhodium cluster was formed. Monomeric rhodium species are recovered during hydrogenation reactions in water.

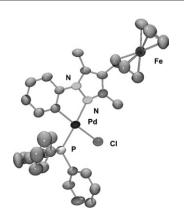


## Asensio González, Concepción López, Xavier Solans, Mercè Font-Bardía, Elies Molins

I. Organomet. Chem. 693 (2008) 2119

Cyclopalladation of N-phenyl-4-ferrocenylmethylpyrazoles: Crystal structure of  $[Pd\{\kappa^2-C,N-C_6H_4-1-[(3,5-Me_2-C_3N_2)-CH_2-(\eta^5-C_5H_4)Fe(\eta^5-C_5H_5)]\}Cl(PPh_3)]\cdot CH_2Cl_2$ 

The synthesis, characterization and study of the electrochemical properties of the N-phenyl-4-ferrocenylmethylpyrazoles [ $C_6H_4$ -4-R-1-{(3,5-Me<sub>2</sub>- $C_3N_2$ )-CH<sub>2</sub>-( $\eta^5$ - $C_5H_4$ )Fe-( $\eta^5$ - $C_5H_5$ )] (1) [with R = OMe or H] are reported together with the study of their reactivity with Pd(AcO)<sub>2</sub> that has allowed the obtention of mono- and dimeric five- or nine-membered palladacycles.



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## Sergio Muñoz, Josefina Pons, Xavier Solans, Merce Font-Bardia, Josep Ros

J. Organomet. Chem. 693 (2008) 2132

New *N*-pyrazole, *P*-phosphinite hybrid ligands and corresponding Rh(I) complexes: X-ray crystal structures of complexes with [Rh, N, P-phosphinite, Cl, (CO)]

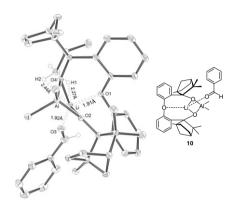
Rh(I) complexes with three *N*-pyrazole, *P*-phosphinite hybrid ligands have been prepared and characterised. <sup>1</sup>H NMR spectroscopic studies of the complexes prove the rigid conformation of the ligands when they are complexed. Two structures of Rh(I) with [N, P-phosphinite, Cl, (CO)] *core* are presented.

# Francis Soki, Jörg-Martin Neudörfl, Bernd Goldfuss

J. Organomet. Chem. 693 (2008) 2139

Homo- vs. heterometallic organoaluminum fencholates: Structures and selectivities

A new heterometallic aluminum lithium-fencholate gives rise to a dramatic increase of the enantioselectivity in comparison to its homometallic aluminum-fencholate analogue, i.e. from 19% ee to 62% ee in the methylation of benzaldehyde. Benzaldehyde coordinates to a fencholate-based lithium dimethyl aluminate, this X-ray crystal structure is shown.



## Iván Dorado, Román Andrés, Ernesto de Jesús, Juan Carlos Flores

J. Organomet. Chem. 693 (2008) 2147

Palladium(II) complexes of phosphane ligands with ammonium-functionalized carbosilane substituents

Ammonium-functionalized mono and diphosphane ligands were synthesized as models of potentially water-soluble dendritic carbosilane ligands, but the solubility brought about by the quaternized *N*-trimethylanilinium groups is scarce. Their palladium(II) complexes have been tested in the Hiyama cross-coupling reaction in aqueous sodium hydroxide solution.

## Olivier Pélerin, Céline Olivier, Thierry Roisnel, Daniel Touchard, Stéphane Rigaut

J. Organomet. Chem. 693 (2008) 2153

A ruthenium(II) allenylidene complex with a 4,5-diazafluorene functional group: A new building-block for organometallic molecular assemblies The synthesis of the new chelating ruthenium(II) allenylidene complex [ClRu(dppe)<sub>2</sub>—C—C— $C_{11}H_6N_2$ ][OTf] (dppe = 1,2-bis-(diphenylphosphino)ethane) along with its further coordination to ruthenium and rhenium centres are reported. This work shows that this complex is an attractive molecular clip for the access to original redox-active multi-component supramolecular assemblies.

$$\begin{array}{c} Ph_2P \\ PPh_2 \\ CI-Ru=C=C=C \\ Ph_2P \\ PPh_2 \end{array}$$

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## Metin Zora, Özlem Velioğlu

J. Organomet. Chem. 693 (2008) 2159

Synthesis of ferrocenyl quinolines

A convenient one-pot synthesis of ferrocenyl-substituted quinolines via a molecular iodine-catalyzed reaction of ferrocenylimines with enolizable aldehydes is described.

$$R_1$$
 +  $R_3$  Dioxane  $R_1$  +  $R_3$   $R_2$   $R_3$   $R_2$   $R_3$   $R_2$   $R_3$ 

## Bożena Adrjan, Teresa Szymańska-Buzar

J. Organomet. Chem. 693 (2008) 2163

Photochemical reactions of [W(CO)<sub>4</sub>( $\eta^4$ -nbd)] with hydrosilanes: Generation of new hydrido complexes of tungsten and their reactivity

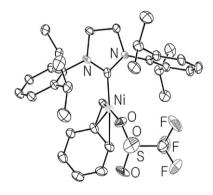
Photochemically activated  $[W(CO)_4(\eta^4-nbd)]$  (1) reacts with the Si–H bond of secondary and tertiary silanes (Cl<sub>3</sub>SiH, Et<sub>3</sub>SiH, Et<sub>2</sub>SiH<sub>2</sub>, Ph<sub>2</sub>SiH<sub>2</sub>) to yield hydride complexes and the hydrosilylation products of the  $\eta^4$ -nbd ligand. In reaction of complex 1 with silanes, the seven-coordinate complex  $[WH(SiCl_3)(CO)_3(\eta^4-nbd)]$  and other hydride complexes were identified by NMR spectroscopic methods.

## Sujith S, Eun Kyung Noh, Bun Yeoul Lee, Jin Wook Han

J. Organomet. Chem. 693 (2008) 2171

Synthesis, characterization, and norbornene polymerization of  $\eta^3$ -benzylnickel(II) complexes of N-heterocyclic carbenes

 $\eta^3$ -benzylnickel complexes of N-heterocyclic carbenes are prepared and characterized in this study. While the imidazolinylidene complexes are inactive, the imidazolylidene-based  $\eta^3$ -benzyl complexes exhibit good activity for norbornene homopolymerization without the requirement of any activator.



## Juntao Liu, Yinuo Wu, Xingshu Li, Albert S.C. Chan

J. Organomet. Chem. 693 (2008) 2177

Structure effect of TsDPEN derivatives on enantioselectivity of asymmetric transfer hydrogenation

TsDPEN derivative (3,3′,5,5′-TM TsDPEN) was synthesized and applied in asymmetric transfer hydrogenation of ketones. The influence of chiral ligands' NCCN dihedral angles to the enantioselectivities of the reaction was discussed.

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#### Konrad Kowalski, Rainer F. Winter

J. Organomet. Chem. 693 (2008) 2181

The synthesis, structures, and electrochemistry of 1'-heteroaryl-2,5-dimethylaza-ferrocenes

A synthetic route to 1'-heteroaryl substituted 2,5-dimethylazaferrocene derivatives is reported along with their crystallographical and electrochemical characterization.

## Jialiang Wang, Zhenyu Zhu, Wen Huang, Mingli Deng, Xigeng Zhou

J. Organomet. Chem. 693 (2008) 2188

Air-initiated hydrosilylation of unactivated alkynes and alkenes and dehalogenation of halohydrocarbons by tris(trimethylsilyl)-silane under solvent-free conditions

An efficient air-initiated highly regio- and stereoselective hydrosilylation of unactivated alkynes and alkenes and dehalogenation reaction of organic halides with tris(trimethylsilyl)silane as a reducing agent has been developed under solvent-free conditions.

$$\begin{array}{c} R - \frac{\square}{\square} \\ \text{or} \\ \text{RX} \end{array} + (\text{TMS})_3 \text{SiH} \begin{array}{c} 2 \text{ mol } \% \text{ Air} \\ \hline \text{Solvent-free} \end{array} \begin{array}{c} R \\ \text{or} \\ \text{RH} \end{array}$$

## Anna Kowalewska

J. Organomet. Chem. 693 (2008) 2193

Dendronized polystyrene supports for new catalytic systems

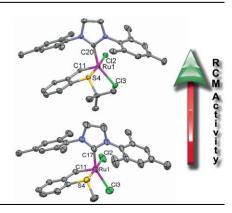
New Pt catalytic systems based on poly(styrene)-co-[1,1,1-tris(dimethylvinyl)ethylstyrene] as the polymeric support were prepared. Modification of poly(styrene-co-chloromethylstyrene) with LiC(SiMe<sub>2</sub>CH= CH<sub>2</sub>)<sub>3</sub> was followed by coordination of platinum to vinyl groups located on carbosilane grafts. The catalytic system was used in hydrosilylation of vinylsilanes, and proved to be an interesting alternative for heterogenous Pt catalysts as well as Karstedt's catalyst.

#### Note

## Tamar Kost, Mark Sigalov, Israel Goldberg, Amos Ben-Asuly, N. Gabriel Lemcoff

J. Organomet. Chem. 693 (2008) 2200

Latent sulfur chelated ruthenium catalysts: Steric acceleration effects on olefin metathesis By systematically modifying the substituent group bulkiness at the chelating sulfur atom, catalyst activity at different temperatures was fine tuned; larger substituents fomented activity at lower temperatures.



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