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# Contents

## Communications

## Yutaka Nishigaichi, Takayuki Orimi, Akio Takuwa

J. Organomet. Chem. 694 (2009) 3837

Photo-allylation and photo-benzylation of carbonyl compounds using organotrifluoroborate reagents Allyl- and benzyl-trifluoroborates can be applied to the photoreaction of carbonyl compounds to afford the corresponding alcoholic adducts in acceptable yields via a photo-induced single electron transfer pathway. These results were confirmed from the reaction selectivity and the negative free energy change for the electron transfer process.



#### D.Y. Mikhaylov, Y.H. Budnikova, T.V. Gryaznova, D.V. Krivolapov, I.A. Litvinov, D.A. Vicic, O.G. Sinyashin

J. Organomet. Chem. 694 (2009) 3840

Electrocatalytic fluoroalkylation of olefins

An efficient nickel-catalyzed method devoted to the direct addition of perfluoroalkyl halides (I, Br) to  $\alpha$ -methylstyrene is described. This procedure allows for synthesis of compounds resulting from additiondimerization in good yields.



## **Regular Papers**

## Fang-Hui Wu, Taike Duan, Lude Lu, Qian-Feng Zhang, Wa-Hung Leung

J. Organomet. Chem. 694 (2009) 3844

Synthesis and reactivity of ruthenium complexes with 1,1'-dithiolate ligands

Reaction of  $[RuCl_2(PPh_3)_3]$  with tetramethylthiuram disulfide  $[Me_2NCS_2]_2$  gave a Ru(III) dithiocarbamate complex  $[Ru(PPh_3)_2(S_2CNMe_2)Cl_2]$ . This reaction involved oxidation of ruthenium(II) to ruthenium(III) by the disulfide group in  $[Me_2NCS_2]_2$ . Treatment of  $[Ru(PPh_3)_2(S_2CN-Me_2)Cl_2]$  with 1 equiv. of  $[M(MeCN)_4]-[ClO_4]$  (M = Cu, Ag) afforded the stable cationic ruthenium(III)-alkyls  $[Ru\{C(NMe_2)-QC(NMe_2)S\}(S_2CNMe_2)(PPh_3)_2][ClO_4]$  (Q = O, S) with ruthenium–carbon bonds.



#### Zorica D. Petrović, Vladimir P. Petrović, Dušica Simijonović, Svetlana Marković

J. Organomet. Chem. 694 (2009) 3852

Mechanistic pathways for oxidative addition of aryl iodides to the low-ligated diethanolamine palladium(0) complex in phosphine-free Heck reactions

A set of reactions of different activated olefins and aryl iodides with the trans-dichlorobis(diethanolamine-N)palladium(II) complex (trans-[PdCl<sub>2</sub>(DEA)<sub>2</sub>]) as a precatalyst was performed, in the presence of diethanolamine (DEA) as a weak base, and NaOEt as a strong base. It was established that the presence of NaOEt slightly lowered the yields, but significantly accelerated the reactions. This experimental finding is in agreement with

#### Laxhmaiah Alakonda, Mariappan Periasamy

J. Organomet. Chem. 694 (2009) 3859

Copper(I) catalysis: Synthesis of N,N'diarylated and N-aryl,N'-formylated chiral  $C_2$ -symmetric diamines our computational investigation that shows that significantly higher activation barrier is required for the preactivation reaction in the presence of a weak base than in the presence of a strong base. The reaction between the catalytically active DEA-Pd(0)-Cl complex, formed in the preactivation reaction, and iodobenzene was investigated using density functional theory. Two mechanisms for the oxidative addition of the activated complex were found. The first mechanism is based on a nucleophilic attack of Pd on I of iodobenzene, and yields an intermediate tetracoordinated Pd complex (aI2). The second mechanism begins with a nucleophilic attack of Pd on the benzene ring, and vields a tricoordinated intermediate complex (bI4). It was concluded, on the basis of structural and energetical properties of al2 and bl4, that the second mechanism is significantly more favorable. It was shown that the oxidative addition requires noticeable lower activation energy than that required for the preactivation process. Thus, our investigations indicate that oxidative addition is not the rate determining step for the Heck reactions investigated in this work, but preactivation step.

Chiral *N*,*N*'-diaryl  $C_2$ -symmetric diamines and *N*-formyl, *N*'-phenyl-*trans*-(1*R*,2*R*)-diaminocyclohexane are readily accessed by copper catalyzed *N*-arylation of *trans*-(1*R*,2*R*)-diaminocyclohexane with aryl bromides. The reaction using (*R*)-1,1'-binaphthyl-2,2'-diamine and iodobenzene gave the corresponding (*R*)-*N*,*N*'-diphenyl-1,1'-binaphthyl-2,2'-diamine derivative in 83% yield.





### M. Angeles Alvarez, M. Esther García, Alberto Ramos, Miguel A. Ruiz

J. Organomet. Chem. 694 (2009) 3864

Reactivity of the 30-electron dimolybdenum anion  $[Mo_2(\eta^5-C_5H_5)_2(\mu-PCy_2)(\mu-CO)_2]^-$  towards  $\beta,\gamma$ -unsaturated organic halides: Alkenyl, allenyl and alkoxycarbyne derivatives

Rare 2,1-hydrogen shifts or decarbonylation processes occur readily at room temperature in the reactions of the title anion with organic halides having a  $\beta$ , $\gamma$ -double bond, to give unsaturated alkenyl derivatives. Other reaction pathways, as the electrophilic attack at the O(carbonyl) atoms of the anion to give an alkoxycarbyne derivative, are only marginally competitive.



## Pradhumn Singh, Monika Singh, Ajai K. Singh

J. Organomet. Chem. 694 (2009) 3872

Half sandwich complexes of Ru(II) and complexes of Pd(II) and Pt(II) with seleno and thio derivatives of pyrrolidine: Synthesis, structure and applications as catalysts for organic reactions *N*-{2-(phenylseleno)ethyl}pyrrolidine (**L1**), *N*-{2-(phenylthio)ethyl}pyrrolidine (**L2**), and bis{2-pyrrolidene-*N*-yl}ethyl selenide (**L3**) and complexes [Pd/PtCl<sub>2</sub>**L**] [RuCl( $\eta^6$ -C<sub>6</sub>H<sub>6</sub>/ $\eta^6$ -*p*-cymene) **L**][PF<sub>6</sub>](**L = L1** or **L2**) [Ru( $\eta^6$ -*p*-cymene)(**L1**)(CH<sub>3</sub>CN)][P-F<sub>6</sub>]<sub>2</sub>·CH<sub>3</sub>CN and [RuCl( $\eta^6$ -*p*-cymene)(**NH**<sub>3</sub>)<sub>2</sub>][PF<sub>6</sub>] have been synthesized and characterized by NMR (Proton, C-13 and Se-77) and X-ray crystallography (for some). The Pd–Se/Ru–Se bond length is 2.353(2)/2.4770(5)–2.4918(9) Å. Catalytic Heck and Suzuki–Miyaura coupling reactions using Pd complexes show TON up to 85 000. [RuCl( $\eta^6$ -C<sub>6</sub>H<sub>6</sub>)(**L**)][PF<sub>6</sub>] catalyzes oxidation of primary/ secondary alcohols with *N*-methylmorpholine-*N*-oxide [TON = 8.0 × 10<sup>4</sup>–9.7 × 10<sup>4</sup>].



#### Saphidabha L. Nongbri, Babulal Das, K. Mohan Rao

J. Organomet. Chem. 694 (2009) 3881

Arene ruthenium  $\beta$ -diketonato triazolato derivatives: Synthesis and spectral studies ( $\beta$ -diketones: 1-phenyl-3-methyl-4-benzoyl pyrazol-5-one, acetylacetone derivatives)

Arene ruthenium azide complexes bearing functionalized  $\beta$ -diketonato ligands have been synthesized. These complexes undergo 3 + 2 cycloaddition reactions with activated alkynes to yield triazolato compounds. These complexes were characterized by spectral studies and representative complexes by single crystal X-ray studies.



#### Liladhar B. Kumbhare, Amey P. Wadawale, Vimal K. Jain, Siddharth Kolay, Munirathinam Nethaji

J. Organomet. Chem. 694 (2009) 3892

Palladium(II) and platinum(II) complexes of  $\beta$ -functionalized ethyl selenolates: Effect of substitution on synthesis, reactivity, spectroscopy, structures and thermal behavior

A series of mono-, bi- and poly-nuclear palladium and platinum complexes have been synthesized by employing  $\beta$ -substituted ethylselenolate ligands.  $\beta$ -Substitution results in different nucleophilicity of ethylselenolate ligands which is reflected on reactivity, structures and thermal behavior of palladium and platinum complexes. Presence of protic groups in XCH<sub>2</sub>CH<sub>2</sub>Se<sup>-</sup> (X = OH, COOH) modified the solid state structures which exhibited functional group mediated aggregation via hydrogen-bonding.



#### Oussama M. El-Kadri, Mary Jane Heeg, Charles H. Winter

J. Organomet. Chem. 694 (2009) 3902

Synthesis, structure, properties, volatility, and thermal stability of molybdenum(II) and tungsten(II) complexes containing allyl, carbonyl, and pyrazolate or amidinate ligands The synthesis, structure, dynamic NMR spectra, volatility, and thermal stability of the molybdenum(II) and tungsten(II) complexes  $M(allyl)(X)(CO)_2(py)_n$  and  $[M(allyl)(X)(CO)_2]_2$  are described, where X is an amidinate or pyrazolate ligand and n = 0, 1, or 2.



## Peter B. Kraikivskii, Hans-Friedrich Klein, Vitaly V. Saraev, Reinhard Meusinger, Ingrid Svoboda, Mikhail Pashchanka

J. Organomet. Chem. 694 (2009) 3912

Conversion of imine ligands in allyl-nickel(II) complexes

The reaction of  $bis(\pi-allyl)nickel$  with phenanthroline results in dearomatization of one heteroaromatic ring and formation of an imine(amide)nickel complex.



#### Szymon Rogalski, Cezary Pietraszuk, Bogdan Marciniec

J. Organomet. Chem. 694 (2009) 3918

Synthesis of siloxy-modified second generation Hoveyda–Grubbs catalysts and their catalytic activity

Efficient syntheses of the first ruthenium alkylidene complexes bearing siloxide ligands are described. The complexes obtained exhibit catalytic activity in selected metathesis transformations.





#### Habib Firouzabadi, Nasser Iranpoor, Soghra Farahi

J. Organomet. Chem. 694 (2009) 3923

Highly efficient chemo- and regioselective silylation of –OH groups and cyanosilylation of aldehydes promoted by TiCl<sub>2</sub>(OTf)–SiO<sub>2</sub> as a new recyclable catalyst

TiCl<sub>2</sub>(OTf)–SiO<sub>2</sub> as a non-hygroscopic, easy handling recyclable catalyst was applied for trimethylsilylation of diethyl  $\alpha$ -hydroxyphosphonates, alcohols and phenols with high selectivity using HMDS as a silylating agent. Cyanotrimethylsilyl ethers were also obtained in excellent yields from treatment of aldehydes with TMSCN in the presence of this catalyst.



## Richard S. Herrick, Christopher J. Ziegler, Saovalak Sripothongnak, Natalie Barone, Roshinee Costa, William Cupelo, Americo Gambella

J. Organomet. Chem. 694 (2009) 3929

Preparation and characterization of rhenium (I) tricarbonyl dithiocarbamate compounds; Re(CO)<sub>3</sub>(S<sub>2</sub>CNMe<sub>2</sub>)(L)

Rhenium (I) tricarbonyl dimethyldithiocarbamate compounds with a neutral ligand have been prepared yielding eight Re- $(CO)_3(S_2CNMe_2)(L)$  derivatives. A one-pot procedure was employed. All new compounds have been spectroscopically and crystallographically characterized. Compounds were tested for physiological stability; derivatives with a phosphine as the sixth ligand were stable under physiological conditions.



Milan D. Joksović, Violeta Marković, Zorica D. Juranić, Tatjana Stanojković, Ljiljana S. Jovanović, Ivan S. Damljanović, Katalin Mészáros Szécsényi, Nina Todorović, Snežana Trifunović, Rastko D. Vukićević

J. Organomet. Chem. 694 (2009) 3935

Synthesis, characterization and antitumor activity of novel N-substituted  $\alpha$ -amino acids containing ferrocenyl pyrazole-moiety

A series of the novel *N*-[(3-ferrocenyl-1-phenylpyrazol-4-yl)methyl]  $\alpha$ -amino acids were synthesized, fully characterized by different spectroscopic techniques and tested for their cytotoxic potential against cervix adenocarcinoma HeLa, melanoma Fem-x and myelogenous leukemia K562 cell lines using the MTT method.



#### Thomas Gathy, Daniel Peeters, Tom Leyssens

J. Organomet. Chem. 694 (2009) 3943

Mechanism of ketone hydrosilylation by Cu(I) catalysts: A theoretical study

DFT calculations confirm the plausibility of the catalytic cycle suggested for the hydrosilylation of ketones by Cu(I) hydrides. A model system made up of a CuH(PH<sub>3</sub>)<sub>2</sub> catalyst, acetone and SiH<sub>4</sub> gives us the necessary insight into the intrinsic reactivity of the system. Computations show the activation of the copper fluoride pre-catalyst, as well as both steps of the catalytic cycle to involve a 4 center metathesis transition state as suggested from experimental data.



#### Laura Rodríguez, Montserrat Ferrer, Oriol Rossell, Silverio Coco

J. Organomet. Chem. 694 (2009) 3951

New rhodium(I) supramolecular structures containing pyridyl and bipyridyl ligands

The [RhCl(CO)<sub>2</sub>]<sub>2</sub> compound has been used as acceptor unit in self-assembly reactions with different pyridine derivatives for the construction of mono-, bi- and threedimensional novel rhodium(I) derivatives. It has been demonstrated that the size and length of the used ligand clearly determinate the structure of the final product.

3D- Rh(I) metallosupramolecular structures



 ${[RhCl(CO)]_2(\mu-4,4'-bipy)}_2(\mu-dppm)_4$ 

### Xiao Qiu, Hongli Zhao, Minbo Lan

J. Organomet. Chem. 694 (2009) 3958

Novel ferrocenyl nitroxides: Synthesis, structures, electrochemistry and antioxidative activity Novel ferrocenyl cyclic nitroxides with different linkages were synthesised. The modification of the linkage was found to be able to effectively improve the redox property and the antioxidative activity.



#### Rolando Luna-García, Berenice M. Damián-Murillo, Victor Barba, Herbert Höpfl, Hiram I. Beltrán, Luis S. Zamudio-Rivera

J. Organomet. Chem. 694 (2009) 3965

Structure and conformational motion of seven-coordinate diorganotin(IV) complexes derived from salen and salan type ligands

Four seven-coordinate diorganotin complexes have been prepared from ONNNOtype salen and salan ligands, which occupy the equatorial sites of a pentagonal bipyramid and show the tendency to adopt a curved conformation. Thus, the conformational motion observed in solution resembles the flapping of butterfly wings.





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