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## Journal of Organometallic Chemistry

journal homepage: www.elsevier.com/locate/jorganchem

# Contents

## Communication

## Sergey E. Lyubimov, Ilya V. Kuchurov, Andrei A. Vasil'ev, Andrey A. Tyutyunov, Valery N. Kalinin, Vadim A. Davankov, Sergei G. Zlotin

J. Organomet. Chem. 694 (2009) 3047

The use of a new carboranylamidophosphite ligand in the asymmetric Pdcatalysed allylic alkylation in organic solvents and supercritical carbon dioxide A novel *P*-monodentate ligand based on carboranyl alcohol and (S)-2-(anilino-methyl)pyrrolidine provides high enantio-selectivities (ee's up to 95%) in the Pd-catalyzed allylic alkylation of (E)-1,3-diphenylallyl acetate. The first example of the Pd-catalysed allylic alkylation in super-critical carbon dioxide is also described.

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## **Regular Papers**

## Guoping Ge, Jing He, Haiqing Guo, Fuzhi Wang, Dechun Zou

J. Organomet. Chem. 694 (2009) 3050

Highly efficient phosphorescent iridium (III) diazine complexes for OLEDs: Different photophysical property between iridium (III) pyrazine complex and iridium (III) pyrimidine complex The synthesis and luminescence of four new iridium (III) diazine complexes (**1–4**) were investigated. The results suggest that the iridium pyrimidine complexes show a significantly blue-shift of the emission band, compared with iridium pyrazine complexes. The device with these complexes showed high performance.



## Ning Luo, Zhengkun Yu

J. Organomet. Chem. 694 (2009) 3058

Multiple reactivities of dithranol towards 1-alkynyl Fischer carbene complexes  $(CO)_5M=C(OEt)C=CPh$  (M = Cr, W) – Efficient chemical synthesis of aromatic polyketides

Multiple reactivities of dithranol were unveiled in its reactions with 1-alkynyl Fischer carbene complexes (CO)<sub>5</sub>M= $C(OEt)C\equiv CPh (M = Cr, W)$  under controlled conditions, directing formation of polyphenolic organic and/or organometallic mono-and triscarbene complexes.





## Miao Zhao, Zhengkun Yu, Shenggang Yan, Yang Li

I. Organomet. Chem. 694 (2009) 3068

Ruthenium(II) complex catalysts bearing a pyridyl-supported pyrazolyl-imine ligand for transfer hydrogenation of ketones

Ruthenium(II) complexes bearing a unsymmetrical 2-(1-arylimino)-6-(pyzazol-1-yl)pyridine ligand exhibited good to excellent catalytic activity in the transfer hydrogenation of ketones in refluxing 2-propanol.



## Jin Woo Lee, Won Ho Jo

J. Organomet. Chem. 694 (2009) 3076

Chemical structure-stereospecificity relationship of internal donor in heterogeneous Ziegler-Natta catalyst for propylene polymerization by DFT and MM calculations

Theoretical investigation on the effect of 1,3-diether on the performance of Ziegler-Natta catalyst reveals that the primary function of 1,3-diether is to prevent the formation of aspecific site on the  $(1 \ 1 \ 0)$ surface, without significant decrease in the number of the isospecific active site created on the (1 0 0) surface.



on the (100) surface

on the (110) surface

### Ashish Kumar Singh, Sudhakar Dhar Dwivedi, Santosh Kumar Dubey, Sanjay Kumar Singh, Sanjeev Sharma, Daya Shankar Pandey, Ru-Qiang Zou, Qiang Xu

J. Organomet. Chem. 694 (2009) 3084

Synthesis and reactivity of homobimetallic Rh and Ir complexes containing a N,O-donor Schiff base

Rhodium and iridium complexes [ $\{(\eta^5 C_5Me_5)MCl_2(\mu-bsh)$ ] (M = Rh, Ir) containing N,N'-bis(salicylidine)hydrazine (H<sub>2</sub>bsh) have been prepared. These complexes reacted with  $EPh_3$  (E = P, As) to afford the complexes  $[(\eta^5 - C_5 Me_5)M(EPh_3)(\kappa^2 - Hbsh)]$ -PF<sub>6</sub> which have been employed as a metallo-ligand in the synthesis of heterobimetallic complexes.



## Yong-chun Liu, Zheng-yin Yang

J. Organomet. Chem. 694 (2009) 3091

Synthesis, crystal structure, antioxidation and DNA binding properties of binuclear Ho(III) complexes of Schiff-base ligands derived from 8-hydroxyguinoline-2carboxyaldehyde and four aroylhydrazines Coordination sphere of ORTEP diagrams (30% probability ellipsoids) of [HoL1- $(NO_3)(DMF)_2]_2$  complex. Ho(III) and the ligand can form a binuclear nine-coordination Ho(III) complex with an 1:1 metal-toligand stoichiometry. Dimerization of the monomeric unit occurs through the phenolate oxygen atoms leading to a central planar four-membered (HoO)<sub>2</sub> ring.



#### Contents

## Paula Barbazán, Rosa Carballo, Inmaculada Prieto, Margarita Turnes, Ezequiel M. Vázquez-López

J. Organomet. Chem. 694 (2009) 3102

Synthesis and characterization of several rhenium(I) complexes of 2-acetylpyridine and ferrocenyl carbaldehyde derivatives of 2-hydroxybenzoic acid hydrazide The rhenium(I) carbonyl halide (X = Cl and Br) complexes of the ligands derived from 2-acetylpyridine and ferrocenyl carbaldehyde derivatives of 2-hydroxybenzoic acid hydrazide have been prepared. The ligand forms a five-membered chelate ring but in the pyridine ligands it is Npyridine,N'bidentate while it is O,N-bidentate in the ferrocene complexes.



#### Daniel Olsson, Ola F. Wendt

J. Organomet. Chem. 694 (2009) 3112

Suzuki reaction catalysed by a  $PC_{sp3}P$  pincer Pd(II) complex: Evidence for a mechanism involving molecular species

Based on a mechanistic investigation of the Suzuki reaction catalysed by an aliphatic PCP palladium pincer complex an alternative parallel reaction mechanism based on soluble palladium(II) species only is proposed.



### Mitsushiro Nomura, Eriko Tsukano, Chikako Fujita-Takayama, Toru Sugiyama, Masatsugu Kajitani

J. Organomet. Chem. 694 (2009) 3116

Organometallic dithiolene complexes of benzenedithiolate analogues with  $\pi$ -coordinating and  $\pi$ -interacting Cp\* ligand

Organometallic dithiolene complexes, which were formulated as  $[Cp^*M(dcbdt)]$ and  $[Cp^*M(dcdmp)]$  (M = Co, Rh, Ir; dcbdt = 4,5-dicyanobenzene-1,2-dithiolate, dcdmp = 2,3-dicyano-5,6-dimercaptopyrazine) were prepared. The monomeric  $[Cp^*Co(dcbdt)]$  (**3a**),  $[Cp^*Co(dcdmp)]$  (**4a**) and dimeric  $[Cp^*Rh(dcbdt)]_2$  (**3b**) were structurally determined by X-ray diffraction. Some plane-to-plane intermolecular interactions were observed such as benzene···benzene (**3a**),  $Cp^*...$ benzene (**3a**), and pyrazine···pyrazine (**4a**).



## Tomohide Saita, Hiroyuki Nitadori, Akiko Inagaki, Munetaka Akita

J. Organomet. Chem. 694 (2009) 3125

Syntheses and photophysical properties of visible-light-absorbing Ru(II) polypyridyl complexes possessing (pyridylpyrazolyl)-metal tethers

Novel Ru(II) polypyridyl complexes with pendant pyridylpyrazolyl ligands were synthesized and their complexation with various organometallic precursors gave a series of di- (Ru···M) and trinuclear (M···Ru···M) complexes containing organometallic fragments. Their electrochemical and photophysical properties were compared with those of the corresponding parent complexes.



## Ludmila Vigo, Pekka Salin, Raija Oilunkaniemi, Risto S. Laitinen

J. Organomet. Chem. 694 (2009) 3134

Formation and structural characterization of mercury complexes from  $Te(R)CH_2SiMe_3$ (R = Ph, CH\_2SiMe\_3) and HgCl<sub>2</sub> The treatment of HgCl<sub>2</sub> with Te(R)CH<sub>2</sub>-SiMe<sub>3</sub> [R = CH<sub>2</sub>SiMe<sub>3</sub> (1), Ph (2)] yielded mononuclear or dinuclear complexes [HgCl<sub>2</sub>{Te(R)CH<sub>2</sub>SiMe<sub>3</sub>}<sub>2</sub>] (R = Ph, **3a**; R = CH<sub>2</sub>SiMe<sub>3</sub>, **3b**) and [Hg<sub>2</sub>Cl<sub>2</sub>( $\mu$ -Cl)<sub>2</sub>{Te(R)-CH<sub>2</sub>SiMe<sub>3</sub>}<sub>2</sub>] (R = Ph, **4a**; R = CH<sub>2</sub>SiMe<sub>3</sub>, **4b**). Depending on the workup and recrystallization conditions, [HgCl{Te(Ph)CH<sub>2</sub>Si-Me<sub>3</sub>}<sub>3</sub>]Cl-2EtOH (**5a**·2EtOH), and [HgCl<sub>2</sub>-{Te(CH<sub>2</sub>SiMe<sub>2</sub>})]·2HgCl<sub>2</sub>·CH<sub>2</sub>Cl<sub>2</sub> (**6b**·2Hg-Cl<sub>2</sub>·CH<sub>2</sub>Cl<sub>2</sub>) were also obtained.



#### Gabriele Albertin, Stefano Antoniutti, Stefano Paganelli

J. Organomet. Chem. 694 (2009) 3142

Trichlorostannyl complexes of iridium with both P-donor and N-donor ligands: Preparation and activity as hydrogenation catalysts The preparation of a series of trichlorostannyl complexes of iridium(III), containing both phosphine and pyrazole or 1,2-bipyridine as supporting ligands, is described. The activity of the iridium complexes as hydrogenation catalysts is also discussed.



 $[Ir] = IrHCIP_3$ ,  $IrHCI(HRpz)P_2$ , IrHCI(bpy)PP = phosphine or phosphite

#### Ivan A. Portnyagin, Mikhail S. Nechaev

J. Organomet. Chem. 694 (2009) 3149

Germylene and stannylene (Me<sub>2</sub>NCH<sub>2</sub>-CH<sub>2</sub>O)<sub>2</sub>E as strong  $\sigma$ -donor ligands for transition metal complexes [ML(CO)<sub>n</sub>] (E = Ge, Sn; M = Cr, Mo, W, n = 4 or 5; M = Fe, n = 4). Synthesis, spectroscopic and theoretical study It was shown using experimental and calculation data that germylene and stannylene ( $Me_2NCH_2CH_2O$ )<sub>2</sub>E (E = Ge, Sn) are promising ligands for preparation of metal complexes. They (i) exhibit relatively high binding energies to transition metals, (ii) are very strong donors, stronger than imidazolium-based NHCs, and (iii) possess tunable steric properties.



M = Ge, Sn TM - transition metal

## Michael J. Geier, Christopher M. Vogels, Andreas Decken, Stephen A. Westcott

J. Organomet. Chem. 694 (2009) 3154

The transition metal catalyzed hydroboration of enamines The addition of catecholborane (HBcat) to 9-vinylcarbazole can give either the branched or linear hydroboration product selectively depending upon the judicious choice of metal catalyst used in these reactions. Hydroborations with 1-pyrrolidino-1-cyclopentene, 1-pyrrolidino-1-cyclohexene and 1-vinyl-2-pyrrolidinone, however, all gave products arising from competing dehydrogenative borylation pathways.



### Bing Yan, Kai Qian, Hai-Feng Lu

J. Organomet. Chem. 694 (2009) 3160

Chemically bonded metallic (Eu, Tb, Zn) hybrid materials through sulfide linkage: Molecular construction, physical characterization and photophysical properties Sulfhydryl group (2-mercaptonicotinic acid) is modified with four silane crosslinking reagents to achieve four new kinds of functionalized molecular bridge (Pi (I = 1-4)). Subsequently, four novel series of chemically bonded hybrid materials which named as Ln (Zn)–Mi (I = 1-4) have been assembled via chemical bonds.



## Tao Cai, Xiaoniu Chen, Fan Xu, Yong Zhang, Yingming Yao, Qi Shen

J. Organomet. Chem. 694 (2009) 3167

Synthesis and molecular structures of lanthanocene amide complexes and their catalytic activity for addition of amines to nitriles A series of lanthanide amide complexes stabilized by two methylcyclopentadienyl ligands were synthesized and well characterized. These lanthanocene amide complexes were found to serve as efficient catalysts for addition of amines to nitriles to give the monosubstituted *N*-arylamidines.



## Bo Liang, Lei Wang, Xuhui Zhu, Huahong Shi, Junbiao Peng, Yong Cao

J. Organomet. Chem. 694 (2009) 3172

Application of heteroleptic iridium complexes with fluorenyl-modified 1-phenylisoquinoline ligand for high-efficiency red polymer light-emitting devices We designed and synthesized a new cyclometalating ligand: 1-(3-(9,9-dimethylfluoren-2-yl)phenyl)isoquinoline. Three new high-efficiency red iridium complexes were synthesized using different ancillary ligands. The electroluminescent performance of these complexes shows efficiency of saturated red phosphorescent devices processed by spin-coating from polymer host reaching the level comparable with the small molecules OPhLEDs.



## Włodzimierz Buchowicz, Anna Makal, Krzysztof Woźniak

J. Organomet. Chem. 694 (2009) 3179

The bis(trifluoroacetate) analogue of the first-generation Grubbs catalyst: Synthesis, X-ray structure, and metathesis activity of  $[Ru(CF_3CO_2)(\eta^2-CF_3CO_2)(=CHPh)(PCy_3)_2]$ 

The bis(trifluoroacatete) counterpart of the first-generation Grubbs catalyst, i.e.  $[Ru(CF_3CO_2)_2(=CHPh)(PCy_3)_2]$ , was synthesized in high yield by addition of PCy<sub>3</sub> to  $[Ru_2(CF_3CO_2)_2(=CHPh)_2(PCy_3)_2-(\mu-H_2O)]$ . The new complex is octahedral, with one monodentate and one bidentate carboxylic ligand. The very low metathesis activity of this complex clearly demonstrates that replacement of chlorides with trifluoroacetates in Grubbs catalyst results in a drastic decrease of the catalytic activity.



## Oleg V. Chernov, Aleksandr Yu. Smirnov, Ivan A. Portnyagin, Victor N. Khrustalev, Mikhail S. Nechaev

J. Organomet. Chem. 694 (2009) 3184

Heteroleptic tin (II) dialkoxides stabilized by intramolecular coordination Sn(OCH<sub>2</sub>-CH<sub>2</sub>NMe<sub>2</sub>)(OR) (R = Me, Et, <sup>i</sup>Pr, <sup>t</sup>Bu, Ph). Synthesis, structure and catalytic activity in polyurethane synthesis A straightforward method of synthesis of heteroleptic tin (II) alkoxides stabilized by one intramolecular coordination bond was developed. These compounds are active catalysts of polyurethane formation.



Marta Arroyo, M. Teresa García-de-Prada, Carolina García-Martín, Vanesa García-Pacios, Raúl García-Rodríguez, Patricia Gómez-Iglesias, Fernando Lorenzo, Isaac Martín-Moreno, Daniel Miguel, Fernando Villafañe

J. Organomet. Chem. 694 (2009) 3190

*fac*-Acetato-bis(pyrazole) complexes: A systematic study on intra- and intermole-cular hydrogen bonds

A systematic study on the hydrogen bonds observed in the crystal structures of *fac*acetato-bis(pyrazole) Mo, Mn, and Re complexes reveals that depend on the pyrazole used: dimethylpyrazole complexes show the same pattern of intramolecular hydrogen bonds, whereas intra- and intermolecular are found in the pyrazole complexes.





## Alessia Bacchi, Paolo Pelagatti, Corrado Pelizzi, Dominga Rogolino

J. Organomet. Chem. 694 (2009) 3200

Diastereomeric half-sandwich Ru(II) cationic complexes containing amino amide ligands. Synthesis, solution properties, crystal structure and catalytic activity in transfer hydrogenation of acetophenone A series of half-sandwich Ru(II) complexes containing two different amino amides (Lproline amide and L-phenylalanine amide), two different arenes (*p*-cymene and indane), two different coordinated halogens (Cl and I) and three different uncoordinated anion (Cl, I or PF<sub>6</sub>) have been synthesised and characterized both in solution and in the solid state. They show reasonable activity in the enantioselective reduction of acetophenone.



Ar = p-cymene or indane NO = L-proline amide or L-phenylalanine amide X = Cl, I Y = Cl, I, PF<sub>6</sub>

## Notes

Nobu Kato, Takanobu Sanji, Masato Tanaka, Tetsuya Fukasawa, Shintaro Ishida, Soichiro Kyushin

J. Organomet. Chem. 694 (2009) 3212

A ladder polysilane wrapped with amylose

A mixture of tricyclic ladder polysilane and amylose, upon pH adjustment of aqueous media from very basic to neutral, affords a supramolecular complex in which a preferential twisted (helical) conformation is induced on the ladder polysilane to display optical activity.

Si(i-Pr)2 or Si(i-Pr)

## Chan Sik Cho, Wen Xiu Ren

J. Organomet. Chem. 694 (2009) 3215

A recyclable copper catalysis in quinoxaline synthesis from  $\alpha$ -hydroxyketones and o-phenylenediamines  $\alpha$ -Hydroxyketones are oxidatively cyclized with *o*-phenylenediamines under a recyclable copper catalytic system (CuCl<sub>2</sub>/MS 4A) to give quinoxalines.





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