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# Contents

### **Regular papers**

# Tushar S. Basu Baul, Archana Mizar, Xueqing Song, George Eng, Robert Jirásko, Michal Holčapek, Rudolph Willem, Monique Biesemans, Ingrid Verbruggen, Ray Butcher

J. Organomet. Chem. 691 (2006) 2605

Dibenzyltin(IV) complexes of the 5-[(E)-2-(aryl)-1diazenyl]quinolin-8-olates: Synthesis and an investigation of structures by X-ray diffraction, solution and solid-state tin NMR, <sup>119</sup>Sn Mössbauer and electrospray ionization MS A series of *cis*-bis{5-[(*E*)-2-(aryl)-1-diazenyl]quinolinolato}dibenzyltin(IV) complexes have been synthesized by reacting sodium salts of 5-[(*E*)-2-(aryl)-1-diazenyl]quinolin-8-ol (LH) and dibenzyltin dichloride. These complexes have been characterized by <sup>1</sup>H, <sup>13</sup>C, <sup>119</sup>Sn NMR, ESI-MS in solution and by IR and <sup>119m</sup>Sn Mössbauer, <sup>117</sup>Sn CP-MAS NMR spectroscopy in the solid state. The structures of three dibenzyltin(IV) complexes, viz.,  $Bz_2Sn(L^3)_2$  (2),  $Bz_2Sn(L^3)_2$  (3), and  $Bz_2Sn(L^5)_2$  (5) were determined by single-crystal X-ray diffraction and revealed that the complexes adopt a distorted *cis*-octahedral geometry around central Sn atom.



### M.C. Torralba, M. Cano, J.A. Campo, J.V. Heras, E. Pinilla, M.R. Torres, J. Perles, C. Ruiz-Valero

J. Organomet. Chem. 691 (2006) 2614

Molecular architectures of cationic  $[Pd(\eta^3-C_3H_5)(pz^{bp2}py)]^+$  complexes and  $BF_4^-$  and  $CF_3SO_3^-$  as counteranions  $(pz^{bp2}py = 2-[3,5-bis(4-butoxyphenyl)pyrazol-1-yl]pyridine)$ 

The crystal structures of the complexes  $[Pd(\eta^3-C_3H_5)(pz^{bp2}py)]A$   $(pz^{bp2}py = 2-[3,5-bis(4-bu$  $toxyphenyl)pyrazol-1-yl]pyridine; <math>A = BF_4^- 1$ ,  $CF_3SO_3^- 2$ ) have been solved. The crystal packing revealed that the counteranion and the  $pz^{bp2}py$  ligand function as a source of hydrogen-bonding interactions, resulting in a <sup>2</sup>D network built through weak C-H···F/O interactions. The layers so generated exhibited interdigitation between the substituent-chains at the pyrazole group. These compounds constitute new examples of the importance of considering these or other weak interactions when designing supramolecular assemblies.



J. Organomet. Chem. 691 (2006) 2623

Copper(II) complexes containing chiral substituted 2-(4-isopropyl-4-methyl-4,5-dihy-dro-1*H*-imidazol-5-one-2-yl)pyridine ligands: Synthesis, X-ray structural studies and asymmetric catalysis

New chiral *N*,*N*-bidentate ligands derived from substituted 2-(4-isopropyl-4-methyl-4,5dihydro-1*H*-imidazol-5-on-2-yl)pyridines have been prepared and characterised by means of <sup>1</sup>H, <sup>13</sup>C NMR spectroscopy and optical rotation. Their Cu(II) complexes were characterised by means of elemental analysis, <sup>1</sup>H NMR spectroscopy and MS. By means of Xray diffraction, molecular geometry of the complex of 2-(1-methyl-4-isopropyl-4-methyl-4,5-dihydro-1*H*-imidazol-5-one-2-yl)pyridine with copper(II) chloride was determined.



### Jan Chalupa, Karel Handlíř, Ivana Císařová, Robert Jirásko, Jiří Brus, Antonín Lyčka, Aleš Růžička, Jaroslav Holeček

J. Organomet. Chem. 691 (2006) 2631

Structural study of bis(triorganotin(IV)) esters of 4-ketopimelic acid

The set of six bis(triorganotin(IV)) esters of 4ketopimelic acid was prepared. Their structures were studied using IR, NMR and X-ray crystallographic techniques both in solution and the solid state.



### **R.M.G.** Roberts

J. Organomet. Chem. 691 (2006) 2641

Synthesis of  $(\eta^6$ -arene) $(\eta^5$ -cyclopentadienyl) iron (II) complexes with heteroatom and carbonyl substituents. Part I: Oxygen and carbonyl substituents Synthesis of new arene–cyclopentadienyl iron complexes with hydroxyl and carbonyl substituents by microwave-mediated reactions and other methods.



### Nicoletta Panziera, Paolo Pertici, Ilaria Fratoddi, Alessandra La Groia, Maria Vittoria Russo

J. Organomet. Chem. 691 (2006) 2648

 The novel dialkynylated complexes  $Ru(\eta^6-arene)(\eta^4-COD)$  [arene = 1,4-diethynylbenzene and 4,4'-bis(ethynyl)biphenyl; COD = cycloocta-1,5-diene] have been prepared in high yield by desilylation of the corresponding  $Ru[\eta^6-(trimethylsilyl)arene](\eta^4-COD)$  derivatives obtained by the arene exchange reaction with the compound  $Ru(\eta^6-naphthalene)(\eta^4-COD)$ .



Uwe Klingebiel, Mathias Noltemeyer, Annette Wand

J. Organomet. Chem. 691 (2006) 2657

 $Dipheno-sily limin oquinones-A\ 14\pi\text{-system}$ 

Lithium salts of amino-2.6-diisopropylphenyl-(di-*tert*-butylfluorosilanes) thermally lose LiH. Iminosilanes with a  $14\pi$ -system are isolated.



#### M.Z. Kassaee, S.M. Musavi, M. Ghambarian

J. Organomet. Chem. 691 (2006) 2666

From halo-azasilylenes to halo-phosphasilylenes (X-CNSi vs. X-CPSi) at ab initio and DFT levels Thermodynamic and structural data for 24 singlet (s) and triplet (t) states of X-CPSi halophosphasilylenes, confined to the three structures, are studied at eight ab initio and DFT levels and compared with their haloaza-silylene analogues.



### Natalya V. Kirij, Wieland Tyrra, Ingo Pantenburg, Daniela Naumann, Harald Scherer, Dieter Naumann, Yurii L. Yagupolskii

J. Organomet. Chem. 691 (2006) 2679

Trifluoromethylselenato(0) and trifluoromethyltellurato(0) complexes of platinum(II) The series of *cis/trans*-trifluoromethylselenato complexes  $[Pt(SeCF_3)_{2-x}Cl_x(PPh_3)_2]$  (x = 0, 1) was identified by NMR spectroscopic methods. Molecular structures of *cis*- and *trans*-[Pt(SeCF\_3)\_2(PPh\_3)\_2] and *cis*-[Pt(TeCF\_3)\_2-(PPh\_3)\_2] are discussed in comparison with related compounds.



# Jianbing Liu, Lichun Li, Hong Dai, Zhun Liu, Jianxin Fang

J. Organomet. Chem. 691 (2006) 2686

Synthesis and biological activities of new 1*H*-1,2,4-triazole derivatives containing ferrocenyl moiety

Some new 1*H*-1,2,4-triazole derivatives containing ferrocenyl moiety were synthesized. Their structures of all these new compounds have been confirmed with <sup>1</sup>H NMR, IR, MS and elemental analysis. Their results of bioassay showed that some title compounds exhibited some degree of antifungal and plant growth regulatory activities.



#### Mitsushiro Nomura, Masatsugu Kajitani

J. Organomet. Chem. 691 (2006) 2691

Formations and structures of cobalt dithiolene complexes with nitrogen group-substituted cyclopentadienyl ligands

The acid hydrolysis, base hydrolysis and *N*-methylation of the cobalt dithiolene complex having the sulfonylamide-substituted Cp ligand [(C<sub>5</sub>H<sub>4</sub>-NHTs)Co{S<sub>2</sub>C<sub>2</sub>(COOMe)<sub>2</sub>}] (1) gave the cobalt dithiolene complexes **2–6**. The crystal structures, intermolecular hydrogen bondings and  $\pi$ - $\pi$  interactions in these cobalt dithiolene complexes were described.



### J.T. Lim, C.H. Jeong, J.H. Lee, G.Y. Yeom, H.K. Jeong, S.Y. Chai, I.M. Lee, W.I. Lee

J. Organomet. Chem. 691 (2006) 2701

Synthesis and characteristics of bis(2,4dimethyl-8-quinolinolato)(triphenylsilanolato)aluminum (III): A potential hole-blocking material for the organic light-emitting diodes The 5-coordinated bis(2,4-dimethyl-8-quinolinolato)aluminum (III) (24MeSAlq) was synthesized and characterized by various analyses. The high hole-blocking property of 24MeSAlq in the organic light-emitting devices (OLEDs) was enhanced by the high HOMO (highest Occupied Molecular Orbital) energy level. Its HOMO level was proved by cyclic voltammogram.



### Elena Mas-Marzá, Patrícia M. Reis, Eduardo Peris, Beatriz Royo

J. Organomet. Chem. 691 (2006) 2708

Dioxomolybdenum(VI) complexes containing *N*-heterocyclic carbenes

Compound MoO<sub>2</sub>Cl<sub>2</sub>(THF)<sub>2</sub> reacts with two equivalents of 1,3-dialkyl substituted 4,5-dimethylimidazol-2-ylidenes to give the dioxomolybdenum(VI) complexes MoO<sub>2</sub>Cl<sub>2</sub>(L<sup>R</sup>)<sub>2</sub> [R = Me (1), *i*-Pr (2)]. Treatment of MoO<sub>2</sub>Cl<sub>2</sub>(THF)<sub>2</sub> with one equivalent of the *N*-heterocyclic carbenes L<sup>Me</sup>, L<sup>*i*-Pr</sup> and <sup>Cl</sup>L<sup>*n*-Bu</sup> affords the monocarbene adducts MoO<sub>2</sub>Cl<sub>2</sub>-(L<sup>R</sup>) [R = Me (3), *i*-Pr (4)] and MoO<sub>2</sub>Cl<sub>2</sub>-(<sup>Cl</sup>L<sup>*n*-Bu</sup>) (5), respectively.



### Macarena Poyatos, Aline Maisse-François, Stéphane Bellemin-Laponnaz, Eduardo Peris, Lutz H. Gade

J. Organomet. Chem. 691 (2006) 2713

Synthesis and structural chemistry of areneruthenium half-sandwich complexes bearing an oxazolinyl-carbene ligand Ruthenium complexes bearing an oxazolinyl-NHC ligand,  $[RuCl(oxcarb)(p-cymene)]PF_6$ (**2a,b**) have been synthesized and converted to the dicationic aqua complexes  $[Ru(H_2O)-(oxcarb)(p-cymene)](PF_6)_2$  (**3a,b**). Their potential as transfer hydrogenation and Lewis acid catalysts has been probed.



### Javier Martínez, Luis A. Adrio, José M. Antelo, Juan M. Ortigueira, M<sup>a</sup> Teresa Pereira, Jesús J. Fernández, Alberto Fernández, José M. Vila

J. Organomet. Chem. 691 (2006) 2721

 $\label{eq:cyclometallated thiosemicarbazone palladium-(II) compounds: The first crystal and molecular structures of mononuclear complexes with a <math display="inline">\eta^1\text{-}diphosphine \ ligand$ 

Cyclometallated palladium thiosemicarbazone compounds with short or long "bite"  $\eta^1$ -diphosphines may be obtained by modulating the reaction conditions or the nature of the phosphine ligand. The first crystal and molecular structures of compounds bearing  $\eta^1$ -diphosphines,  $Ph_2PCH_2PPh_2$  and cis-Ph\_2PCH=CHPPh\_2, are reported.



### Fatma Alper, Ceyhan Kayran, Saim Özkar

J. Organomet. Chem. 691 (2006) 2734

A stable carbonyl–pyrazine–metal(0) complex: Synthesis and characterization of *cis*-tetracarbonylpyrazinetrimethylphosphitetungsten(0) The pentacarbonylpyrazinetungsten(0), (CO)<sub>5</sub>-W(pyz), is soluble in polar solvents such as acetone or dichloromethane, however, exists at equilibrium with the bimetallic complex, (CO)<sub>5</sub>W(pyz)W(CO)<sub>5</sub> plus free pyrazine (pyz) in solution. Using the quantitative <sup>1</sup>H NMR spectroscopy, the equilibrium constant could be determined to be  $K_{eq} = (5.9 \pm 0.8) \times 10^{-2}$  at 25 °C. Introducing trimethylphosphite as donor ligand into the molecule stabilizes the metal–pyrazine bond, so that *cis*-W(CO)<sub>4</sub>-[P(OCH<sub>3</sub>)<sub>3</sub>](pyz), could be isolated and characterized.



### Takashi Tsuno, Henri Brunner, Syushi Katano, Naoto Kinjyo, Manfred Zabel

J. Organomet. Chem. 691 (2006) 2739

Synthesis of chiral-at-metal half-sandwich ruthenium(II) complexes with the CpH-  $(PN_{Ment})$  tripod ligand

Treatment of the chiral tripod ligand  $(L_{Ment}, S_C)$ -CpH(PN<sub>Ment</sub>) with (Ph<sub>3</sub>P)<sub>3</sub>RuCl<sub>2</sub> in ethanol afforded the two chiral-at-metal diastereomers ( $L_{Ment}, S_C, R_{Ru}$ )- and ( $L_{Ment}, S_C, S_{Ru}$ )-[Cp(PN<sub>Ment</sub>)Ru(PPh<sub>3</sub>)Cl] (70% de) in which the cyclopentadienyl group and the P atom of the ligand coordinated at the metal center. The ( $L_{Ment}, S_C, R_{Ru}$ )-diastereomer was isolated by crystallization from ethanol– pentane and its structure was established by X-ray crystallography. Furthermore, the substitution reaction [Cp(PN<sub>Ment</sub>)Ru(PPh<sub>3</sub>)Cl] with nitriles or amines as monodentate ligands in the presence of NH<sub>4</sub>PF<sub>6</sub> is discussed.



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

J. Organomet. Chem. 691 (2006) 2748

Bis(silylaminodiarylphosphoranylsilylmethyl- *C*,*N*)-tin(II) and -lead(II) complexes and their precursors; structures of H(LL'), H(LL''), Sn(LL'')<sub>2</sub> and Pb(LL'')<sub>2</sub>; [LL']<sup>-</sup> = [CH(SiMe<sub>3</sub>)P(Ph)<sub>2</sub>=NSiMe<sub>3</sub>]<sup>-</sup>, [LL'']<sup>-</sup> = [CH-(SiMe<sub>3</sub>) $\overline{P(Ph)}$ {=NSi(Me<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>-1,2}]<sup>-</sup> A number of new derivatives of the 1-aza-2-phospha(V)allyl ligands [LL']<sup>-</sup> and [LL'']<sup>-</sup> were obtained, including their conjugate acids H(LL') (III) and H(LL'') (IV) and their complexes [Li(LL')]<sub>2</sub> (1a), [Li(LL'')]<sub>2</sub> (2), Pb(LL')<sub>2</sub> (3a), Pb(LL'')<sub>2</sub> (4), SnCl(LL') (5) and Sn(LL'')<sub>2</sub> (6); the X-ray structures of III, IV, 4, and 6 are presented; those of 1a, 2 and 3a were published earlier.



# Nicholas C. Lloyd, Brian K. Nicholson, Alistair L. Wilkins

J. Organomet. Chem. 691 (2006) 2757

Six-coordinate organotin(IV) complexes formed using the Kläui ligands; [CpCo- $\{P(OR')_2O\}_3$ ]SnR<sub>3-n</sub>Cl<sub>n</sub>

The Kläui ligands have been used to prepare six-coordinate organo-halo-tin(IV) complexes which have been characterised structurally and by <sup>1</sup>H, <sup>13</sup>C, <sup>31</sup>P and <sup>119</sup>Sn NMR spectroscopy.



### Contents

### Cheng-Hsien Yang, Kai-Hung Fang, Wei-Lin Su, Shao-Pin Wang, Shih-Kang Su, I-Wen Sun

J. Organomet. Chem. 691 (2006) 2767

Color tuning of iridium complexes for organic light-emitting diodes: The electronegative effect and  $\pi$ -conjugation effect

A novel red phosphorescent emitter (bis(4phenylquinazolinato- $N, C^2$ )iridium(acetylacetonate)) has been synthesized and characterized. Device using this emitter was fabricated and compared with devices using other emitters. The density functional theory (DFT) was applied successfully to illustrate the remarkable N(1) electronegative atom effect of this new emitter.



#### Stefan Buck, Gerhard Maas

J. Organomet. Chem. 691 (2006) 2774

Diruthenium(I,I) saccharinate complexes: Synthesis, molecular structure, and evaluation as catalysts for carbenoid reactions of diazoacetates The first dinuclear Ru(I,I) complexes with bridging saccharinate ligands ( $[Ru_2(\mu-sac)_2-(CO)_4L_2]_n$ , L = CO, CH<sub>3</sub>CN, PPh<sub>3</sub>) have been prepared. XRD analysis revealed the existence of regioisomers with head–head and head–tail arrangement, respectively, of the sac ligands. Complexes 1 and 2 catalyze the cyclopropanation of nucleophilic alkenes with methyl diazoacetate in good to fair yields.



# Carolina Villalonga-Barber, Barry R. Steele, Veronika Kovač, Maria Micha-Screttas, Constantinos G. Screttas

J. Organomet. Chem. 691 (2006) 2785

New stable, isolable triarylmethyl based dyes absorbing in the near infrared

Stable carbocationic dyes absorbing in the near infrared have been prepared from triarylmethanol derivatives containing 2,6dimethoxy-4-[2-(ferrocenyl)ethenyl]phenyl or 2,6-dimethoxy-4-[2-[4-(dimethylamino)phenyl]ethenyl]phenyl groups. These carbinols on treatment with acid deposit dark-purple crystals which display long-term stability in the solid state.



### Snigdha Panda, Sanjio S. Zade, Arunashree Panda, Harkesh B. Singh, Ray J. Butcher

J. Organomet. Chem. 691 (2006) 2793

Anion binding with some 22- and 28membered selenaaza macrocycles: Structural aspects and <sup>77</sup>Se NMR studies The anion adduct formation properties of two selenaaza macrocycles of different ring sizes with various anions such as halides,  $SO_4^{2-}$ ,  $CIO_4^-$ ,  $PO_4^{3-}$ ,  $CF_3COO^-$  and  $NO_3^-$  have been studied. The <sup>77</sup>Se NMR spectrum of the sulfate adduct of the 22-membered selenaaza macrocycles shows a considerable upfield shift (difference ~241 ppm) compared to the free ligand, indicating a strong interaction of the sulfate ion with the protonated macrocycle. The crystal structures of adducts show extensive hydrogen bonding between protonated macrocycles and the anions.



### Sumit Bhaduri, Sami Mukhopadhyay, Sudhir A. Kulkarni

J. Organomet. Chem. 691 (2006) 2810

Role of titanium oxidation states in polymerization activity of Ziegler–Natta catalyst: A density functional study The role of titanium oxidation states (+4, +3, +2) in ethylene and propylene polymerization activity of Ziegler–Natta catalyst has been investigated using density functional calculations at B3LYP/LANL2DZ and higher basis set on the simple [TiCl<sub>2</sub>CH<sub>3</sub>]<sup>n</sup> (n = +1, 0, -1) model catalysts.



Olefin insertion steps in the M-R(alkyl) bond with M = Ti in +2, +3, +4 oxidation states and  $Me=CH_3$ 

#### Kenji Ueura, Sawako Miyamura, Tetsuya Satoh, Masahiro Miura

J. Organomet. Chem. 691 (2006) 2821

Rhodium-catalyzed addition of arylboron compounds to nitriles, ketones, and imines

Nitriles, ketones, and imines efficiently undergo intermolecular phenylation with use of sodium tetraphenylborate under rhodium catalysis. The addition of  $H_2O$  and  $NH_4Cl$  is crucial to smoothly conduct the reaction of nitriles and of the latter two substrates, respectively.



# Sunita Jeram, William Henderson, Brian K. Nicholson, T.S. Andy Hor

J. Organomet. Chem. 691 (2006) 2827

Moderating the nucleophilicity of the sulfide ligands in the dinuclear  $\{Pt_2S_2\}$  metalloligand system using triphenylarsine

The complex  $[Pt_2(\mu-S)_2(AsPh_3)_4]$ , which is the triphenylarsine analogue of the extensively studied metalloligand  $[Pt_2(\mu-S)_2(PPh_3)_4]$ , has been synthesised and its chemistry studied, primarily using the technique of electrospray ionisation mass spectrometry. The results point towards a complex that contains somewhat less basic and nucleophilic sulfide centres, that together with the presence of labile arsine ligands modifies the chemistry of this complex towards alkylating agents.



### Marcin Konkol, Dirk Steinborn

J. Organomet. Chem. 691 (2006) 2839

On the reactivity of  $[IrCl(N_2)(PPh_3)_2]$  with alkynylsilanes – A new route to vinylidene iridium(I) complexes

The dinitrogen iridium complex [IrCl- $(N_2)(PPh_3)_2$ ] (1) was found to react with alkynylsilanes RC=CSiR'\_3 (R = Me, <sup>*i*</sup>Pr, Bn, Ph, SiMe\_3, SiEt\_3, C(O)Me, CO\_2Et; R' = Me, Et) to form vinylidene iridium(I) complexes *trans*-[IrCl{=C=CR(SiR'\_3)}(PPh\_3)\_2] (3), being the first examples of Werner's type complexes with other than P<sup>*i*</sup>Pr\_3 co-ligands. With R = C(O)Me and CO\_2Et the intermediate  $\eta^2$ alkyne iridium complexes *trans*-[IrCl{ $\eta^2$ -RC=CSiMe\_3}(PPh\_3)\_2] (2) were isolated.



# László Jánosi, László Kollár, Piero Macchi, Angelo Sironi

J. Organomet. Chem. 691 (2006) 2846

Synthesis of platinum-iodo-alkyl/aryl complexes in ligand-exchange reactions: Determination of the structure of  $Pt\{(S,S)$ bdpp $\}(X)I$  complexes (X = Me, I) by X-ray crystallography  $Pt{(S,S)-bdpp}(X)I$  (X = I, Me; bdpp = 2,4bis(diphenylphosphino)pentane) complexes were synthesised in ligand exchange reactions and their structure was determined by X-ray crystallography. Three different platinumbdpp chelate conformations have been identified.



# Note

### François Y. Pétillon, Françoise Robin-Le Guen, René Rumin, Philippe Schollhammer, Jean Talarmin, Kenneth W. Muir

J. Organomet. Chem. 691 (2006) 2853

Reactions of  $[Fe_3Cp_2(CO)_3(\mu$ -CO)( $\mu_3$ -CO)( $\mu_3$ -CF\_3C\_2CF\_3)] with diphosphines: X-ray structure of a complex in which two tri-iron clusters are linked only by Ph\_2PCH\_2CH\_2PPh\_2

Reactions of the trinuclear iron cluster  $[Fe_3Cp_2(CO)_3(\mu-CO)(\mu_3-CO)(\mu_3-CF_3C_2CF_3)]$ (1) with diphosphines yield mainly the hexanuclear compound in which two tri-iron cluster units are linked by the diphosphine.





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