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Regular papers

Yong Nie, Hans Pritzkow, Hubert Wadepohl, Walter Siebert

J. Organomet. Chem. 690 (2005) 4531

Halogen exchange at boron in $\mathit{nido}\text{-}C_4B_2$ carboranes

The Pd(PPh₃)₄-catalyzed reaction of 1-iodo-6phenylethynyl-2,3,4,5-tetraethyl-2,3,4,5-tetracarba-*nido*-hexaborane (1a) with arylzinc reagents (generated *in situ* from arylbromides) leads to 1-bromo-6-phenylethynyl-2,3,4,5tetraethyl-2,3,4,5-tetracarba-*nido*-hexaborane (2a) and related compounds. The composition of the products follows from NMR and MS data and a single crystal X-ray analysis of 2a.



Nigel J. Sweeney, Oscar Mendoza, Helge Müller-Bunz, Clara Pampillón, Franz-Josef K. Rehmann, Katja Strohfeldt, Matthias Tacke

J. Organomet. Chem. 690 (2005) 4537

Novel benzyl substituted titanocene anticancer drugs Bis-[(*p*-methoxybenzyl)cyclopentadienyl]titanium (IV) dichloride is a promising candidate for an anti-cancer drug and was synthesised starting from 6-(*p*-methoxyphenyl)fulvene and Super Hydride. Herein, we present the synthesis and X-ray structure of the titanocene followed by MTT-based cytotoxicity tests on pig kidney carcinoma (LLC-PK) cells.



Peter Butler, John F. Gallagher, Anthony R. Manning, Helge Mueller-Bunz, C. John McAdam, Jim Simpson, Brian H. Robinson

J. Organomet. Chem. 690 (2005) 4545

The spectra, structures and electrochemistry of Ni(η^5 -C₅H₅)(PPh₃)-C=C-Ar complexes, and their reactions with Co₂(CO)₈

The structures, spectroscopy and electrochemistry of Ni(η^{5} -C₅H₅)(PPh₃)–C=C–Ar complexes suggest that there is only limited interaction between the Ni and the aryl groups via the acetylide linkage.



Yan Wang, Zheng-Yin Yang, Qin Wang, Qi-Kuan Cai, Kai-Bei Yu

J. Organomet. Chem. 690 (2005) 4557

Crystal structure, antitumor activities and DNA-binding properties of the La(III) complex with Phthalazin-1(2H)-one prepared by a novel route Phthalazin-1(2H)-one was prepared by a novel route, its La(III)-complex, $[La(NO_3)_3 \cdot 4H_2O \cdot C_8H_7N_2O] \cdot H_2O$, was synthesized and characterized on X-ray crystallography. Comparative antitumor activities of La(III)-complex was investigated by HL-60 and A-549. IC₅₀ = 2.6×10^{-8} , 3.3×10^{-5} mg/mL are given.



Janine T. Chantson, Maria Vittoria Verga Falzacappa, Sergio Crovella, Nils Metzler-Nolte

J. Organomet. Chem. 690 (2005) 4564

Antibacterial activities of ferrocenoyl- and cobaltocenium-peptide bioconjugates

Ferrocenoyl- and cobaltocenium-peptide bioconjugates of varing length (3–5 amino acids) were prepared by solid phase peptide synthesis and their antibacterial properties against *Escherichia coli*, *Staphylococcus aureus* and *Pseudomonas aeruginosa* were determined by minimum inhibition concentration (MIC) tests.



Gabriele Albertin, Stefano Antoniutti, Alessia Bacchi, Giancarlo Pelizzi, Marika Tollon

J. Organomet. Chem. 690 (2005) 4573

Preparation of rhenium hydride complexes with pyrazole and pyrazolato ligands

The synthesis of rhenium hydride Re-H(*R*pz)(H*R*pz)(NO)(PPh₃)₂ complexes containing both pyrazole and pyrazolato as supporting ligands is described. An intramolecular hydrogen bond N–H···N between the pyrazolato and the pyrazole ligands is present both in the solid state and in solution. Acetylide pyrazolato Re(C=CAr)(*R*pz)(H*R*pz)-(NO)(PPh₃)₂ complexes were also prepared by reacting the ReH(*R*pz)(H*R*pz)(NO)(PPh₃)₂ hydrides with terminal alkynes.



Nolwenn Cabon, François Y. Pétillon, Pierre-Yves Orain, Philippe Schollhammer, Jean Talarmin, Kenneth W. Muir

J. Organomet. Chem. 690 (2005) 4583

Controlled nucleophilic activation of different sites in $[Mo_2Cp_2L_2(\mu-SMe_2)_2(\mu-L')]^+$ cations $(L = Bu'NC, xyINC, CO; L' = SMe \text{ or }PPh_2)$ Factors governing nucleophilic attacks at various electrophilic sites in bis-cyclopentadienyl dimolybdenum cations have been investigated.



Paolo Pelagatti, Alessia Bacchi, Francesca Calbiani, Mauro Carcelli, Lisa Elviri, Corrado Pelizzi, Dominga Rogolino

J. Organomet. Chem. 690 (2005) 4602

Inverted piano-stool dimers of half-sandwich Ru(II) complexes with (*R*)-phenylglycine methylester and (*S*)-phenylalanineamide: An X-ray structural study and preliminary catalytic results

The complexes $[Ru(\eta^6-p\text{-}cymene)(\kappa^1-N\text{-}(rac)-phenylglycine methylester)Cl_2]$ (1) and $[Ru(\eta^6-p\text{-}cymene)(\kappa^2-N,N'\text{-}(S)\text{-}phenylalanineamido)-Cl]$ (2) have been synthesized and structurally characterized. The overall shape of 1 and 2 may be defined as a piano-stool geometry. The crystal architecture of 2 is characterized by two opposite helices of akin diastereoisomers, connected through strong intermolecular hydrogen bonds between the amine and carbonyl groups.

Maria Helena Araujo, Regina M.S. Pereira, Maria D. Vargas, Dario Braga, Fabrizia Grepioni

J. Organomet. Chem. 690 (2005) 4611

X-ray molecular structures and multinuclear NMR studies of the tetranuclear iridium clusters $[Ir_4(CO)_7(\mu_4-\eta^3-PhCC(H)CCPh)(\mu-PPh_2)_3]$ and $[Ir_4(CO)_7(\mu_3-\eta^2-HCCPh)(\eta^1-CCPh)(\mu-PPh_2)_3]$ Thermolysis of $[HIr_4(CO)_8(Ph_2PC=CPh)_2(\mu-PPh_2)]$ (1) gives $[Ir_4(CO)_7(\mu_4-\eta^3-PhCC(H)-CCPh)(\mu-PPh_2)_3]$ (2) and $[Ir_4(CO)_7(\mu_3-\eta^2-HCCPh)(\eta^1-CCPh)(\mu-PPh_2)_3]$ (3), similarly constituted of a spiked metal triangle, and a butadienic chain (compound 2) or two fragments of this ligand (compound 3); although directed in the appropriate fashion to generate the chain of compound 2, these fragments do not react.





Silvia Arévalo, Ernesto de Jesús, F. Javier de la Mata, Juan C. Flores, Rafael Gómez, María-Melia Rodrigo, Susana Vigo

J. Organomet. Chem. 690 (2005) 4620

Ethylene polymerization behavior of monometallic complexes and metallodendrimers based on cyclopentadienyl-aryloxy titanium units Monometallic complexes and titaniumcontaining carbosilane dendrimers of type nG-Si[(CH₂)₃[{C₆H_{4-y}(OMe)_y}O]Ti(C₅H₅)Cl₂]_x were used in ethylene polymerization. Fresh toluene solutions of these dendrimers in conjunction with MAO behaved as moderate active systems. However, in the case of complexes in which the phenoxy group is attached to the dendrimer in *para* position, their aged toluene solutions, when they were activated with MAO, became highly active catalysts as result of dendrimer aggregation processes.



Hamida Akter, Antony J. Deeming, G.M. Golzar Hossain, Shariff E. Kabir, Dwijendro N. Mondol, Ebbe Nordlander, Ayesha Sharmin, Derek A. Tocher

J. Organomet. Chem. 690 (2005) 4628

Triphenylphosphine-substituted selenido and sulfido clusters of osmium derived from $Ph_3P=Se$ or $Ph_3P=S$

Cleavage of P=Se bonds occurs readily at room temperature on treating $[Os_3(CO)_{10}$ -(MeCN)₂] with Ph₃P=Se to givethree new compounds, $[Os_3(\mu_3-Se)_2(CO)_8(PPh_3)]$ (2), $[Os_3(\mu_3-Se)(\mu_3-CO)(CO)_7(PPh_3)_2]$ (5), and $[Os_3(\mu-H)_2(CO)_8(PPh_3)_2]$ (6), and three known compounds, $[Os_3(\mu_3-Se)_2(CO)_9]$ (1), $[Os_3-(\mu_3-Se)(\mu-CO)_2(CO)_7(PPh_3)]$ (3) and 1,2- $[Os_3-(CO)_{10}(PPh_3)_2]$ (4). Both compounds 1 and 2 react with PPh₃ in the presence of trimethylamine-*N*-oxide at ambient temperature to give $[Os_3(\mu_3-Se)_2(CO)_7(PPh_3)_2]$ (10).



Nicholas J. Beach, Andrew E. Williamson, Gregory J. Spivak

J. Organomet. Chem. 690 (2005) 4640

A comparison of Cp*- and Tp-ruthenium carbyne complexes prepared via site selective electrophilic addition to neutral ruthenium vinylidenes

Ruthenium(IV) carbyne complexes supported by either pentamethylcyclopentadienyl (Cp*) or hydridotris(pyrazolyl)borate (Tp) ligands, and bearing various carbyne ligand substituents, are described and compared.



Daniel Schönfelder, Oskar Nuyken, Ralf Weberskirch

J. Organomet. Chem. 690 (2005) 4648

Heck and Suzuki coupling reactions in water using poly(2-oxazoline)s functionalized with palladium carbene complexes as soluble, amphiphilic polymer supports Three amphiphilic, water-soluble diblock copolymers based on 2-oxazoline derivatives with pendant N-heterocyclic carbene/palladium catalysts in the hydrophobic block. The copolymers were studied in the Heck coupling of iodobenzene with styrene indicating high activities with turn over frequencies (*TOF*) of up to 2700 h⁻¹ at 110 °C. In addition, the Suzuki coupling reaction of phenylboronic acid was studied in detail with iodobenzene and various bromoarenes.



Bożena Biernat, Teresa Szymańska-Buzar

J. Organomet. Chem. 690 (2005) 4656

Photochemical synthesis and spectroscopic characteristic of the first vinylsilane carbonyl complexes of tungsten(0) A series of new vinylsilane complexes of the type [W(CO)₅(η^2 -H₂C=CHSiR₃)] (1a–e) and *trans*-[W(CO)₄(η^2 -H₂C=CHSiR₃)₂](2a–e) (R = Me, OMe, OCH₂CH₂OMe, and Cl) have been synthesized photochemically and characterized by IR and ¹H, ¹³C and ²⁹Si NMR spectroscopy. The bis(vinylsilane) complexes 2a–e are shown to exist in several isomeric forms.



Vincenzo G. Albano, Luigi Busetto, Fabio Marchetti, Magda Monari, Stefano Zacchini, Valerio Zanotti

J. Organomet. Chem. 690 (2005) 4666

New bridging ligands from methylation reactions of μ -vinyliminium diiron complexes

Methyllithium addition at the Cp ligand of the diiron vinyliminium complexes 1 is followed by hydrogen migration from the C_5H_5Me ring to the iminium carbon. Bridging vinylcarbene complexes of type 2 are consequently formed. Treatment of 2 with MeSO₃CF₃ selectively produces the methylation of the nitrogen atom, affording the ammonium μ -allylidene 5.



Jeong Hyun Kim, Seung-Hyun Kang, Joon Soo Han, Myong Euy Lee, Do Hyun Moon, Myoung Soo Lah, Bok Ryul Yoo

J. Organomet. Chem. 690 (2005) 4677

Synthesis and structures of bis(alkyldihydroxysilyl)methanes Bis(alkyldihydroxysilyl)methanes **1** [R(HO)₂-SiCH₂Si(OH)₂R: R = methyl (**a**) and cyclopentyl (**b**)] were prepared in 65% and 86% yields by the hydrolysis of the corresponding bis(alkyldichlorosilyl)methanes. In single crystal X-ray structures, the molecules of **1a** and **1b** crystallize in the tetragonal (a = b = 22.884 Å, c = 6.1485 Å; $\alpha = \beta = \gamma = 90^{\circ}$ in a unit cell) and triclinic [a = 5.1729(14) Å [$\alpha = 89.133(4)^{\circ}$], b = 11.394(3) Å [$\beta = 85.065(4)^{\circ}$], c = 12.548(3) Å [$\gamma = 79.956(4)^{\circ}$ in a unit cell] space groups, respectively.

CI CI R-Si-CH ₂ -Si-R + 4 H ₂ O CI CI	0 °C/4 aniline in ethyl ether	OH R-Si-CH ₂ OH	OH -Si-R OH
R = Me, cyclopentyl		1a, 65% 1b, 86%	

Mingqiang Xue, Yingming Yao, Qi Shen, Yong Zhang

J. Organomet. Chem. 690 (2005) 4685

The salt-free diamido complexes of lanthanide supported by β -diketiminate: Synthesis, characterization, and their catalytic activity for the polymerization of acrylonitrile and ϵ -caprolactone

Treatment of β -diketiminate lanthanide dichloride LLnCl₂(THF)₂ (L = *N*,*N*'-bis(2,6dimethylphenyl)-2,4-pentanediiminate) [Ln = Yb (1), Nd (2)] with freshly prepared solutions of LiNPh₂ in THF gave LLn(NPh₂)₂(THF) [Ln = Yb (3), Nd (4)] in good yield as crystalline solids. Both of these lanthanide amides supported by β -diketiminate ligand were found to exhibit high activity for the polymerization of acrylonitrile and ring-opening polymerization of ε -caprolactone at room temperature.



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

J. Organomet. Chem. 690 (2005) 4692

In search of triplet ground state GeCNX germylenes (X = H, F, Cl, and Br): An ab initio and DFT study

Two triplet germylenes 2_{t-H} and 3_{t-H} appear more stable than their corresponding singlet states. This is found through the comparison of singlet-triplet energy splittings for 24 GeCNX germylenes at 10 levels of theory (X = H, F, Cl, and Br).



Hongkyu Kang, Bo Keun Park, Md. Arzu Miah, Hyunjoon Song, David G. Churchill, Sangwoo Park, Moon-Gun Choi, Joon T. Park

J. Organomet. Chem. 690 (2005) 4704

The synthesis and characterization of Re₃- $(\mu$ -H)₃(CO)_{9-n}(PMe₃)_n(μ ₃- η ²: η ²: η ²-C₆₀) (*n* = 2, 3) complexes

The reaction of $\text{Re}_3(\mu-\text{H})_3(\text{CO})_9(\mu_3-\eta^2;\eta^2;\eta^2-C_{60})$ (1) with PMe₃ in the presence of Me₃NO produces di- and tri-substituted stereoisomeric compounds having the general formula $\text{Re}_3(\mu-\text{H})_3(\text{CO})_{9-n}(\text{PMe}_3)_n(\mu_3-\eta^2;\eta^2;\Omega^2-C_{60})$ (n = 2, 2a and 2b; 3, 3a and 3b), depending on the stoichiometry of Me₃NO. Single crystal X-ray structures were obtained for 2a and 3b. Ligand arrangements for 2b and 3a are proposed based on assigning one PMe₃ ligand in an axial position and remaining PMe₃ ligands according to low energy equatorial site exchanges known in related metal cluster complexes, and were verified by ¹H NMR spectroscopic methods.



Contents

Alexandra M.J. Rost, Horst Schneider, Jochen P. Zoller, Wolfgang A. Herrmann, Fritz E. Kühn

J. Organomet. Chem. 690 (2005) 4712

Methyltrioxorhenium heterogenized on commercially available supporting materials as cyclooctene metathesis catalyst

Methyltrioxorhenium (MTO) is easily immobilized on various commercially available supporting materials, reaching Re loadings of up to 10 wt%. The obtained materials can be utilized as catalysts for cyclooctene metathesis. The selectivity of such systems with respect to the desired low molecular weight products is, however, not very high.



I.S. Butler, J.F. Meng, D.F.R. Gilson, J.A. Kozinski

J. Organomet. Chem. 690 (2005) 4719

Pressure-tuning vibrational spectra of the heterobimetallic complexes, $Ph_3MCo(CO)_4$ (M = Sn, Pb)

High-pressure vibrational spectroscopic measurements on two heterobimetallic organometallic complexes are reported that may afford a new and useful way in which to probe π -backbonding interactions in organometallic complexes.



Jeremy C. Stephens, Masood A. Khan, Kenneth M. Nicholas

J. Organomet. Chem. 690 (2005) 4727

Cyclopentadienyliron complexes of nitrosobenzene: Preparation, structure and reactivity with olefins Two novel CpFe-nitrosobenzene complexes have been prepared and structurally characterized. {[CpFe- μ -(η^2 -(N,O)-PhNO)]₂- μ -NH-Ph}BF₄ (2) features bridging PhNO and PhNH-units, whereas [CpFe(CO)₂(η^1 -Ph-NO)]SbF₆ (3) exhibits η^1 -N(O)Ph coordination. The possible intermediacy of 3⁺ in [CpM(CO)₂]₂-catalyzed allylic amination of alkene by nitroarenes is evaluated via reactions with a representative alkene and diene.



Tong Ren, Damon A. Parish, Guo-Lin Xu, Martin H. Moore, Jeffrey R. Deschamps, Jie-Wen Ying, Steven K. Pollack, Terence L. Schull, Ranganathan Shashidhar

J. Organomet. Chem. 690 (2005) 4734

Synthesis and characterization of wire-like $Ru_2(ap)_4$ -[σ -oligo(phenylene ethynyl)] compounds

Reported herein are the synthesis, electrochemical and structural characterization of wirelike Ru₂-alkynyl compounds, $Ru_2(ap)_4(Ln)_x$, where *ap* is 2-anilinopyridinate, and L*n* is $-(C \equiv CC_6H_4)_nSCH_2CH_2SiMe_3$ with n = 1 (1) and 2 (2), and *x* can be 1 (a) and 2 (b).



Maddalena Pizzotti, Claudia Zucchi, Angiola Chiesi-Villa, Roland Boese, Gyula Pályi

J. Organomet. Chem. 690 (2005) 4740

Surface organometallic chemistry: Facile μ_2 carbene to μ_3 -carbyne transformation of organocobalt carbonyls on silica surface μ_2 -[ROC(O)C(R)]- μ_2 -(CO)Co₂(CO)₅ (R = Me, *i*Pr, *t*Bu, Ph) bridging carbene-type dinuclear cobalt carbonyls (1) undergo a facile surfacemediated clusterification while chromatographed on silica gel, yielding [μ_3 -RC(O)OC]-Co₃(CO)₉ (**2a**) complexes transformed into (μ_3 -RC)Co₃(CO)₉ (**2b**) derivatives by silicamediated decarboxylation.



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Vladimir I. Meshcheryakov, Peter S. Kitaev, Konstantin A. Lyssenko, Zoya A. Starikova, Pavel V. Petrovskii, Zbyněk Janoušek, Maddalena Corsini, Franco Laschi, Piero Zanello, Alexander R. Kudinov

J. Organomet. Chem. 690 (2005) 4745

(Tetramethylcyclobutadiene)cobalt complexes with monoanionic carborane ligands [9-L-7,8- $C_2B_9H_{10}$]⁻ (L = SMe₂, NMe₃ and py)

Simple procedures for the preparation of *nido*-carboranes 9-SMe₂-7,8-R₂-7,8-C₂B₉H₉ (R = H, Me), 9-NMe₃-7,8-C₂B₉H₁₁ and 9-NC₅H₅-7,8-C₂B₉H₁₁ were developed. Their deprotonation with NaH affords sodium salts of the carborane monoanions [9-L-7,8-R₂-7,8-C₂B₉H₈]⁻, which react further with Cb*Co-(CO)₂I or [Cb*Co(MeCN)₃]⁺ (Cb* = C₄Me₄) to give complexes Cb*Co(η -9-L-7,8-R₂-7,8-C₂B₉H₈). The structures of three compounds were investigated by X-ray diffraction. Electrochemistry of the cobalt complexes was studied.



Mohammad G. Assadi, Mehrdad Mahkam, Zohreh Tajrezaiy

J. Organomet. Chem. 690 (2005) 4755

Synthesis and characterization of some organosilicon derivatives of poly 2-hydroxyethyl methacrylate with cubane as a cross-linking agent

Silyl monomer of 2-hydroxyethyl methacrylate was synthesized. Free radical copolymerization and cross-linking copolymerization of resulting monomers with HEMA were done. Cubane-1,4-dicarboxylic acid linked to two HEMA groups is the cross-linking agent. The effects of silyl groups in polymers were studied.

Reza Ghiasi

J. Organomet. Chem. 690 (2005) 4761

A computational study of the arsabenzenes: Structure, properties and aromaticity The structure and properties of the arsabenzenes series have been investigated using B3LYP theory. Measures of aromatic character derived from structure, molecular orbital and chemical shift. Energetic criteria suggest that As123, As12 and As1234 enjoy conspicuous stabilization. By magnetic criteria, these systems are among the least aromatic. As13, As135, and As1235 isomers are the most aromatic using magnetic criteria.

 C_6H_6

C_i, Asl

C_s As As13

C_s As12

As 123

C_{2s} II

As1234

As14

As135

As As

As1245

Roberto Della Pergola, Luigi Garlaschelli, Mario Manassero, Mirella Sansoni, Annalisa Sironi, Donatella Strumolo

J. Organomet. Chem. 690 (2005) 4768

C–H and C–C bonds activation by iridium clusters: Synthesis and solid state structure of $[Ir_6(CO)_{14}(\mu_3-\eta^1:\eta^2:\eta^1-C_7H_8)]$

The reaction between norbornene (C_7H_{10}) and $Ir_6(CO)_{16}$ in refluxing toluene yields the substituted cluster [$Ir_6(CO)_{14}(C_7H_8)$]. To be coordinated to the metal centers, the two vinylic carbon atoms lose two hydrogen atoms via a double oxidative addition of its C–H bonds, followed by elimination of a hydrogen molecule from the cluster. As a result, the C_7H_8 fragment is coordinated through a 1,2-vinylidene unit. In accordance, the bonding parameters of the Ir₃C₂ unit closely match those found in other alkyne-substituted complexes.



M. Assunta Girasolo, Clelia Di Salvo, Domenico Schillaci, Giampaolo Barone, Arturo Silvestri, Giuseppe Ruisi

J. Organomet. Chem. 690 (2005) 4773

Synthesis, characterization, and in vitro antimicrobial activity of organotin(IV) complexes with triazolo-pyrimidine ligands containing exocyclic oxygen atoms Organotin(IV) derivatives of oxo-substituted triazolopyrimidines were synthesized and spectroscopically characterized. The complexes adopt polymeric structures with organotin moieties bridged by anionic ligands. Antimicrobial activity tests evidenced interesting antifungal and antibiofilm properties for *n*-Bu₃Sn(HtpO₂).



Samuel W. Coghlan, Richard L. Giles, Judith A.K. Howard, Leonard G.F. Patrick, Michael R. Probert, Gillian E. Smith, Andrew Whiting

J. Organomet. Chem. 690 (2005) 4784

Synthesis and structure of potential Lewis acid–Lewis base bifunctional catalysts: 2-*N*,*N*-Diisopropylaminophenylboronate derivatives

Directed *ortho*-metallation is used to introduce a boron function into *N*,*N*-diisopropylbenzamide, resulting in the formation of both borinate and boronate derivatives. *N*,*N*-Diisopropylbenzamide *ortho*-boronate pinacol ester can be reduced with sodium borohydride– TMSC1 resulting in *N*,*N*-diisopropylbenzylamino *ortho*-boronic acid; X-ray crystallography and ¹¹B NMR shows that the hindered isopropylamino groups are sufficient to prevent B–N intramolecular coordination, which contrasts with *N*,*N*-dimethylbenzylamino *ortho*-boronic acid.



Chungkyun Kim, Hyeseon Kim, Kyungrae Park

J. Organomet. Chem. 690 (2005) 4794

Preparation and Diels-Alder reaction of carbosilane dendrimer with conjugated diene

The carbosilane dendrimers with 12, 36, 108 and 324 diene groups on the periphery have been prepared. The first generation with 12 diene groups which react with enes such as *N*ethylmaleimide, 1,4-naphtoquinone, and tetracyanoethene has produced the Diels–Alder products (DA) on the dendritic periphery.





José A. Fernandes, Sérgio Lima, Susana S. Braga, Paulo Ribeiro-Claro, José E. Rodriguez-Borges, Cátia Teixeira, Martyn Pillinger, José J.C. Teixeira-Dias, Isabel S. Gonçalves

J. Organomet. Chem. 690 (2005) 4801

Inclusion complex formation of diferrocenyldimethylsilane with β -cyclodextrin Inclusion complex formation of diferrocenyldimethylsilane with β -cyclodextrin (β -CD) was studied experimentally (in the solid state by powder X-ray diffraction, thermogravimetric analysis and MAS NMR spectroscopy) and theoretically (by ab initio calculations in vacuo). The results are consistent with the formation of an inclusion compound with an overall host:guest molar ratio of 1.5 and channel-type packing of β -CD molecules.



Katsunori Nishide, Hongze Liang, Shigekazu Ito, Masaaki Yoshifuji

J. Organomet. Chem. 690 (2005) 4809

Preparation and properties of palladium(II) complexes of 3-oxo-1-(2,4,6-tri-*t*-butyl- phenyl)-1,3-diphosphapropenes

Kinetically stabilized 3-oxo-1,3-diphosphapropenes were prepared and used as P, O-unsymmetrical bidentate ligands of dichloropalladium(II) complexes. The chelate complexes were characterized and the catalytic activity for some cross-coupling reactions was investigated.



$$\begin{split} \mathsf{Mes}^* &= 2,4,6\text{-}t\text{-}\mathsf{Bu}_3\mathsf{C}_6\mathsf{H}_2\\ \mathsf{R} &= \mathsf{Ph},\, p\text{-}\mathsf{MeC}_6\mathsf{H}_4,\, p\text{-}\mathsf{MeOC}_6\mathsf{H}_4,\, n\text{-}\mathsf{Bu} \end{split}$$

Jahar lal Pratihar, Debprasad Patra, Surajit Chattopadhyay

J. Organomet. Chem. 690 (2005) 4816

Syntheses, characterization, structure and redox properties of new Rh(III) cyclo-metallates incorporating azoimine ligands

Reaction of 2-(arylazo) aniline, HL-NH₂, with Wilkinson's catalyst afforded the new orthometallated complexes of Rh(III) upon oxidative addition. This has relevance with the C–H bond activation in azo compounds by Wilkinson's catalyst. The electron transfer process of the new Rh(III) cyclometallates have been examined.

 $\begin{array}{c} & \overset{H}{\underset{N \longrightarrow N}{\longrightarrow}} R \overset{Rh(PPh_{1}),Cl}{\underset{N \longrightarrow N}{\longrightarrow}} & \overset{H}{\underset{N \longrightarrow N}{\longrightarrow}} R \overset{PPh_{2}}{\underset{N \longrightarrow N}{\longrightarrow}} R \overset{Cl}{\underset{N \longrightarrow N}{\longrightarrow}} R \overset{PPh_{2}}{\underset{N \longrightarrow N}{\longrightarrow}} R \overset{PPh_{$

Jean-Pierre Djukic, André de Cian, Nathalie Kyritsakas Gruber

J. Organomet. Chem. 690 (2005) 4822

Unprecedented ligand anti-bis-benzylation upon thermolytic treatment of 2,3-diphenylbenzo[g]quinoxaline with (η^1 -benzyl) pentacarbonylmanganese The treatment of 2,3-diphenylbenzo[g]quinoxaline with $PhCH_2Mn(CO)_5$ in boiling *n*-heptane affords significant amounts of a biscyclomanganated 5,10-anti-bis-benzylation product, which structure was assessed by X-ray diffraction analysis.



Rosa Fandos, Carolina Hernández, Antonio Otero, Ana Rodríguez, Maria José Ruiz

J. Organomet. Chem. 690 (2005) 4828

Synthesis and characterization of titanium and tantalum complexes with di(2-pyridyl)amine (dpa): Molecular structures of $Cp*TaCl_3(dpa)$ and $Ti(NMe_2)_2(dpa)_2$

New titanium and tantalum complexes with the assisted amide ligand dpa (di(2-pyridyl)-amide) have been synthesized.



C. Croix, A. Balland-Longeau, H. Allouchi, M. Giorgi, A. Duchêne, J. Thibonnet

J. Organomet. Chem. 690 (2005) 4835

Organogold(I) complexes: Synthesis, X-ray crystal structures and aurophilicity

The synthesis of RAuPPh₃ (R = aryl) from ClAuPPh₃ and Grignard RM reagents (M = Li or MgX) is described. New (vinylphenyl)gold(I) and other arylgold(I) complexes were characterized by ¹H, ¹³C, ³¹P, ¹⁹F NMR, melting point determination, and X-ray diffraction. Crystallographic studies of some organogold(I) complexes indicate an aurophilic Au(I)...Au(I) attraction.



Lucia Calucci, Ulli Englert, Guido Pampaloni, Calogero Pinzino, Manuel Volpe

J. Organomet. Chem. 690 (2005) 4844

Reactivity of $bis(\eta^6$ -arene) derivatives of titanium, vanadium and niobium with fulvenes bearing electron-withdrawing substituents

The reaction of $M(\eta^6\text{-arene})_2$ (M = Ti, V, Nb; arene = MeC_6H_5 or 1,3,5-Me₃C₆H₃) with "pentacarbomethoxycyclopentadiene" (pcmcpH), 1-benzoyl-6-hydroxy-6-phenyl fulvene, and 1-benzoyl-3-nitro-6-hydroxy-6-phenyl fulvene proceeds with evolution of dihydrogen and oxidation of the metal to coordination compounds containing *O*,*O*'-coordinated cyclopentadienyl anions. The reactivity of the arene derivatives of Groups 4 and 5 is compared to that of the corresponding chromium and molybdenum derivatives.



Marina Gay, Angel M. Montaña, Virtudes Moreno, Mercè Font-Bardia, Xavier Solans

J. Organomet. Chem. 690 (2005) 4856

Synthesis and structure of new trichloroplatinum π -complexes: Reactivity of nitrogen lone-pair versus C–C double bond π -electrons in ligands, effect of steric hindrance Two trichloroplatinum π -complexes and a diammonium tetrachloroplatinate (II) salt have been unexpectedly isolated during the attempt of the synthesis of the corresponding cisplatinum square-planar complexes of tertiary cyclohexene diamines. This could be explained as due to the higher availability of the π -electrons of C=C double bond than the electron lone pairs of nitrogen atoms from the tertiary amino groups.



F. Micoli, L. Salvi, A. Salvini, P. Frediani, C. Giannelli

J. Organomet. Chem. 690 (2005) 4867

Mononuclear ruthenium complexes containing two different phosphines in *trans* position: I. Synthesis and spectroscopic characterization Mononuclear ruthenium complexes $Ru(CO)_2$ -(Y)(Y')(PⁿBu₃)[P(p-XC₆H₄)₃] (Y, Y' = H, CH₃COO; X = CH₃O, CH₃, H, F, Cl), containing a PⁿBu₃ in *trans* position to a triarylphosphinic ligand were synthesized and spectroscopically characterized. The presence of two different phosphines seems an interesting model to study the "*trans* effect" for octahedral species.



Mahammad Ali, Sumana Gangopadhyay, Md. Mijanuddin

J. Organomet. Chem. 690 (2005) 4878

Transition metal carbene chemistry 5: Kinetic studies on the nucleophilic substitution reactions of $(CO)_5M=C-(SCH_3)CH_3$ (M = Cr and W) with primary amines in aqueous acetonitrile

A kinetic study of the aminolysis of M–S (M = Cr and W) with primary aliphatic amines in 50% MeCN–50% H₂O (v/v) at 25 °C is reported. The reactions proceed in a step-wise fashion with $\beta_{nuc}(k_1) 0.31 \pm 0.02$ and 0.29 ± 0.02 for Cr–S and W–S, respectively.



Fausto Calderazzo, Francesco Masi, Guido Pampaloni, Vincenzo Passarelli, Roberto Santi, Anna Sommazzi, Silvia Spera, Francesca Tumminia

J. Organomet. Chem. 690 (2005) 4886

Perfluorofluorenyl anions and their use as co-catalysts in the zirconocene-promoted polymerization of olefins 1,2,3,4,5,6,7,8-Octafluoro-9-(pentafluorophenyl)-9H-fluorene, $C_{19}HF_{13}$, is deprotonated by NaH, LiR in polar solvents to the $[C_{19}F_{13}]^$ anion. By reaction with [*rac*-ethylene-bis(η^5 -4,5,6,7-tetrahydroindenyl)](diallyl)zirconium-(IV) an ethylene-polymerization catalytic precursor is obtained.



Jorge Bravo, Jesús Castro, Soledad García-Fontán, Manuel Iglesias, Pilar Rodríguez-Seoane

J. Organomet. Chem. 690 (2005) 4899

Preparation and characterization of chloroand polyhydride complexes of rhenium: Variable-temperature NMR spectroscopy and protonation studies The rhenium complexes *fac*-[ReOCl₃L] [1; L = 1,3-bis(diphenylphosphanyloxy)propane], [ReOCl₂(OEt)L] (2), and *mer*-[ReCl₃LL'] [3; L' = P(OEt)₃ in **3a**, PPh(OEt)₂ in **3b**, PPh₂(OEt) in **3c**] were prepared. Reaction of complexes **1** and **3a–c** with excess NaBH₄ gave [ReH₇L] (4) and [ReH₅LL'] (**5a–c**), respectively. Protonation of these polyhydrides with HBF₄ · OMe₂ yields cationic polyhydride complexes characterized as non-classical species.



Richard L. Cordiner, David Albesa-Jové, Rachel L. Roberts, Julian D. Farmer, Horst Puschmann, Deborah Corcoran, Andrés E. Goeta, Judith A.K. Howard, Paul J. Low

J. Organomet. Chem. 690 (2005) 4908

Syntheses and molecular structures of group 8 benzonitrile complexes

The molecular structures of eight nitrile complexes of general form $[M(NCC_6H_4R-4)(L_2)Cp']PF_6$ $[M = Fe, Ru; L_2 = dppe, (PPh_3)_2; Cp' = Cp, Cp^*]$ are reported and discussed in terms of the nature of the M–N interaction. Data are consistent with a predominantly σ -interaction, similar to that found in related acetylide complexes, with little evidence for metal to nitrile π -back bonding interactions.



Chao-Yu Wang, Duan-Ming Tan, Kin Shing Chan, Yi-Hong Liu, Shei-Ming Peng, Shiuh-Tzung Liu

J. Organomet. Chem. 690 (2005) 4920

Copolymerization of olefins and CO catalyzed by new chiral arsine–oxazoline palladium complexes Chiral arsine–oxazoline palladium complex mediates the insertion of CO and olefins leading to the chiral copolymers.



Liping Ma, Jie Zhang, Ruifang Cai, Zhenxia Chen, Linhong Weng, Xigeng Zhou

J. Organomet. Chem. 690 (2005) 4926

Synthesis and reactivity of organolanthanide complexes containing phenothiazine ligand toward carbodiimide and isothiocyanate

Four new organolanthanide phenothiazine complexes were synthesized, and their reactivities toward carbodiimide or isothiocyanate were investigated, indicating that carbodiimide or isothiocyanate readily mono-inserts into the lanthanide–nitrogen bonds to give the corresponding insertion products. All the reactions provide an alternative synthetic strategy for the modification of the phenothiazine ligand.

Soh-Keang Loh, Geok-Kheng Tan, Lip Lin Koh, S. Selvaratnam, Pak-Hing Leung

J. Organomet. Chem. 690 (2005) 4933

Organopalladium complex promoted asymmetric synthesis of a P-chiral phosphanorbornene in ionic liquids and in organic solvents The organopalladium complex bearing the (*S*)ortho-palladated (1-(dimethylamino)-ethyl)naphthylalene successfully promoted the asymmetric *endo*-cycloaddition reaction between coordinated 3,4-dimethyl-1-phenylphosphole and acrolein to give complex **2** in both ionic liquid and organic solvent.



Fredrick Erdman III, Daniel B. Lawson

J. Organomet. Chem. 690 (2005) 4939

The aromaticity of tungstenacyclobutadiene, Cl₃W(–ButC–CMe–CMe–): A DFT/NICS study

B3LYP and MP2 are used to investigate the geometry and aromaticity of tungstenacyclobutadiene, W[C-t-BuCMeCMe]Cl₃. Nucleusindependent chemical shift is used as an index of aromaticity for this experimentally observed metallacyclobutadiene. Additionally, charge effects are explored by characterizing the aromaticity of the tungstenacyclobutadiene fragment ions, WC₃H₃⁺³ and WC₃H₃⁺¹. CMO-NICS analysis provides the contribution of each B3LYP orbital to the aromaticity and allows differentiation between orbitals of σ and π symmetries.



Sandra Bolaño, Jorge Bravo, Jesús Castro, Soledad García-Fontán, M^a Carmen Marín, Pilar Rodríguez-Seoane

J. Organomet. Chem. 690 (2005) 4945

New bromo-, triflato-, and hydridotricarbonylrhenium(I) complexes with diphosphinite ligands: Structural, spectral and protonation studies of various hydrides The synthesis and characterization of different bromo-, triflato- and hydridocarbonyl rhenium(I) complexes bearing diphosphinite ligands L [L = Ph₂PO(CH₂)₃OPPh₂ (L¹), ⁱPr₂PO-(CH₂)₂OPⁱPr₂ (L²), Cy₂PO(CH₂)₂OPCy₂ (L³)] are described. The structures of three bromoand three hydrido complexes are established by X-ray crystallography.



Christopher Imrie, Elago R.T. Elago, Nadia Williams, Cedric W. McCleland, Pieter Engelbrecht

J. Organomet. Chem. 690 (2005) 4959

Synthesis of ferrocenoate esters, amides and other ferrocenoyl derivatives using ferrocenoyl fluoride. A comparison of the reactions of ferrocenoyl fluoride in [bmim][BF₄] with the microwave-promoted solvent-free reactions of ferrocenoyl fluoride Simple, efficient and convenient routes for the synthesis of ferrocenoyl derivatives are described. They involve either the reaction of nucleophilic compounds and DMAP with ferrocenoyl fluoride in $[bmim][BF_4]$ or the solvent-free reactions of nucleophilic compounds with ferrocenoyl fluoride promoted by microwaves.



Michael G.S. Londesborough, Michael J. Carr, John D. Kennedy

J. Organomet. Chem. 690 (2005) 4967

An interesting metallacarborane cage closure and dismantling reaction including the facile halogenation of a cluster carbon atom: Structure of $[1,2-(\eta^5-C_5Me_5)_2-\mu-1,2-H-closo-1,2,3-Rh_2CB_4H_4-3-I]$

With an approximately molar equivalent of iodine and excess of triethylamine $[2,5-(\eta^5-C_5Me_5)_2-10-Me-\mu-2,5-H-nido-2,5,1-Rh_2CB_6H_8]$ expels two boron cluster vertices and undergoes a cage-closure reaction, resulting in the formation of a seven-vertex *closo* species of constitution $[1,2-(\eta^5-C_5Me_5)_2-\mu-1,2-H-closo-1,2,3-Rh_2CB_4H_4-3-I]$ (see figure), isolatable in good yield (79%).



William Henderson, Brian K. Nicholson, Alistair L. Wilkins

J. Organomet. Chem. 690 (2005) 4971

Facile syntheses of four-membered aurathietane dioxide [Au–CHR-SO₂-CHR] ring systems, and the first isonitrile insertion reaction into a gold(III)–carbon bond A series of complexes containing the Au-CHR-SO₂-CHR [R = C(O)Ph or CN] ring system have been synthesised from the parent gold-(III) dichloride complexes (which contain cyclo-aurated amine or pyridine ligands), by reaction with the sulfone RCH₂SO₂CH₂R (R = COPh or CN) and Me₃N base. The insertion reaction of one complex with *t*butylisonitrile is described.



Notes

Mannar R. Maurya, L. Keith Woo

J. Organomet. Chem. 690 (2005) 4978

Metalloporphyrin as a ligand in organometallic complexes: Synthesis and characterization of a nickel(II) porphyrin complex of 1,5-cyclooctadienedichlo- roruthenium(II) A method for the synthesis of dinuclear metal complexes has been developed which utilizes the multichelating porphyrin ligand, α, α -5,15bis(*o*-nicotinoylphenyl)-2,8,12,18-tetraethyl-3, 7,13,17-tetramethylporphyrin, H₂[DPE](py)₂-(di[*o*-nicotinoylphenyl]etioporphyrin). The versatility of this ligand is demonstrated by fabricating a heterobimetallic complexes, [Ni(DPE)(py₂)]Ru(COD)Cl₂, composed of a porphyrin coordination complex linked to an organometallic fragment.

N. Faux, B. Caro, F. Robin-Le Guen, P. Le Poul, K. Nakatani, E. Ishow

J. Organomet. Chem. 690 (2005) 4982

 γ -Methylene chalcogenapyrans and benzopyrans as proaromatic donors in "push–pull" Fischer type carbene complexes: Influences of chalcogen atom and chain length on the electronic and N.L.O. properties of these molecules N.L.O. properties of a new class of "push– pull" Fischer type carbene complexes bearing γ -methylene chalcogenapyran and benzopyran nucleus as proaromatic donors have been investigated. The influence of the unsaturated chain length, of the presence of the fused aromatic ring and of the chalcogen atom on the first hyperpolarizability values are shown. H₃CO W(CO)₅ X = 0, S, TeR'' n'' = 3, X = 0, R = Ph, R' = Ph, R'' = H $\mu\beta = 2894 \ 10^{-48} \text{ esu}$

Ashfaq A. Bengali

J. Organomet. Chem. 690 (2005) 4989

Displacement of the heptane solvent from $(\eta^5-C_5H_5)Re(CO)_2$ (heptane): A flash photolysis study using infrared detection

Substitution of the heptane solvent molecule from $(\eta^5-C_5H_5)Re(CO)_2(heptane)$ by several ligands, L, has been studied using time resolved infrared spectroscopy. The displacement reaction appears to proceeds through an I_d mechanism and the activation parameters suggest a lower limit of 57.3 ± 0.9 kJ/mol for the strength of the Re–heptane interaction.





Guanmin Wu, David R. Glass, Daniel May, William H. Watson, David Wiedenfeld, Michael G. Richmond

J. Organomet. Chem. 690 (2005) 4993

Reaction of 2,3-bis(methylthio)pyrrolo[1,2*a*lbenzimidazol-1-one with BrRe(CO)₃-(THF)2: X-ray diffraction structure, redox chemistry, and luminescence behavior of fac-BrRe(CO)₃{N,S-2,3-bis(methylthio)pyrrolo-[1,2-*a*]benzimidazol-1-one}

The ligand substitution chemistry of the heterocyclic ligand 2,3-bis(methylthio)pyrrolo[1, 2-a]benzimidazol-1-one with fac-BrRe(CO)3-(THF)₂ has been examined and found to give fac-BrRe(CO)₃(N,S-heterocycle). The new rhenium(I) compound has been isolated and characterized in solution by IR and NMR spectroscopies, and the chelation of the heterocycle to the rhenium center through the nitrogen and 3-methylthio groups was established by X-ray crystallography. The redox properties, MO data, and photophysical behavior of fac- $BrRe(CO)_3(N,S-heterocycle)$ are reported.



Holger Braunschweig, Frank M. Breitling, Krzysztof Radacki, Fabian Seeler

J. Organomet. Chem. 690 (2005) 5000

Synthesis and molecular structure of boronbridged constrained geometry complexes of zirconium and hafnium

In the present paper, we report the synthesis of the first boron-bridged constrained geometry complexes (CGCs) of zirconium and hafnium, which was achieved via amine elimination reaction. The new compounds were fully characterised in solution and by means of Xray diffraction.





Sipra Naskar, Manish Bhattacharjee

J. Organomet. Chem. 690 (2005) 5006

Ruthenium cationic species for transfer hydrogenation of aldehydes: Synthesis and catalytic properties of [(PPh₃)₂Ru(CH₃CN)₃- $Cl]^{+}[A]^{-} \{A = BPh_4 \text{ or } ClO_4\}$ and structure of $[(PPh_3)_2Ru(CH_3CN)_3 - Cl]^+[BPh_4]^-$

have been synthesized, which are found to be effective catalyst for transfer hydrogenation of aldehydes.



5011

5012

R' = H or Alkyl or Ary

Erratum

Erratum

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