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Contents

Communication

SEVIER

Irene Piras, Reiko Jennerjahn, Ralf Jackstell, Wolfgang Baumann, Anke Spannenberg, Robert Franke, Klaus-Diether Wiese, Matthias Beller

J. Organomet. Chem. 695 (2010) 479

Synthesis of novel rhodium phosphite catalysts for efficient and selective isomerization-hydroformylation reactions

New modular bisphosphite ligands have been conveniently synthesized. The corresponding rhodium complexes are highly active catalysts for isomerization-hydroformylation reactions of internal olefins. The active catalysts have been characterized by in situ NMR studies.

,СНО P, H Rh-CO P CO

Regular Papers

Elisabetta Maccaroni, Hailin Dong, Olivier Blacque, Helmut W. Schmalle, Christian M. Frech, Heinz Berke

J. Organomet. Chem. 695 (2010) 487

Water soluble phosphine rhenium complexes

Various water soluble nitrosyl rhenium (I) complexes bearing PTA ligands were prepared. PTA substituted complexes were probed in reactions with olefins, hydride reagents and hydrogen to form hydride complexes. The hydrides were tested for catalytic hydrogenation of olefins.



L = PTA(3), MeCN(4), CH₂CH₂(5a), PhCHCH₂(5b)

 $L = CH_2CH_2(7)$

Kota Thirumala Prasad, Bruno Therrien, Steven Geib, Kollipara Mohan Rao

J. Organomet. Chem. 695 (2010) 495

Mono and dinuclear half-sandwich platinum group metal complexes bearing pyrazolyl-pyrimidine ligands: Syntheses and structural studies

Reactions of η^5 - and η^6 -cyclic hydrocarbons of platinum group metal complexes with pyrazolyl-pyrimidine ligands have resulted in the formation of mono and dinuclear complexes.



 $[{(\eta^6 - p^{-i} PrC_6 H_4 Me) RuCl}_2(L3)](PF_6)_2$

Kazem D. Safa, Yones Mosaei Oskoei

J. Organomet. Chem. 695 (2010) 505

Functionalisation of the upper rim of calix[4]arene via alcoholysis and hydro-silylation reactions

Metalation of calixarene 1 with *n*-BuLi in THF at -78 °C gave organolithium reagent, which reacted with Me₂HSiCl to give calixarene 2. The Si–H groups of calixarene 2 were treated with various alcohols in the presence of Karstedt catalyst to give the corresponding calixarene 3. Calixarene 2 was functionalized with a variety of alkenes using Karstedt catalyst to give the corresponding organosilylated calixarene 4.



Kamlesh Kumar, Sarvendra Kumar, B.D. Gupta

J. Organomet. Chem. 695 (2010) 512

Weak interactions between furfuryl and equatorial dioxime ligand in furfuryl(O₂)-Co(dmgH)₂Py: NMR, X-ray and DFT calculations

The crystal and molecular structure of furfuryl(O₂)Co(dmgH)₂Py (1) has been determined by X-ray diffraction analysis. The furfuryl ring oxygen in 1 is pointing inwards and is very close to one of the dmgH (Me) (2.625 Å) and shows unusual C-H…O weak interaction. This is responsible for the observed 1:3 ratio of dmgH methyl protons in NMR spectrum. These observations have also been confirmed by DFT level calculations.



Claude H. Yoder, Allison K. Griffith, Alaina S. DeToma, Cameron J. Gettel, Charles D. Schaeffer Jr.

J. Organomet. Chem. 695 (2010) 518

Hypercoordination in triphenyl oxinates of the group 14 elements

The Group 14 triphenyl oxinates show 5coordinate structures for tin and lead with two fluxional geometric isomers. The silicon and germanium analogs are 4-coordinate. These conclusions, derived from multinuclear NMR studies, are corroborated by DFT modeling.



Xiu-Hui Lu, Xin Che, Jun-Feng Han, Le-Yi Shi, Zhen-Xia Lian

J. Organomet. Chem. 695 (2010) 524

Ab initio study of mechanism of forming germanic bis-heterocyclic compound between germylene carbene (H₂Ge=C:) and acetone

The potential energy surface for the cycloaddition reactions between germylene carbene and acetone with CCSD (T)//MP2/ $6-31G^*$ method. On the basis of the potential energy surface, we can predict reaction (5) [namely: $R1 + R2 \rightarrow INT4^{+R2}$ INT5 $\stackrel{TS5}{\longrightarrow}$ P5P] is dominant reaction pathways of the cycloadditional reaction of forming germanic bis-heterocyclic compound between singlet germylene carbene and acetone.



Andrey I. Poddel'sky, Ivan V. Smolyaninov, Nikolay V. Somov, Nadezhda T. Berberova, Vladimir K. Cherkasov, Gleb A. Abakumov

J. Organomet. Chem. 695 (2010) 530

Antimony(V) catecholato complexes based on 4,5-dialkylsubstituted *o*-benzoquinone. The spectroscopic and electrochemical studies. Crystal structure of $[Ph_4Sb]^+$ - $[Ph_2Sb(4,5-Cat)_2]^-$ New triphenyl- (1) and triethylantimony(V) (2) catecholates R₃Sb(Cat) based on 4,5-(1,1,4,4-tetramethyl-butane-1,4-diyl)-o-benzoquinone have been prepared and characterin details. Triphenylantimony(V) ized catecholate transforms to ionic complex $[Ph_4Sb]^+[Ph_2Sb(4,5-Cat)_2]^-$ (3) in polar solvents. Molecular structure of [Ph₄Sb]⁺-[Ph₂Sb(4,5-Cat)₂]⁻ was confirmed by X-ray analysis. Cyclic voltammometry of 1 and 3 shows that both complexes undergo reversible one-electron oxidation to quite stable osemiquinonato cationic [Ph₃Sb(4,5-SQ)]⁺ and neutral [Ph₂Sb(4,5-SQ)(4,5-Cat)] species which were also detected by EPR spectroscopy.

of $[Ph_4Sb]^+$ med by X-ray ry of 1 and 3 ndergo reversiquite stable *o* $o(4,5-SQ)]^+$ and Cat)] species *v* EPR spectro-

Lucie Červenková Šťastná, Jan Čermák, Petra Cuřínová, Jan Sýkora

J. Organomet. Chem. 695 (2010) 537

Synthesis and fluxional behaviour of new "heavy fluorous" cyclopentadienes

The synthesis and fluxional behaviour of new "heavy fluorous" cyclopentadienes, substituted with three and six ponytails, is reported. Special emphasis is placed on the assignment of individual isomers and their interconversion.

isomers and

Giuseppe Ruisi, Loredana Canfora, Giuseppe Bruno, Archimede Rotondo, Teresa F. Mastropietro, Eugenio A. Debbia, Maria A. Girasolo, Bartolomeo Megna

J. Organomet. Chem. 695 (2010) 546

Triorganotin(IV) derivatives of 7-amino-2-(methylthio)[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylic acid. Synthesis, spectroscopic characterization, in vitro antimicrobial activity and X-ray crystallography

Xiangai Yuan, Siwei Bi, Yangjun Ding, Lingjun Liu, Min Sun, Dongdong Dong

J. Organomet. Chem. 695 (2010) 552

A DFT study on the effect of hydrogen bonding on the reaction of a $\mu\text{-benzo-quinone}$ diruthenium complex with acetylene

Triorganotin(IV) complexes of the 7-amino-2-(methylthio)[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxylic acid (HL), Me₃SnL(H₂O), (1), [*n*-Bu₃SnL]₂(H₂O), (2), Ph₃SnL(MeOH), (3), were synthesized and characterized by elemental analysis, ¹H, ¹³C and ¹¹⁹Sn NMR, IR, Raman and ¹¹⁹Sn Mössbauer spectroscopic techniques. Single crystal X-ray diffraction data are reported for compounds (2) and (3). Antimicrobial tests are reported for compounds (1) and (2).



The mechanisms and the effect of hydrogen bonding on the reaction of a μ -benzoquinone diruthenium complex with acetylene were studied with the help of DFT.



Susana Quintal, M. Concepción Gimeno, Antonio Laguna, Maria José Calhorda

J. Organomet. Chem. 695 (2010) 558

Silver(I) and copper(I) complexes with ferrocenyl ligands bearing imidazole or pyridyl substituents

Ferrocenyl derivatives containing an imidazole or pyridine nitrogen atom react with AgPF₆, AgOTf, or $[Cu(NCCH_3)_4]PF_6$, leading to new polynuclear complexes. The triflate counter ion appears to contribute to the formation of weak Ag \cdots Ag interactions in the solid, which are not observed with PF₆.



Ashish Kumar Singh, Prashant Kumar, Mahendra Yadav, Daya Shankar Pandey

J. Organomet. Chem. 695 (2010) 567

Synthesis, characterisation and theoretical studies on some *piano-stool* ruthenium and rhodium complexes containing substituted phenyl imidazole ligands

Present work deals with the synthesis, spectral and structural characterisation of a series of mononuclear complexes containing the $(\eta^6\text{-arene})Ru\text{-}$ and $(\eta^5\text{-}C_5Me_5)Rh\text{-}$ moieties and imidazole based ligands. The resulting complexes have been characterised by elemental analyses and various spectral studies. Crystal structure of the representative complex [$(\eta^5\text{-}C_5Me_5)\text{-}RhCl_2(NOPI)$] has been determined crystal-lographically.



Gabriele Albertin, Stefano Antoniutti, Jesús Castro

J. Organomet. Chem. 695 (2010) 574

The reaction of organic azide ArCH₂N₃ with the half-sandwich complexes of ruthenium and osmium $MCl_2(\eta^6-p-cymene)(PR_3)$, leading to imine derivatives $[MCl(\eta^6-p-cymene)\{h^1-NH=C(H)Ar\}-(PR_3)]BPh_4$ (PR₃ = phosphite), is described. Benzophenone-imine complexes $[MCl(\eta^6-p-cymene)-\{h^1-NH=CPh_2\}(PR_3)]BPh_4$ are also reported.



Jinliang Liu, Bing Yan

J. Organomet. Chem. 695 (2010) 580

Rare-earth (Eu³⁺, Tb³⁺) hybrids through amide bridge: Chemically bonded selfassembly and photophysical properties This work focuses on the construction of a series of chemically bonded rare-earth/ inorganic/organic hybrid materials using TCH–Si as an organic bridge molecule that can both coordinate to rare-earth ions (Eu³⁺ and Tb³⁺) and form an inorganic Si– O–Si network with tetraethoxysilane (TEOS) after cohydrolysis and copolycondensation through a sol–gel process.



Longjin Li, Wei Zhou, Guozheng Zhang, Zhen Pang

J. Organomet. Chem. 695 (2010) 588

Chelate ring closing and opening behavior in cyclopentadienyl cobalt(III) complexes with pendant nitrogen functional group Chelate ring closing and opening process of diiodomonocarbonyl cyclopentadienyl cobalt(III) complexes bearing pendant Nfunctional group is studied. The rate of chelation is determined by electronic density on the donor atom and the strength of forming chelated bond via associative pathway while chelate ring opening is via dissociative pathway.



Kirill Nikitin, Yannick Ortin, Helge Müller-Bunz, Marie-Aude Plamont, Gérard Jaouen, Anne Vessières, Michael J. McGlinchey

J. Organomet. Chem. 695 (2010) 595

Organometallic SERMs (selective estrogen receptor modulators): Cobaltifens, the (cyclobutadiene)cobalt analogues of hydroxytamoxifen A novel organometallic cobalt sandwich analogue of tamoxifen demonstrates antiproliferative activity in vitro against standard breast cancer cell lines. Unexpectedly, the introduction of a second dialkylaminoalkyl chain at the other oxygen markedly enhances the effect.



M. Assunta Girasolo, Simona Rubino, Patrizia Portanova, Giuseppe Calvaruso, Giuseppe Ruisi, Giancarlo Stocco

J. Organomet. Chem. 695 (2010) 609

New organotin(IV) complexes with L-Arginine, N_{α} -t-Boc-L-Arginine and L-Alanyl-L-Arginine: Synthesis, structural investigations and cytotoxic activity

A wide array of organotin(IV) derivatives of L-Arg, Boc–Arg–OH and L-Ala-L-Arg was obtained by direct reaction of organotins with aminoacids and dipeptide. The structural characterization was accomplished by use of FT-IR, Mössbauer in the solid state and by ¹H, ¹³C, ¹¹⁹Sn and ¹H–¹H COSY NMR spectroscopy. In vitro cytotoxic activities against HT29 cells are also reported.

 $\begin{array}{l} R_{1}SnO+H_{2}Ala_{2}Arg\rightarrow R_{3}Sn(Ala_{4}Arg)+H_{2}O \end{array}$



Michael I. Bruce, Alexandre Burgun, Christian R. Parker, Brian W. Skelton

J. Organomet. Chem. 695 (2010) 619

Some ruthenium complexes of fluorinated alkynylcyclopentenes

Reactions between 1,2-dichlorohexafluorocyclopentene and Ru(C \equiv CH)(dppe)Cp* or Ru(C \equiv CC \equiv CLi)(dppe)Cp* have given Ru(C \equiv C-c-C₅F₆Cl-2)(dppe)Cp* 4 and Ru(C \equiv CC \equiv Cc-C₅F₆Cl-2)(dppe)Cp* 7, respectively. Ready hydrolysis of 4 to Ru{C \equiv C[c-C₅F₄Cl(O)]}(dppe)Cp* 5 occurs, which can be converted to Ru{C \equiv C(c-C₅F₄Cl[=C(CN)₂])}(dppe)Cp* 6 by treatment with CH₂(CN)₂/basic alumina. Spectroscopic, electrochemical and XRD structural studies for 4–7 are reported: the cyanated fluorocarbon ligand in 6 is a very powerful electron-withdrawing group.



Notes

Ulrich Siemeling, Frauke Bretthauer, Clemens Bruhn

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Oxidative addition of asparagusic acid based disulfides to Pt^0

[Pt(PPh₃)₄] reacts smoothly and swiftly at room temperature with asparagusic acid and with selected amide and ester derivatives of this cyclic disulfide to afford Pt^{II} dithiolate chelates of the type *cis*-[Pt{CRR'(CH₂S)₂}(PPh₃)₂]. The crystal structures of three such products are reported.



Raji Raveendran, Samudranil Pal

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Ruthenium(II) complexes with 2-(benzylimino-methyl)-4-R-phenol containing the *trans*(PPh₃),*cis*(CO,Cl)-{Ru(PPh₃)₂(CO)Cl}⁺ unit Ru(II) complexes *trans*(PPh₃),*cis*(CO,Cl)-[Ru(^RL)(PPh₃)₂(CO)Cl] (H^RL, 2-(benzylimino-methyl)-4-R-phenol (R = H, Cl, Br and OMe)) are reported. The complexes display a metal centred oxidation. X-ray structures reveal an intramolecular C-H··· π interaction between the *ortho*-C-H of the benzyl group phenyl ring of ^RL⁻ and a phenyl ring of PPh₃.



Gregory J. Grant, Desirée A. Benefield, Donald G. VanDerveer

J. Organomet. Chem. 695 (2010) 634

Antimony–Carbon bond activation in a Pt(II) complex: The crystal structure of $[Pt(9S3)(SbPh_3)(Ph)](PF_6)$ -CH₃NO₂

Cleavage of a phenyl group from a triphenylstibine ligand in a Pt(II) thiacrown complex results in the formation of a σ coordinated phenyl ligand.



Natalia V. Belina, Alexander N. Kornev, Vyacheslav V. Sushev, Georgy K. Fukin, Eugene V. Baranov, Gleb A. Abakumov

J. Organomet. Chem. 695 (2010) 637

The rearrangement of phosphitohydrazide ligand [(ArO)₂P–NPh–NPh–] into iminophosphoranate anion [(PhN=P(OAr)₂–NPh–] {(ArO)₂P = [CH₂(^tBuMeC₆H₂O)₂P]} in coordination sphere of divalent cobalt

The rearrangement of phosphitohydrazide ligand { $(ArO)_2P-NPh-NPh-$ } into iminophosphoranate anion, PhN=P(OAr)_2-NPh-{ $(ArO)_2P = CH_2(6-Bu-4-Me-C_6H_2O)_2P$ }, which takes place in coordination sphere of Co(II), is described.



Erratum



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