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# **Contents**

#### Communication

Sergey E. Lyubimov, Vadim A. Davankov, Pavel V. Petrovskii, Evamarie Hey-Hawkins, Andrey A. Tyutyunov, Evgeny G. Rys, Valery N. Kalinin

J. Organomet. Chem. 693 (2008) 3689

Chiral carborane-derived thiophosphites: A new generation of ligands for Rh-catalyzed asymmetric hydrogenation

A new class of chiral monodentate ligands – carborane-containing thiophosphites have been synthesized and tested in the Rh-catalyzed asymmetric hydrogenation of prochiral olefins with the result of up to 99% ee. The dependence of the enantioselectivity on the electronic properties of the carboranyl substituent has been studied.

#### **Regular Papers**

#### Xuming Guo, Jin Zhou, Xiaoyan Li, Hongjian Sun

J. Organomet. Chem. 693 (2008) 3692

Synthesis and catalytic applications of sulfonate  $\beta$ -ketoimine and  $\beta$ -diimine in the Suzuki reaction in aqueous phase

A series of sulfonated  $\beta$ -ketoimine and  $\beta$ -diimine compounds were synthesized and characterized. They were used in the Suzuki cross-coupling reaction with PdCl<sub>2</sub> as catalyst in aqueous phase. The new catalytic system can tolerate a wide range of substrates. This result provides environmentally benign preparations of diaryl compounds.

# Hakim Ahmed, John E. McGrady

J. Organomet. Chem. 693 (2008) 3697

On the role of the indenyl effect in controlling intramolecular hydride transfer in iron carbonyl complexes

Density functional theory reveals multiple pathways for intramolecular hydride migration between metal and ligand in cyclopentadienyl and indenyl iron carbonyl complexes. Facile ring slippage in the indenyl case opens up a low-energy channel for transfer of hydride from CO to iron, and hence for decomposition of transient formyl species.

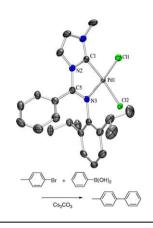
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#### Kjetil Andreas Netland, Alexander Krivokapic, Markus Schröder, Klaus Boldt, Fredrik Lundvall, Mats Tilset

J. Organomet. Chem. 693 (2008) 3703

Synthesis, X-ray structures, and catalytic applications of palladium(II) complexes bearing *N*-heterocyclic iminocarbene ligands

Pd(II) *N*-heterocyclic iminocarbene complexes (C–N)PdCl<sub>2</sub> that contain 5- and 6-membered chelate rings have been evaluated as catalysts for the Suzuki–Miyaura coupling reaction.



#### Nicola E. Cameron, Rachael A. Linklater, William Henderson, Brian K. Nicholson, T.S. Andy Hor

J. Organomet. Chem. 693 (2008) 3711

Spanning  $[Pt_2(\mu-S)_2(PPh_3)_4]$  metalloligands with 1,4-dimercurated durene

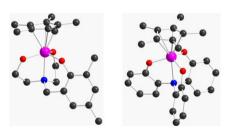
Reaction of  $[Pt_2(\mu-S)_2(PPh_3)_4]$  with 0.5 mol equivalents of durene-1,4-bis(mercuric acetate) [AcOHgC<sub>6</sub>Me<sub>4</sub>HgOAc] in methanol gives the polynuclear complex  $[\{Pt_2(\mu-S)_2(PPh_3)_4\}_2(\mu-1,4-C_6Me_4Hg_2)]^{2+}$ ; a single-crystal X-ray structure determination on the BPh<sub>4</sub> salt shows that the cation crystallises on a centre of symmetry, with structural features that are comparable to those of the previously characterised complex  $[Pt_2(\mu-S)_2(PPh_3)_4HgPh]BPh_4$ .

# Junseong Lee, Younjin Hong, Jeong Hee Kim, So Han Kim, Youngkyu Do, Young Kook Shin, Youngjo Kim

J. Organomet. Chem. 693 (2008) 3715

Synthesis, characterization, and polymerization activity of (pentamethylcyclopentadienyl)titanatranes containing  $\{(O-2,4-Me_2C_6H_2-6-CH_2)_nN(CH_2CH_2O)_{3-n}\}^{3-}$  (n=0-2) or  $\{N(C_6H_4-2-O)_3\}^{3-}$ 

New (pentamethylcyclopentadienyl)titanatranes,  $Cp^*Ti\{(O-2,4-Me_2C_6H_2-6-CH_2)_n-N(CH_2CH_2O)_{3-n}\}$  (n=0-2) and  $Cp^*Ti\{(0-2-C_6H_4)_3N\}$  were synthesized from  $Cp^*TiCl_3$  with the corresponding tri-hydroxy chelating ligands in the presence of NEt<sub>3</sub>. These compounds exhibited good catalytic activity for the syndiospecific polymerization of styrene at various polymerization conditions.



#### Yuanzhi Xia, Yahong Li, Wu Li

J. Organomet. Chem. 693 (2008) 3722

Theoretical study on the consecutive 1,2-hydroboration and 1,1-organoboration reactions of alkyn-1-yl(vinyl)silane with borane

The detailed reaction mechanism for the formation of 1-silacyclopent-2-ene from alkyn-1-yl(vinyl)silane with borane was studied by means of DFT calculations. The chemo- and regioselectivities, kinetic and thermodynamic properties of the consecutive 1,2-hydroboration and 1,1-organo-boration reactions, and the Si-H-B interactions of the product were analyzed.

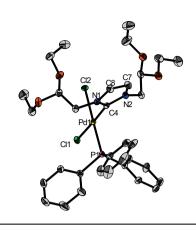
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#### Wei-Hsuan Yang, Chen-Shiang Lee, Sachindranath Pal, Yan-Nian Chen, Wen-Shu Hwang, Ivan J.B. Lin, Ju-Chun Wang

J. Organomet. Chem. 693 (2008) 3729

Novel Ag(I), Pd(II), Ni(II) complexes of N,N'-bis-(2,2-diethoxyethyl)imidazole-2-ylidene: Synthesis, structures, and their catalytic activity towards Heck reaction

Ag(I), Pd(II), Ni(II) complexes derived from tetra-ether substituted imidazolium salt have been synthesized. Mononuclear Pd-NHC complex, chlorobridged dinuclear Pd-NHC complex, and Pd(II) complex with mixed NHC and phosphine ligands provided an excellent activity toward Heck coupling reaction.

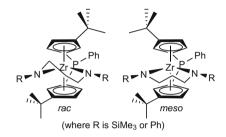


#### Jonathan C. Axtell, Susan D. Thai, Laurel A. Morton, William S. Kassel, William G. Dougherty, Deanna L. Zubris

J. Organomet. Chem. 693 (2008) 3741

Syntheses of rac/meso-{PhP(3-t-Bu- $C_5H_3$ ) $_2$ }-Zr{RN(CH $_2$ ) $_3$ NR}, structural analyses of rac-{PhP(3-t-Bu- $C_5H_3$ ) $_2$ }Zr{RN-(CH $_2$ ) $_3$ NR} (where R is SiMe $_3$  or Ph), and meso to rac isomerization

Phosphine-linked *ansa*-zirconocenes of the form *rac/meso*-{PhP(3-*t*-Bu-C<sub>5</sub>H<sub>3</sub>)<sub>2</sub>}Zr{RN-(CH<sub>2</sub>)<sub>3</sub>NR} (where R is SiMe<sub>3</sub> (*rac-3/meso-3*), Ph (*rac-4/meso-4*)) were prepared and characterized by <sup>1</sup>H, <sup>13</sup>C{<sup>1</sup>H}, and <sup>31</sup>P{<sup>1</sup>H} NMR spectroscopy; *rac-3* and *rac-4* were also examined via single crystal X-ray crystallography. Observations of *meso* to *rac* isomerization in these systems are also presented.



# Wei Zhong, Giuseppe Zampella, Zhimei Li, Luca De Gioia, Yinqiu Liu, Xirui Zeng, Qiuyan Luo, Xiaoming Liu

J. Organomet. Chem. 693 (2008) 3751

Synthesis, characterisation of two hexairon clusters with  $\{Fe_2S_2(CO)_x\}$  (x = 5 or 6) fragments and investigation into their inter-conversion

Two hexa-iron clusters **1** and **2**, synthesised from the reaction of a trithiol ligand with Fe<sub>3</sub>(CO)<sub>12</sub>, can interconvert into each other following a two-step mechanism as revealed by DFT calculations.

# Andrea Biffis, Giancarlo Gioia Lobbia, Grazia Papini, Maura Pellei, Carlo Santini, Elena Scattolin, Cristina Tubaro

J. Organomet. Chem. 693 (2008) 3760

Novel scorpionate-type triscarbene ligands and their silver and gold complexes

Novel silver(I) carbene complexes were obtained starting from scorpionate-type *N*-heterocyclic carbene ligand precursors {[HB(RImH)<sub>3</sub>]Br<sub>2</sub>} (R = Bn, Mes and *t*-Bu) and {[HC(MeBImH)<sub>3</sub>](BF<sub>4</sub>)<sub>3</sub>}. The tris-imidazolylborate silver(I) complexes were successfully employed as carbene transfer reagents in the synthesis of related gold(I) complexes by transmetallation reaction. The silver(I) complexes also proved to be active catalysts of the coupling of aryl iodides with terminal alkynes (the Sonogashira reaction).

# Peter B. Hitchcock, Michael F. Lappert, Zhong-Xia Wang

J. Organomet. Chem. 693 (2008) 3767

Synthesis and characterisation of six Fe(II or III), Co(II) or Zr(IV) complexes containing the ligand  $[CH(SiMe_2R)P(Ph)_2NSiMe_3]^-$  (R = Me, NEt<sub>2</sub>) and of  $[Co\{N(SiMe_3)-C(Ph)C(H)P(Ph)_2NSiMe_3\}_2]$ 

The iminophosphoranylmethyl complexes  $Fe(L)_2$ ,  $Co(L)_2$ ,  $ZrCl_3(L)$ ,  $Fe(L)_3$ ,  $Fe(L)_2$ ,  $Co(L)_2$  and the iminophosphoranyl-1-azaallyl compound  $Co\{N(SiMe_3)C(Ph)C(H)P(Ph)_2-NSiMe_3\}_2$  are reported;  $[CH(SiMe_2R)P(Ph)_2-NSiMe_3]$  L (R = Me), L'  $(R = NEt_2)$ .

# Zhifang Li, Chenjun Yang, Hongfang Zheng, Huayu Qiu, Guoqiao Lai

I. Organomet. Chem. 693 (2008) 3771

Selective mono- and di-allylation and allenylation of chlorosilanes using indium

Allyl and allenyl groups have been introduced into silicon systems by the allylation and allenylation of chlorosilanes using allyl bromide or propargyl bromide with indium. The allylation of chlorosilanes afforded a variety of aryl, aralkyl, and alkenyl substituted allylsilanes. By applying this method, the reactions of 1-bromo-3-methylbut-2-ene, 3-bromo-2-methylprop-1-ene and 3-bromobut-1-ene with chlorosilanes also proceed smoothly to give regioselectively allylic rearrangement products in good yields. Mediated by indium, dichlorosilanes (R<sub>2</sub>SiCl<sub>2</sub>) and trichlorosilanes (RSiCl<sub>3</sub>) can either afford monoallylated silanes or diallylated silanes depending on the amount of allyl bromide and indium used.

$$R_1$$
  $R_4$   $R_2$   $R_3$   $R_4$   $R_2$   $R_3$   $R_4$   $R_2$   $R_3$   $R_3$   $R_4$   $R_4$   $R_5$   $R_5$ 

# Rajkumar Jana, M. Senthil Kumar, Nem Singh, Anil J. Elias

J. Organomet. Chem. 693 (2008) 3780

Synthesis, reactivity and structural studies of  $(\eta^5$ -methylcyclopentadienyl) $(\eta^4$ -tetraphenylcyclobutadiene)cobalt and its derivatives

 $(\eta^5\text{-methylcyclopentadienyl})(\eta^4\text{-tetraphenylcyclobutadiene}) cobalt and a variety of its 1,2 and 1,3 disubstituted derivatives have been prepared and structurally characterized. The selectivity for the formation of 1,2 and 1,3-isomers has been studied with various substituents. Reactivity of some of the derivative has also been explored and compared with non-methylated analogues.$ 

