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Contents

Communication

Meritxell Casadesus, Michael P. Coogan, Sarah Oakley, Elenna Davies, Li-ling Ooi

J. Organomet. Chem. 691 (2006) 3715

A oxygen-dependent reductive dechlorination of chloroform by (Bisdiphenylphosphinomethane) cobalthexacarbonyl Co₂(CO)₆(dppm) The reduction dechlorination with $Co_2(\mu-dppm)(CO)_6$ requires oxygen for all steps not only for the formation of the phosphine oxide.



Review

Christelle Freund, Marta Abrantes, Fritz E. Kühn

J. Organomet. Chem. 691 (2006) 3718

Monomeric cyclopentadiene molybdenum oxides and their carbonyl precursors as epoxidation catalysts

Monomeric cyclopentadiene molybdenum oxides are receiving increased interest both concerning their preparation and reaction chemistry and with regard to possible catalytic applications. The use of the title compounds as epoxidation catalysts in homogeneous phase and after immobilization has been examined in some detail and is also summarized here.



Regular papers

Tatiana A. Stromnova, Oleg N. Shishilov, Mikhail V. Dayneko, Kirill Yu. Monakhov, Andrei V. Churakov, Ludmila G. Kuz'mina, Judith A.K. Howard

J. Organomet. Chem. 691 (2006) 3730

Palladium(I) carbonyl carboxylate clusters cyclo-[Pd₂(μ -CO)₂(μ -OCOR)₂]_n (n = 2 or 3): Structure and reactivity

The interaction of palladium(+1) cluster $Pd_4(\mu$ -CO)_4(\mu-OAc)_4 with saturated and unsaturated carboxylic acids was studied. It was found, that the substitution of acetates groups on others carboxylates leads to the clusters with different nuclearity. According to X-ray data all clusters possess cyclic planar metal cores with alternate pairs of μ -carbonyl and μ carboxylate ligands.



Achim Hiller, Jörg T. Patt, Jörg Steinbach

J. Organomet. Chem. 691 (2006) 3737

On the reaction of 4-substituted trimethyltin aromatics with perchlorylfluoride

The reactivity of 4-substituted trimethyltin aromatic compounds towards $FCIO_3$ was studied.



Mohammad El-khateeb, Khaled Shawakfeh, Tobias Rüffer, Heinrich Lang

J. Organomet. Chem. 691 (2006) 3743

Monomeric and dimeric ruthenium thiooxalate complexes: Structures of CpRu(PPh_3)_2-SCOCO_2Me and CpRu(dppe)SCOCO_2Et The complexes CpRu(L)(L')SH react with *O*alkyl oxalyl chlorides to form the corresponding *O*-alkylthiooxalate complexes CpRu(L)(L')SCOCO₂R (L = L' = PPh₃ (1), $\frac{1}{2}$ dppe (2); L = PPh₃, L' = CO (3); R = Me (a), Et (b)). The reactions of the hydrosulfido complexes with half equivalent of oxalyl chloride produce [CpRu(L)(L')SCO]₂ (L = L' = PPh₃ (4), $\frac{1}{2}$ dppe (5); L = PPh₃, L' = CO (6)). The crystal structures of CpRu(PPh₃)₂SCOCO₂Me (1a) and CpRu-(dppe)SCOCO₂Et (2b) are reported.



Hayati Türkmen, Bekir Çetinkaya

J. Organomet. Chem. 691 (2006) 3749

1,3-Diarylimidazolidin-2-ylidene (NHC) complexes of Pd(II): Electronic effects on cross-coupling reactions and thermal decompositions The efficiency of A as a C–C coupling catalyst and the thermal behavior of **5** and **6** depends on X and the data indicate that saturated [Pd(NHC)] species are catalytically active species. $\begin{array}{c} \overset{\circ}{\underset{Y=Cl \text{ or }Br}{\longrightarrow}} & \overset{A(1,5,5)}{\underset{Y=Cl \text{ or }Br}{\longrightarrow}} & \overset{\circ}{\underset{Y=Cl \text{ or }Br}{\longrightarrow}} & \overset{\circ}{\underset{Y=Cl \text{ or }Br}{\longrightarrow}} & \overset{\circ}{\underset{Y=Cl \text{ or }Br}{\longrightarrow}} & \overset{\circ}{\underset{Z=H, Me, Br, Cl}{\longrightarrow}} & \overset{\circ}{\underset{Z=H, Me, Mh, Cl}{\longrightarrow}} & \overset{\circ}{\underset{Z=H, Mh, Mh, Cl}{\longrightarrow}} & \overset{\circ}{\underset{Z=H, Mh, Mh, Cl}{\longrightarrow} & \overset{\circ}{\underset{Z=H, Mh, Mh, Cl}{\longrightarrow} & \overset{\circ}{\underset{Z=H, Mh, Mh, Cl}{\longrightarrow} & \overset{}{\underset{Z=H, Mh, Mh, Mh, Mh, Cl}$

A.A. Dakhel, Ahmed Y. Ali-Mohamed

J. Organomet. Chem. 691 (2006) 3760

Characterisation and ac-electrical investigation of sublimated bis(dimethylglyoximato)palladium(II) thin films Bis(dimethylglyoximato)palladium(II) complex of chemical formula $Pd(C_4H_7N_2O_2)_2$ with structure shown bellow, was prepared in form of thin film on p-Si substrate by sublimation method. Samples were characterised by X-ray diffraction and fluorescence. Their dielectric properties were studied as a function of frequency.



Contents

Brandon Quillian, Yuzhong Wang, Pingrong Wei, Adele Handy, Gregory H. Robinson

J. Organomet. Chem. 691 (2006) 3765

2,6-Di(4-*t*-butylphenyl)phenyl-group 13 organometallic compounds Reaction of MX₃ (M = Al, Ga, In; X = Br, Cl) with RLi (R = 2,6-(4-t-BuC₆H₄)₂C₆H₃) affords RGaCl₂ · OEt₂, **1**, RAlBr₂ · OEt₂, **2**, R₂GaCl, **3**, and R₃In, **4**. Compounds **1** and **2** are rare (*m*-terphenyl)MX₂ compounds that do not assume dimeric association, while compound **4** is the first tris(*m*-terphenyl)group 13 compound.



Simon G. Bott, Kaiyuan Yang, Michael G. Richmond

J. Organomet. Chem. 691 (2006) 3771

Regiospecific and sequential P–C bond activation/cluster transformations in the reaction of $PhCCo_2MoCp(CO)_8$ with the diphosphine ligands 2,3-bis(diphenylphosphino)maleic anhydride (bma) and 3,4-bis(diphenylphosphino)-5-methoxy-2(5H)-furanone (bmf)

The tetrahedral cluster $PhCCo_2MoCp(CO)_8$ reacts with the diphosphine ligands 2,3-bis(diphenylphosphino)maleic anhydride (bma)

Lirong Zhang, Kin Shing Chan

J. Organomet. Chem. 691 (2006) 3782

Aliphatic carbon—carbon bond activation of ketones by rhodium(II) porphyrin radical

respectively. Thermolysis of these clusters leads to the formation of the bis(phosphido)-bridged clusters $Co_2MoCp(CO)_4[\eta^3,\eta^1,\eta^1-C(Ph)C=CC(O)O-C(O)](\mu-PPh_2)_2$ and $Co_2MoCp(CO)_4[\eta^3,\eta^1,\eta^1-C(Ph)C=CC(O)OCH(OMe)](\mu-PPh_2)_2$, respectively. The molecular structures of all four products have been established by X-ray crystallography, and the regio- and diastereoselectivity that accompany the activation of the bmf ligand are discussed.

and 3,4-bis(diphenylphosphino)-5-methoxy-2(5H)-

furanone (bmf) to give the phosphido-bridged

clusters Co2MoCp(CO)5[µ2,η2,η1-C(Ph)C=C(PPh2)-

C(O)OC(O)](μ -PPh₂) and Co₂MoCp(CO)₅[μ_2, η^2, η^1 -C(Ph)C=C(PPh₂)C(O)OCH(OMe)](μ -PPh₂),

H MeO///////// Ph Ph Ph Ph Ph Ph Ph Ph

Aliphatic carbon—carbon bond activation of both enolizable and non-enolizable ketones occurred successfully with rhodium(II) porphyrin radical to give rhodium porphyrin alkyls. Rh(tmp)+ ketone ligand benzene 130° C, time

Sumit Bali, Ajai K. Singh, J.E. Drake, M.B. Hursthouse, M.E. Light

J. Organomet. Chem. 691 (2006) 3788

Tellurated heterocycles, 2-[(2-thienyltelluro)methyl]tetrahydrofuran (L^1) and [(2-thienyl telluro)methyl]tetrahydro-2H-pyran (L^2): Synthesis and complexation reactions with Pd(II), Pt(II), Hg(II), Ru(II) and Cu(I). Single crystal structures of [Ru(*p*-cymene)Cl₂(L^1)] and *cis*-[PdCl₂(L^2)₂]

The L^1 and L^2 and complexes $[PdCl_2(L^1)_2]$ (1), $[PtCl_2(L^1)_2]$ (2), $[HgBr_2(L^1)_2]$ (3), [Ru(pcymene)Cl₂(L¹)] (4), [CuBr(L¹)] (5), [PdCl₂(L²)₂] (6), [PtCl₂(L²)₂] (7), [HgBr₂(L²)₂] (8) and [Ru(pcymene)Cl₂(L²)₂] (9) have been synthesized and characterized by ¹H and ¹³C NMR spectra which reveal that in all the complexes L¹ and L² coordinate through Te only. This is corroborated by single crystal structures of 4 and 6. The 4 is a half sandwich compound. The Ru–Te bond length is 2.6340(7) Å. In square planar Pd complex 6 two molecules of ligand L² are *cis* to each other [rarely observed with monodentate telluride ligands]. The Pd–Te bond lengths are 2.538(2) and 2.517(2) Å. The crystal of 6 secondary Te···Cl interactions are noticed. The Pd–Pd distance in 6 is 3.188(3) Å (sum of vander Waal's radii 3.26 Å)





Manoja K. Samantaray, Dipankar Roy, Ahindra Patra, Raji Stephen, Mobin Saikh, Raghavan B. Sunoj, Prasenjit Ghosh

J. Organomet. Chem. 691 (2006) 3797

Experimental and theoretical studies of a silver complex of O-functionalized N-heterocyclic carbene

O-Functionalized N-heterocyclic carbene complex of silver has been synthesized and its structural and electronic properties have been studied. Theoretical calculation suggests that the NHC–Ag interaction is predominantly σ -bonding in nature.



Adriana Ionescu, Markus Ruppel, Ola F. Wendt

J. Organomet. Chem. 691 (2006) 3806

Isomerisation of ω -hydroxyalkenes under hydroxycarbonylation conditions in palladium catalysed aqueous phase systems

 ω -Hydroxyolefins primarily undergo isomerisation through a chain walking mechanism under hydroxycarbonylation conditions in water in the presence of PdCl₂(PhCN)₂ and a water soluble phosphine.



Martial Sanz, Tomás Cuenca, Cinzia Cuomo, Alfonso Grassi

J. Organomet. Chem. 691 (2006) 3816

A zirconium dichloro complex supported by an ancillary stereorigid tetradentate bis(phenoxo-imino) Schiff-base-donor ligand: Evidence for a conformational equilibrium between two solution stereoisomers The synthesis of the bis(phenoxo-imino) zirconium dichloro derivative $ZrCl_2[C_6H_4-1,2-\{N=CH-(3,5-^{T}Bu_2C_6H_2-2-O)\}_2]$ is described. This compound has been spectroscopically characterized as a mixture of the C_{2v} - and C_2 -symmetry derivatives. The interconversion between these two species is observed in toluene and chloroform solution and interpreted as a result of the intramolecular isomerization of the ligand. Thermodynamic and kinetic parameters for the equilibrium between **3a** and **3b** have been determined. The alkylation reaction of the bis(phenoxo-imino) zirconium dichloro complex using various alkylation agents under different reaction conditions has been studied.



Dafa Chen, Bin Mu, Shansheng Xu, Baiquan Wang

J. Organomet. Chem. 691 (2006) 3823

Synthesis and structures of the silyl bridged bis(indenyl) diruthenium complexes and a novel indenyl nonanuclear ruthenium cluster $Ru_9(\mu_6-C)(CO)_{14}(\mu_3-\eta^5;\eta^2;\eta^2-C_9H_7)_2$

The silyl bridged bis(indene) ligands $C_9H_7EC_9H_7$ reacted with $Ru_3(CO)_{12}$ in xylene gave the diruthenium complex $(E)[(\eta^5-C_9H_6)Ru(CO)]_2(\mu-CO)_2$ and the desilylation product. A novel nonanuclear ruthenium cluster $Ru_9(\mu_6\text{-}C)(CO)_{14}(\mu_3\text{-}\eta^5\text{-}\eta^2\text{-}C_9H_7)_2$ was also obtained unexpectedly.



Heinrich Lang, Deeb Taher, Bernhard Walfort, Hans Pritzkow

J. Organomet. Chem. 691 (2006) 3834

Linear homobimetallic palladium complexes

The synthesis and reaction chemistry of *trans*-(Ph₃P)₂Pd(C₆H₄-4-I)(X) (X = I, OTf) is discussed. Treatment of *trans*-(Ph₃P)₂Pd(C₆H₄-4-I)(OTf) with bidentate Lewis-bases N[∩]N (N[∩]N = pz, bipy, (C₆H₄-4-C \equiv N)₂, C₅H₄N-4-C \equiv N, C₆H₄-1,4-(C \equiv N)₂) produces, depending on N[∩]N, mono- or homobimetallic species of structural type [*trans*-(C₆H₄-4-X)(Ph₃P)₂Pd-(N[∩]N)]ⁿ⁺(X = I, n = 1;X = PPh₃, n = 2), [*trans*-(C₆H₄-4-X)(Ph₃P)₂Pd \leftarrow N[∩]N \rightarrow Pd(PPh₃)₂-(C₆H₄-4-X)]ⁿ⁺(X = I, n = 2; X = PPh₃, n = 4) and {[(Ph₃P)₂(Ph₃P-4-C₆H₄)Pd(µ-I)]₂}²⁺. The solid state structures of five species is reported.



Anja Bierstedt, George R. Clark, Warren R. Roper, L. James Wright

J. Organomet. Chem. 691 (2006) 3846

A 2-iridafuran from reaction between a 1-iridaindene and methyl propiolate

The 2-iridafuran, **3**, results from reaction of the 1-iridaindene, **1**, first with methyl propiolate and secondly with HI. The reaction proceeds through an initial ring-opening of the iridaindene by the methyl propiolate.



Rui F. Munhá, Sónia Namorado, Sónia Barroso, M. Teresa Duarte, José R. Ascenso, Alberto R. Dias, Ana M. Martins

J. Organomet. Chem. 691 (2006) 3853

Diamido/diamine cyclam-based zirconium and hafnium complexes: Synthesis and characterization

Reactions of Li₂[1,8-Bn₂-1,4,8,11-tetraazacyclotetradecane] (Li₂Bn₂cyclam) with MCl₄-(THF)₂ afforded M(Bn₂cyclam)Cl₂ (M = Zr **3**, Hf **4**). M(CB-cyclam)Cl₂ (M = Zr **8**, Hf **9**; CB = 1,4,8,11-tetraazabicyclo[6.6.2]hexadecane) were synthesized from reactions of MCl₄-(THF)₂ with a cross-bridged cyclam derivative (CB-Li₂cyclam **5**). A comparison of solid-state molecular structures of dianionic cyclam based zirconium complexes is presented.



Camino Bartolomé, Raquel de Blas, Pablo Espinet, Jose Miguel Martín-Alvarez, Fernando Villafañe

J. Organomet. Chem. 691 (2006) 3862

Cationic (fluoromesityl)palladium(II) complexes

Ligand substitution reactions at $[Pd(Fmes)-(NCMe)_3]BF_4$ occur under mild conditions. The results are consistent with the higher *trans* effect of the Fmes group. The experimental results support that thermodynamic and kinetic steric effects can prevail on the purely electronic predictions in this kind of substitution reactions that involve bulky ligands.



Julia L. Brumaghim, Christopher L. Gross, Gregory S. Girolami

J. Organomet. Chem. 691 (2006) 3874

Treatment of the hydride complexes Cp^*Os -(P–P)H with methyl trifluoromethanesulfonate affords the triflate complexes Cp^*Os (P–P)OTf accompanied by the evolution of methane. The coordinated triflate ligand can be displaced by water to form the cationic complexes [Cp^*Os (P–P)(OH₂)][OTf]. The molecular structures of the complexes Cp^*Os (dppm)OTf and [Cp^*Os (dmpm)(OH₂)][OTf] are presented and discussed.



Gianfranco Bellachioma, Giuseppe Cardaci, Alceo Macchioni, Chiara Venturi, Cristiano Zuccaccia

J. Organomet. Chem. 691 (2006) 3881

Reductive elimination of halogens assisted by phosphine ligands in $Fe(CO)_4X_2$ (X = I, Br) complexes

Highly basic phosphine ligands L (L = PMe₃, PEt₃, PMe₂Ph) promote halogen reductive elimination in dihalide complexes of iron $Fe(CO)_4X_2$ (X = I, Br), with formation of equimolar amounts of $Fe(CO)_3L_2$ and phosphonium halide $[LX]^+X^-$. The results of the study on the effect of the concentration, basicity and steric hindrance of L, the halogen and temperature on the reductive elimination support a radical mechanism.



Mark A. Fox, Thomas E. Baines, David Albesa-Jové, Judith A.K. Howard, Paul J. Low

J. Organomet. Chem. 691 (2006) 3889

Improved syntheses of bis(ethynyl)-*para*carboranes, 1,12-(RC \equiv C)₂-1,12-C₂B₁₀H₁₀ and 1,10-(RC \equiv C)₂-1,10-C₂B₈H₈ (R = H or Me₃Si) Reactions of the 12-vertex and 10-vertex *para* carboranes, 1,12- $C_2B_{10}H_{12}$ and 1,10- $C_2B_8H_{10}$, with *trans*-1-iodo-2-chloroethene gave 1, 12-(ClCH=CH)_2-1,12- $C_2B_{10}H_{10}$ and 1,10-(ClCH=CH)_2-1,10- $C_2B_8H_8$, respectively in good yield. These vinyl carboranes can be converted to bis(ethynyl) carboranes, 1,12-(RC=C)_2-1,12- $C_2B_1H_{10}$ and 1,10-(RC=C)_2-1,10- $C_2B_8H_8$ (R = H or Me₃Si), easily, and in high yields.



Alberto Acosta-Ramírez, Miguel Muñoz-Hernández, William D. Jones, Juventino J. García

J. Organomet. Chem. 691 (2006) 3895

Isomerization of 2-methyl-3-butenenitrile with (bis-diphenylphosphinoferrocene)nickel compounds: Catalytic and structural studies

The use of catalytic amounts of $[Ni(COD)_2]$ and bis-diphenylphosphinoferrocene allow the catalytic isomerization of 2-methyl-3-butenenitrile to the linear 3-pentenenitrile with a high yield and selectivity at 100 °C.



Konrad Kowalski, Janusz Zakrzewski, Nicholas J. Long, Sławomir Domagała, Andrew J.P. White

J. Organomet. Chem. 691 (2006) 3902

The synthesis and characterisation of l'ethynyl-2,5-dimethylazaferrocene and derivatives The synthesis of 1'-ethynyl-2,5-dimethylazaferrocene is reported along with its electrochemical behavior and the X-ray structure determination of its $W(CO)_5$ -complex. Basic coordination and organic chemistry of 1'ethynyl-2,5-dimethylazaferrocene is illustrated via derivatives incorporating *cis*-Pt(dppe) and Si(Et)₃ units.



Evdoxia Coutouli-Argyropoulou, Christos Sideris, George Kokkinidis

J. Organomet. Chem. 691 (2006) 3909

Synthesis, structural characterization and electrochemical study of 1,1'-ferrocenylene labeled amino acids

Unsymmetrical 1,1'-disubstituted ferrocenes bearing an alanine or a tyrosine moiety and a conjugated electron density controlling substituent were synthesized conveniently starting from 1,1'-ferrocenedicarbaldehyde. The novel ferrocene amino acid derivatives were completely characterized from their MS, ¹H NMR and ¹³C NMR spectra. Their electrochemical behavior was studied by cyclic voltammetry. Their formal redox potentials $E_{\rm f}$ were slightly influenced by the nature of the amino acid and mainly by the kind of the ethenyl substituent.



Anayive Pérez-Rebolledo, Geraldo M. de Lima, Nivaldo L. Speziali, Oscar E. Piro, Eduardo E. Castellano, José D. Ardisson, Heloisa Beraldo

J. Organomet. Chem. 691 (2006) 3919

 $Tin(IV) \ complexes \ obtained \ by \ reacting \ 2-benzoylpyridine-derived \ thiosemicarbazones \ with \ SnCl_4 \ and \ Ph_2SnCl_2$

Reaction of 2-benzoylpyridine thiosemicarbazone (H2Bz4DH, HL1) and its N(4)-methyl (H2Bz4Me, HL2) and N(4)-phenyl (H2Bz4Ph, HL3) derivatives with SnCl₄ and diphenyltin dichloride (Ph₂SnCl₂) gave [Sn(L1)Cl₃] (1), [Sn(L1)PhCl₂] (2), [Sn(L2)Cl₃] (3), [H₂L2]₂⁺-[Ph₂SnCl₄]²⁻ (4) [Sn(L3)PhCl₂] (5) and [Sn-(L3)Ph₂Cl] (6). The crystal structures of the six tin(IV) complexes have been determined.



Massimo Di Vaira, Maurizio Peruzzini, Stefano Seniori Costantini, Piero Stoppioni

J. Organomet. Chem. 691 (2006) 3931

Hydrolytic disproportionation of coordinated white phosphorus in [CpRu(dppe)(η^1 -P₄)]PF₆ [dppe = 1,2-bis(diphenylphosphino)ethane] The compound $[CpRu(PPh_3)_2(\eta^{1}-P_4)]PF_6$, containing the P_4 molecule bound to the $CpRu(PPh_3)_2$ fragment has been synthesized. The coordinated white phosphorus easily reacts with water at room temperature and some of the reaction products have been identified. Hypotheses are advanced for the attack of the water molecule on the coordinated P_4 .



Robert P. Davies, Andrew E.H. Wheatley, Alexander Rothenberger

J. Organomet. Chem. 691 (2006) 3938

Synthesis of crown ether complexes of alkalimetallated organophosphine oxides and insertion reactions with isonitriles The solid-state structures of the crown-ethersolvated heavier alkali metal complexes [$Ph_2P(O)CH_2$]K \cdot 18-crown-6] and [$Ph_2P(O)-CH_2$]Na \cdot 15-crown-5] are reported together with the insertion reaction of the lithiated organophosphine oxide [$Ph_2P(O)CH_2Li$] with cyclohexylisonitrile which produced [$Ph_2P-(O)CH=CHN(Cy)Li$]₄. $[Ph_{2}P(O)CH_{2}M]_{4}$ $[Ph_{2}P(O)CH_{2}M]_{4}$ $[Ph_{2}P(O)CH_{2}M]_{4}$ $[Ph_{2}P(O)CH_{2}M(crown-ether)]_{4}$

Notes

Daniel B. Werz, Christian Bleiholder, Rolf Gleiter, Frank Rominger

J. Organomet. Chem. 691 (2006) 3943

Strong distortions in hexacarbonyldicobalt complexes by *push-pull* effects

Theoretical considerations lead to the hitherto most distorted hexacarbonyldicobalt complexes that are obtained by reaction of *push-pull* substituted alkynes with $Co_2(CO)_8$.



Tomislav Pintauer

J. Organomet. Chem. 691 (2006) 3948

Synthesis, characterization, and the role of counterion in stabilizing trigonal pyramidal copper(I)/2,2'bipyridine complexes containing electron-poor methyl acrylate

Synthesis, characterization and the role of counterion in stabilizing trigonal pyramidal copper(I)/2, 2'-bipyridine complexes containing electron-poor methyl acrylate are described.





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