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# Contents

#### Communication

## Annika Träff, Göran N. Nilsson, Kálmán J. Szabó, Ludvig Eriksson

J. Organomet. Chem. 692 (2007) 5529

Application of iridium pincer complexes in hydrogen isotope exchange reactions

Iridium pincer complexes have in recent years found use in several reactions based on C–H activation. However, a detailed study of their potential application as catalysts in hydrogen isotope exchange reactions has, to our knowledge, not been performed. We have now found that PCP iridium pincer complexes catalyze selective H/D exchange in aromatic substrates.



### Review

### Kavita R. Jain, Fritz E. Kühn

J. Organomet. Chem. 692 (2007) 5532

Immobilization of organorhenium(VII) oxides

Heterogeneous MTO based systems have been developed with particular emphasis on the supporting materials including inorganic and organic carriers. As a result efficient and selective catalysts are now available for a variety of catalytic reactions like olefin epoxidation in particular and other reactions, e.g. metathesis.



### **Regular Papers**

#### Hiroto Tachikawa, Hiroshi Kawabata

J. Organomet. Chem. 692 (2007) 5541

Structures and electronic states of paramagnetic species in Al–NTCDA co-deposit films

Structures and electronic states of paramagnetic species in co-deposit film of 1,4,5,8-naphthalene-tetracarboxylic-dianhydride (NTCDA) and aluminum (Al) have been investigated by means of hybrid density functional theory (DFT) calculations to determine the species in detail.



Víctor M. Jiménez-Pérez, Carlos Camacho-Camacho, Ángel Ramos-Organillo, Raúl Ramírez-Trejo, Adrián Peña-Hueso, Rosalinda Contreras, Angelina Flores-Parra

J. Organomet. Chem. 692 (2007) 5549

Hypervalent and binuclear silicon and germanium derivatives from bis-(3,5-di-*tert*-butyl-2-phenol)-oxamide

Reactions of bis-(3,5-di-*tert*-butyl-2-phenol)oxamide with R<sub>2</sub>SiCl<sub>2</sub> and R<sub>2</sub>GeCl<sub>2</sub> gave selectively bimetallic hexacyclic symmetric heterocycles bearing pentacoordinated silicon or germanium compounds. The silicon atoms are strongly coordinated by the carbonyl group, in solution, as was deduced from the <sup>29</sup>Si NMR, and in solid state by X-ray diffraction.



#### Ravi Shankar, Atul Pratap Singh, Geeta Hundal, Raymond J. Butcher

J. Organomet. Chem. 692 (2007) 5555

Synthesis, characterization and structural studies of mixed-ligand di-*n*-butyltin alkanesulfonate derivatives,  $[n-Bu_2Sn(X)-OS(O)_2R]_2$  [R = Et, *n*-Pr; X = acac, 4-OMe-O<sub>2</sub>CC<sub>9</sub>H<sub>5</sub>N-2, O<sub>2</sub>CC<sub>9</sub>H<sub>6</sub>N-2, O<sub>2</sub>CC<sub>9</sub>H<sub>6</sub>N-1]

The synthesis and characterization of stable mixed-ligand di-*n*-butyltin alkanesulfonates,  $[n-Bu_2Sn(L)OSO_2R]_2$  (R = Et, *n*-Pr; L = acac, 4-methoxy-2-quinoline/2-quinoline/1-isoquino-line carboxylate) are described.



#### G. Innorta, S. Torroni

J. Organomet. Chem. 692 (2007) 5563

Propane activation by  $MC_5H_5^+$  (M = Ni and Co): An experimental and theoretical work

Hydrogen loss from propane promoted by  $C_5H_5M^{\rm +}$  ions.



## Oleg N. Kadkin, Haksoo Han, Yuri G. Galyametdinov

J. Organomet. Chem. 692 (2007) 5571

Synthesis, computational modelling and liquid crystalline properties of some [3]ferrocenophane-containing Schiff's bases and βaminovinylketone: Molecular geometry–phase behaviour relationship Syntheses of series of mono- and di-substituted [3]ferrocenophane derivatives with various promesogenic molecular shapes are reported in this article. Nematic and smectic mesophases were observed in the synthesized compounds. On the base of computer-generated molecular models the molecular geometry-phase behaviour relationships were examined.



#### Thomas C. Baddeley, Jairo Bordinhão, Nadia M. Comerlato, Laila de Castro Cortás, Glaucio B. Ferreira, R. Alan Howie, James L. Wardell

J. Organomet. Chem. 692 (2007) 5583

Studies of distannylated-1,2-dithiolato compounds: Synthesis of 4,5-bis[(triorganostannylmethyl)thiolato]-1,3-dithiole-2thiones, (R<sub>3</sub>SnCH<sub>2</sub>)<sub>2</sub>(dmit), and 4,5-bis[(triorganostannvlmethvl)thiolatol-1.3-dithiole-2ones, (R<sub>3</sub>SnCH<sub>2</sub>)<sub>2</sub>(dmio) - Crystal structures of (Ph<sub>3</sub>SnCH<sub>2</sub>)<sub>2</sub>(dmit) and (Ph<sub>3</sub>SnCH<sub>2</sub>)<sub>2</sub>(dmio)

#### Martin F. Davis, Marek Jura, William Levason, Gillian Reid, Michael Webster

J. Organomet. Chem. 692 (2007) 5589

Synthesis and coordinating properties of the facultative Sb<sub>2</sub>O- and As<sub>2</sub>O-donor ligands  $O\{(CH_2)_2ER_2\}_2$  (E = Sb or As; R = Ph or Me)

Synthesis and characterization of bis-[(triorganostannylmethyl)thiolato]-1,3-dithiole-2-thiones, (R<sub>3</sub>SnCH<sub>2</sub>)<sub>2</sub>(dmit), and 4,5-bis-[(triorganostannylmethyl)thiolato]-1,3-dithiole-2-ones, (R<sub>3</sub>SnCH<sub>2</sub>)<sub>2</sub>(dmio) compounds.



The preparations and characterisation of four flexible Sb<sub>2</sub>O- and As<sub>2</sub>O-donor ligands,  $O{(CH_2)_2ER_2}_2$  (R = Me or Ph; E = Sb or As), incorporating dimethylene linkages between the donor atoms are described, together with their reactivity with selected late transition metal ions and the crystal structures of representative examples and an unexpected dinuclear Cu(I)-Cu(I) product containing a fragmented ligand.



### G. Brancatelli, M. Saporita, D. Drommi, F. Nicolò, F. Faraone

J. Organomet. Chem. 692 (2007) 5598

Effect of the rigidity and flexibility features of 2-pyridinyl or 8-quinolinyl based N-N\* chiral ligands on the stereochemical properties of  $[Pd(N-N^*)Cl_2]$  complexes

The [Pd(N-N\*)Cl<sub>2</sub>] complexes have been obtained, N-N\* indicate bidentate chiral ligands (S<sub>a</sub>)-1, (S<sub>a</sub>)-2, (S,S)-3, (R,R)-4, containing the rigid 2- pyridinyl or 8-quinolinyl building block skeleton and the C2-symmetric pyrrolidinic and azepinic chiral framework. The compounds [Pd(S,S-3)Cl<sub>2</sub>] and [Pd(R,R-4)Cl<sub>2</sub>] have been characterised by X-ray diffraction. The rigidity and flexibility features of (S,S)-3 and (R,R)-4 ligands induce a different orientation of the trans-2,5-dimethylpyrrolidinyl moiety with respect to the pyridinyl and quinolinyl plane.



# Xuan Pang, Xuesi Chen, Hongzhi Du, Xianhong Wang, Xiabin Jing

J. Organomet. Chem. 692 (2007) 5605

Enolic Schiff-base aluminum complexes and their application in lactide polymerization

Three enolic Schiff-base aluminum complexes derived from  $\beta$ -diketone and diamine were synthesized. These complexes polymerized lactides in good controlled manner and in some cases affording moderately isotactic polylactide. The diimine bridging parts as well as the diketone segment substituents had very close relationship with their performance upon the polymerization process.



R<sub>2</sub>=Ph

# Joyanta Choudhury, D. Krishna Kumar, Sujit Roy

J. Organomet. Chem. 692 (2007) 5614

Generation of Ir–Sn and Rh–Sn bonds from the oxidative addition of tin(IV) halides to  $[Ir(\mu-Cl)(1,5-COD)]_2$  and  $[Rh(\mu-Cl)(1,5-COD)]_2$ 

Facile oxidative addition of SnCl<sub>4</sub>, MeSnCl<sub>3</sub>, and SnBr<sub>4</sub> across Ir(I) and Rh(I) cyclooctadiene complexes resulted in the formation of the corresponding Ir–Sn and Rh–Sn heterobimetallic complexes. A *cis*-addition of Sn–X bond across  $Ir^I/Rh^I$  is proposed from the analysis of the geometrical features of "X–M– Sn" triangular units in the complexes.



#### Balázs Fábián, Veronika Kudar, Antal Csámpai, Tibor Zs. Nagy, Pál Sohár

J. Organomet. Chem. 692 (2007) 5621

Synthesis, IR-, NMR-, DFT and X-ray study of ferrocenyl heterocycles from thiosemicarbazones. Part 21: Study on ferrocenes Thiosemicarbazone-based synthesis, IR and NMR characterization of ferrocenylalkylydenehydrazono-substituted heterocycles were described. Two structures were supported by GIAO NMR calculations at B3LYP/6-311+G(2d,p) level of DFT. For three compounds the stereostructure was also proved by X-ray diffraction revealing non-bonding S–O and S–N interactions in a methoxycarbonylmethylene-substituted thiazolidinone. These interactions were also discernible in the optimized structures obtained by B3LYP/6-31G(d) and B3LYP/6-31G(2d) methods.



### Zdeňka Padělková, Tomáš Weidlich, Lenka Kolářová, Aleš Eisner, Ivana Císařová, Thomas A. Zevaco, Aleš Růžička

J. Organomet. Chem. 692 (2007) 5633

Products of hydrolysis of C,N-chelated triorganotin(IV) chlorides and use of products as catalysts in transesterification reactions

Triorganotin(IV) chlorides containing one  $L^{CN}$  chelating ligand were hydrolyzed with an excess of sodium hydroxide to give appropriate hydroxide and/or stannoxane forms (oxide), whereas alkyltin species react spontaneously and reversibly with carbon dioxide. The catalytic activity of these compounds in transesterification reactions was tested.



### Kerim Serbest, İsmail Değirmencioğlu, Yasemin Ünver, Mustafa Er, Cihan Kantar, Kemal Sancak

J. Organomet. Chem. 692 (2007) 5646

Microwave-assisted synthesis and characterization and theoretical calculations of the first example of free and metallophthalocyanines from salen type Schiff base derivative bearing thiophen and triazole heterocyclic rings Microwave-assisted synthesis and characterization and theoretical calculations of the first example of free and metallophthalocyanines from salen type Schiff base derivative bearing thiophen and triazole heterocyclic rings. Novel metal-free and metallophthalocyanine complexes of Co, Ni, Cu, and Zn have been synthesized by exposure to microwave irradiation and reflux conditions and the products purified by several techniques. The newly prepared compounds have been characterized by elemental analyses, IR, <sup>1</sup>H NMR, MS and UV-Vis spectroscopy. Furthermore, theoretical calculations of metallophthalocyanines CuPc, NiPc, ZnPc and CoPc were carried out to comparatively describe the molecular structures, molecular orbital and UV-Vis spectra of metallophthalocyanine complexes by the HF theory.



#### Graeme Hogarth, John Kilmartin

J. Organomet. Chem. 692 (2007) 5655

Backbone modified small bite-angle diphosphines: Synthesis and molecular structures of  $[M(CO)_4{X_2PC(R^1R^2)PX_2}]$  $(M = Mo, W; X = Ph, Cy; R^1 = H, Me, Et, Pr, allyl, R^2 = Me, allyl)$  Small bite-angle diphosphine complexes,  $[M(CO)_4 \{X_2PC(R^1R^2)PX_2\}]$  (M = Mo, W; X = Ph, Cy; R<sup>1</sup> = H, Me, Et, Pr, allyl, R<sup>2</sup> = Me), have been prepared upon elaboration of the methylene backbones in  $[M(CO)_4(X_2PCH_2PX_2)]$  via successive deprotonation and alkyl halide addition. The crystal structures of nine examples are presented.



# Qing-Xiang Liu, Xiao-Jun Zhao, Xiu-Mei Wu, Jian-Hua Guo, Xiu-Guang Wang

J. Organomet. Chem. 692 (2007) 5671

New mercury(II) and silver(I) complexes containing NHC metallacrown ethers with the  $\pi$ - $\pi$  stacking interactions

The oligoether-linked bis-benzimidazolium salt 1,1'-[1,2-ethanediylbis(oxy-1,2-ethanediyl)]bis[(3-s<sup>ec</sup>butyl)benzimidazolium-1-yl]iodide (H<sub>2</sub>L<sup>1</sup> · I<sub>2</sub>), 1,1'-[1,2-ethanediylbis(oxy-1,2-ethanediyl)]bis](3-ethyl)benzimidazolium-1-yl]iodide (H<sub>2</sub>L<sup>2</sup> · I<sub>2</sub>) and 1,1'-[1,2-ethanediylbis(oxy-1,2-ethanediyl)]bis](3-s<sup>ec</sup>butyl)benzimidazolium-1-yl]hexafluorophosphate (H<sub>2</sub>L<sup>1</sup> · (PF<sub>6</sub>)<sub>2</sub>) and their three new mercury(II) and silver(I) complexes containing NHC metallacrown ethers, HgL<sup>1</sup> · (Hg<sub>2</sub> · I<sub>6</sub>) (1), HgL<sup>2</sup> · I<sub>2</sub> (2) and AgL<sup>1</sup> · PF<sub>6</sub> (3) were prepared and characterized. In the packing diagrams of H<sub>2</sub>L<sup>2</sup> · I<sub>2</sub>, 1, 2 and 3 benzimidazole ring head-totail  $\pi$ - $\pi$  stacking interactions are observed.



#### Note

## Israel Nowik, Heather A. Spinney, Darrin S. Richeson, Rolfe H. Herber

J. Organomet. Chem. 692 (2007) 5680

Static and dynamic disorder in organotin compounds: A bis(amido)stannylene coordinated by *N,N'*-diisopropyl-1,8diamidonaphthalene The dynamics of the Sn atom in a bis(amido)stannylene coordinated by N,N'-diisopropyl-1,8-diamidonaphthalene has been studied by <sup>119</sup>Sn Mössbauer spectroscopy and compared to single crystal X-ray  $U_{i,j}$  values.





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