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Communications

SEVIER

Nasser Iranpoor, Habib Firouzabadi, Roya Azadi

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Imidazolium-based phosphinite ionic liquid (IL-OPPh₂) as Pd ligand and solvent for selective dehalogenation or homocoupling of aryl halides Selective dehalogenation or homocoupling of aryl halides is performed using an imidazolium based phosphinite ionic liquid (IL-OPPh₂) as both solvent and ligand for Pd(II) in the presence of NaOPr^{*i*} or Et₃N respectively.



Ming-Dong Zhou, Shu-Liang Zang, Eberhardt Herdtweck, Fritz E. Kühn

J. Organomet. Chem. 693 (2008) 2473

A (salicylidene)aniline derived Schiff-base adduct of methyltrioxorhenium(VII) – *Cis*- and *trans*-coordination of the ligand

A (salicylidene)aniline derived Schiff-base adduct of MTO is synthesized and its crystal structure is examined. The structure shows that both a *cis*- and a *trans*-isomer with distinct features are present in the solid state, but interchange quickly in solution.



Regular Papers

Gilles Gasser, Leone Spiccia

J. Organomet. Chem. 693 (2008) 2478

Synthesis of a ferrocenyl uracil PNA monomer for insertion into PNA sequences

The synthesis of a new ferrocenyl peptide nucleic acid (PNA) monomer that could potentially be inserted at any chosen position within PNA oligomeric sequences is presented.



Jörg Acker, Klaus Bohmhammel

J. Organomet. Chem. 693 (2008) 2483

Thermodynamic assessment of the copper catalyzed direct synthesis of methylchloro-silanes

The copper catalyzed direct synthesis of methylchlorosilanes is modeled by thermodynamic equilibrium calculations. By the introduction of defined kinetic constrains, which are equivalent to a selective blocking of certain reaction pathways, the experimentally observed product distribution can be modeled. The obtained results are discussed in light of possible reaction pathways, orders of product stabilities, and the impact of varying reaction conditions.

Contents



Maddali L.N. Rao, Varadhachari Venkatesh, Deepak N. Jadhav

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A palladium catalyzed atom-efficient cross-coupling reactivity of triarylbismuths with α , β -unsaturated acyl chlorides An atom-efficient cross-coupling reactivity of triarylbismuths (1 equiv) was demonstrated by cross-coupling reaction with 3 equiv of α , β -unsaturated acyl chlorides under palladium catalysis in the synthesis of a series of functionalized α , β -unsaturated ketones in high isolated yields.



Alexander Betz, Lian Yu, Markus Reiher, Annie-Claude Gaumont, Paul-Alain Jaffrès, Mihaela Gulea

I. Organomet. Chem. 693 (2008) 2499

(*N*,*N*) vs. (*N*,*S*) chelation of palladium in asymmetric allylic substitution using bis(thiazoline) ligands: A theoretical and experimental study

Non-symmetric bis(thiazolines) and oxazoline-thiazolines were synthesized and compared to C_2 -symmetric bis(thiazolines) in the palladium-catalyzed allylic substitution. The experimental results obtained in this study support the hypothesis of a competition between the (*N*,*N*) and the (*N*,*S*) palladium chelation, when sterically hindered bis(thiazolines) are used as ligands. A quantum chemical study performed on the Pd-complexes derived from three selected ligands, two C_2 -symmetric bis(thiazolines) and one oxazoline-thiazoline, also supports this hypothesis.



S.V. Amosova, A.V. Martynov, V.A. Shagun, M.V. Musalov, L.I. Larina, L.B. Krivdin, L.V. Zhilitskaya, M.G. Voronkov

J. Organomet. Chem. 693 (2008) 2509

anti-Markovnikov addition of tellurium tetrachloride to trimethyl ethynyl silane

An investigation of the TeCl_4 interaction with trimethyl ethynyl silane 1 in CHCl_3 has shown that *anti*-Markovnikov adduct [*Z*-1-(trimethylsilyl)-2-chlorovinyl]tellurium trichloride is formed as the only product. In time, it is

hydrolyzed to give [*Z*-1-(trimethylsilyl)-2-chlorovinyl]tellurium(hydroxy)-dichloride which, in turn, is dehydrated to afford bis[(2chloro-1-trimethyl-silylvinyl)dichlorotellurium]oxide. These data revealed that the reaction studied was the first example of *anti*-Markovnikov *syn*-addition of TeCl₄ to terminal acetylenes. A computed simulation of the TeCl₄ interaction with ethynyl silane **1** in a gas state using PES method did not reveal dominating orientation of the addition but showed the conditions at which *anti*-Markovnikov addition can occur and which were probably met in carrying out the reaction in CHCl₃.



Mahmood Payehghadr, Sohaila Yousefi, Ali Morsali

J. Organomet. Chem. 693 (2008) 2514

Thermal, structural and solution studies of a new lead(II) coordination polymer with η^4 Pb-C interactions

A new Pb(II) one-dimensional coordination polymer { $[Pb(PAA)_2]_n$ (1), PAA⁻ = phenylacetate} was synthesized by the reaction of Pb(CH₃COO)₂ · 3H₂O and ligand phenyl acetic acid. Compound 1 was structurally characterized by single-crystal X-ray diffraction. The crystal structure of this

Ahmad R. Esmaeilbeig, Hamid R. Samouei, Mehdi Rashidi

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Organoplatinum(II) complexes with phosphite ligands

compound consists of one-dimensional polymeric units of $[Pb(PAA)_2]$ and the coordination number of Pb^{II} ions is six, the lead atoms have irregular coordination sphere containing stereo-chemically active lone pair and tetra-hapto (η^4) interactions, thus attaining a total hapticity of 10 with environment C₄O₆Pb. The thermal stability of compound 1 was studied by thermal gravimetric (TG) and differential thermal analyses (DTA). The results of studies of the stoichiometry and formation of complex 1 in methanol, ethanol and acetonitrile solutions were found to be in support of their solid state stoichiometry.

[PtMe₂L(SMe₂)] and bis-phosphite com-

 $MeC_6H_4)_2L_2$], in which $L = P(O^iPr)_3$ or $P(OPh)_3$, were synthesized and their reac-

tions with MeI, PPh₃, dppm = bis(diphe-

nylphosphino)methane, and NN = 4,4'-

cis-[PtMe₂L₂]

bipyridine were studied.

complexes

and

cis-

cis-[Pt(p-

Mono-phosphite

plexes





H.J. Breunig, E. Lork, O. Moldovan, C.I. Raţ

J. Organomet. Chem. 693 (2008) 2527

Syntheses of a stable tristibine and of related antimony compounds with the 2,6-dimesitylphenyl (Dmp) substituent

The syntheses of DmpSbX₂ (X = Br, Cl, H, SbMe₂), Dmp(Ph)SbX (X = Br, H, OH), Dmp(Me)SbX (X = H, Sb(Me)Dmp) are reported. DmpSb(SbMe₂)₂ is the first stable *catena* stibine. The molecular structures of DmpSbBr₂, DmpSbI₂, Dmp(Ph)SbX (X = Br, H, OH), and {Dmp(Me)SbH}₂ were determined by X-ray diffraction on single crystal.

 $\begin{array}{cccc} \mathsf{DmpSbH}_2 + \mathsf{Me}_2\mathsf{Sb}^-\mathsf{SbMe}_2 & \xrightarrow{-\mathsf{H}_2} & \underset{\mathsf{Sb}}{\mathsf{Dmp}} \\ \mathsf{Me}_2\mathsf{Sb}^- & \mathsf{SbMe}_2 \\ \mathsf{Dmp} = 2,6\mathsf{-}\mathsf{Mes}_2\mathsf{C}_6\mathsf{H}_3 \end{array}$

Cesar A. Madrigal, Almudena García-Fernández, José Gimeno, Elena Lastra

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Asymmetric transfer hydrogenation of ketones catalyzed by ruthenium(II) complexes bearing a chiral phosphinoferrocenyloxazoline ligand

The catalytic activity in asymmetric transfer hydrogenation of ketones using octahedral and half-sandwich (η^{5} -indenyl and η^{6} -arene) ruthenium(II) complexes containing the chiral

(4S)-2-[(S_p)-2-(diphenylphosphino)ligand ferrocenyl]-4-(isopropyl)oxazoline (FcPN) has been explored. Catalytic studies with complex $fac-[RuCl_2{\eta^2(P,N)-FcPN}(PMe_3)_2]$ (1) show excellent TOF values (9600 h^{-1}). Experiments in the presence of free FcPN, which lead to an increase in conversion rates and ee values when the catalyst is complex $[Ru(\eta^{5}-C_{9}H_{7})\{\kappa^{2}(P,N)-FcPN\}(PPh_{3})][PF_{6}]$ (4) have been carried out. The characterization of the new complexes mer-trans-[RuCl₂{P- $(OMe)_3$ ₂{ $\kappa^2(P,N)$ -FcPN}] and of the watersoluble complexes fac- and mer-trans-[RuCl₂(PTA)₂{ $\kappa^2(P,N)$ -FcPN}] is also reported.



Mala Nath, Hitendra Singh, George Eng, Xueqing Song

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New di- and triorganotin(IV) derivatives of tyrosinylphenylalanine as models for metal-protein interactions: Synthesis and structural characterization. Crystal structure of $Me_2Sn(Tyr-Phe) \cdot MeOH$

Di- and triorganotin(IV) derivatives of tyrosinylphenylalanine (H₂Tyr-Phe) have been synthesized and characterized by various spectroscopic methods. The single crystal X-ray structure of Me₂Sn(Tyr-Phe) · MeOH shows distorted trigonal-bipyramidal arrangement with two methyl groups and peptide nitrogen (N⁻_{peptide}) in the equatorial positions, while the carboxylic oxygen (O⁻_{carboxyl}) and the amino nitrogen (N_{amino}) are at axial positions. One methanol molecule is also present.



Rufen Zhang, Mingqing Yang, Chunlin Ma

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Self-assembly of di- and triorganotin(IV) complexes: Syntheses, characterization and crystal structures of 1D polymeric chain containing *O*,*O*-diethyl or *O*,*O*-diisopropyl phosphoric acid ligands

A series of organotin(IV) complexes with 0,0diethyl phosphoric acid (L¹H) and 0,0-diisopropyl phosphoric acid (L²H) of the types: $[R_3Sn \cdot L]_n$ (L = L¹, R = Ph 1, R = PhCH₂ 2,

Muhammad I. Saleh, Eny Kusrini, Hoong K. Fun, Bohari M. Yamin

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Structural and selectivity of 18-crown-6 ligand in lanthanide–picrate complexes

The mononuclear $[Ln(Pic)_2(18C6)]^+(Pic)^-{Ln} = La-Gd$ and $[Ln(Pic)_3(OH_2)_3] \cdot 2(18C6) \cdot 4H_2O$ {Ln = Tb, Ho} complexes have been synthesized and characterized by reaction of [Ln-(Pic)_2(OH_2)_6]^+(Pic)^- \cdot 6H_2O with the 18C6 ligand in a 1:5 ratio. The current study was evaluated in the solid phase to understand the coordination pattern of Ln(III) with the 18C6

Aleksandr A. Bessonov, Natalia B. Morozova, Nikolay V. Gelfond, Pyotr P. Semyannikov, Iraida A. Baidina, Sergey V. Trubin, Yuriy V. Shevtsov,

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Igor K. Igumenov

Synthesis, crystal structure and thermal behavior of dimethylgold(III) derivatives of salicylaldimine Schiff bases – Novel precursors for gold MOCVD applications R = Me 3, R = Bu 4; L = L², R = Ph 9, R = PhCH₂ 10, R = Me 11, R = Bu 12), [R₂Cl Sn · L]_n (L = L¹, R = Me 5, R = Ph 6, R = PhCH₂ 7, R = Bu 8; L = L², R = Me 13, R = Ph 14, R = PhCH₂ 15, R = Bu 16), have been synthesized. All complexes were characterized by elemental analysis, TGA, IR and NMR (¹H, ¹³C, ³¹P and ¹¹⁹Sn) spectroscopy analysis. Among them, complexes 1, 2, 3, 5, 8, 9 and 11 have been characterized by X-ray crystallography diffraction analysis. In the crystalline state, the complexes adopt infinite 1D infinite chain structures which are generated by the bidentate bridging phosphonate ligands and the five-coordinated tin centers.

ligand. The small differences in the ionic radii of Ln(III) play an important role in the selection of electron rich atoms for the formation of coordination bond. The X-ray crystallographic analysis for the La–Gd complexes indicated the existence of interaction between the Ln(III) ion and the oxygen atoms of the 18C6 ligand in the crystalline state. The ¹H NMR spectra suggested no interaction between the Ln(III) ion and the 18C6 ligand in the solid state and/or solution was observed for the Tb and Ho complexes. Good selectivity of the 18C6 ligand toward Ln(III) in the presence of picrate anion (Pic⁻) which depends on the lanthanide contraction and steric effects were observed.

Dimethylgold(III) derivatives of salicylaldimine Schiff bases were studied as viable MOCVD precursors to gold nanomaterials. Gold nanoparticles 5–15 nm were deposited at temperatures lower than 200 °C by pulse MOCVD.





Luigi Busetto, M. Cristina Cassani, Cristina Femoni, Alceo Macchioni, Rita Mazzoni, Daniele Zuccaccia

J. Organomet. Chem. 693 (2008) 2579

Synthesis, molecular structures and solution NMR studies of *N*-heterocyclic carbene–amine silver complexes

Novel *N*-heterocyclic carbene–amine silver complexes have been prepared and the solid state structures determined by X-ray diffraction analysis have revealed three different bonding motifs: a biscarbene salt $[(NHC-NHBoc)_2Ag]PF_6$ (NHC–NHBoc = 1-(2-BocNH-ethyl)-3-methyl-imidazolin-2ylidene), a tetranuclear complex [Ag(NHC– NHBoc)_2]_2[Ag_2I_4], and a polymeric silver "staircase" [(NHC–NHBoc)_2–Ag_4–I_4]_n, composed of Ag_4I₄ clusters. PGSE and NOE NMR experiments were employed to investigate the level of aggregation and anion–cation relative orientation in solution.



José C. Araujo da Silva, Jean-Paul Pillot, Marc Birot, Jean-Pierre Desvergne, Daniel Liotard, Jean-Claude Rayez, Marie-Thérèse Rayez

J. Organomet. Chem. 693 (2008) 2592

The Si–B chromophore: A joint experimental and theoretical investigation

Organosilylboranes with mesityl groups on boron exhibit an unexpected fluorescence emission band, along with a charge transfer from the silicon atom and the mesityl groups toward the boron atom. MNDO/*d* calculations showed that these phenomena can be ascribed to a large extent to an Si–B HOMO–LUMO transition.



Xia Meng, Yue-Jian Lin, Guo-Xin Jin

J. Organomet. Chem. 693 (2008) 2597

Syntheses and molecular structures of 18/ 16-electron half-sandwich iridium(III) complexes with chelating anilido-imine ligands Sixteen-electron half-sandwich iridium complexes **1b**, **2b**, **2c** and **18**-electron half-sandwich complex **1a** have been synthesized and characterized structurally. **1a** can converted to **1b** by the reaction of **1a** with $AgSO_3CF_3$ in CH₃CN solution.



Felicite Majoumo-Mbe, Peter Lönnecke, Victoria Volkis, Manab Sharma, Moris S. Eisen, Evamarie Hey-Hawkins

J. Organomet. Chem. 693 (2008) 2603

Oligomerization of α -olefins by the dimeric nickel bisamido complex [Ni{1-N(PMes_2)-2-N(μ -PMes_2)C₆H₄- κ^3 N,N',P,- κ^1 P'}]₂ activated by methylalumoxane (MAO) [Ni{1-N(PMes₂)-2-N(μ -PMes₂)C₆H₄- κ^3 N,N', P- κ^1 P'}]₂ after activation by methylalumoxane is a highly active catalyst in the oligomerization and isomerization of α olefins such as ethene, propene, isobutene, 1-hexene and 1,5-hexadiene. To our knowledge this is the most active catalyst for the oligomerization of propene.



Verena Schnitzler, Walter Frank, Christian Ganter

J. Organomet. Chem. 693 (2008) 2610

Straightforward synthesis of phosphametallocenium cations of Rh and Ir The phospharhodocenium and iridocenium cations 7 and 8 were prepared in good yield. The Me₃Si groups of the phosphole prevent the heterocycle from η^1 -P coordination and enforce the formation of the metallocene type structure. The byproduct 9 was also isolated. It features phosphairidocenium and Ir half-sandwich units, which are linked by a bridging phosphole ligand.

Contents



Yu-Pin Wang, Hsien-Li Leu, Hsiu-Yao Cheng, Tso-Shen Lin, Yu Wang, Gene-Hsiang Lee

J. Organomet. Chem. 693 (2008) 2615

Cyclopentadienyl chromium and tungsten complexes with halide, methyl and σ phenylethynyl ligands: Structures of (η^{5} -C₅H₅)Cr(NO)₂(–C=C–C₆H₅), (η^{5} -C₅H₅)Cr (NO)₂I and [(η^{5} -C₅H₄)-COOCH₃]W(CO)₃Cl

With copper(I) iodide as catalyst, CpCr(NO)₂ (C \equiv C-C₆H₅) (**5**), [(η^5 -C₅H₄)-COOCH₃]Cr(NO)₂ (C \equiv C-C₆H₅) (**10**), and [(η^5 -C₅H₄)-COOCH₃]

Haiyan Yang, Linke Li, Yinglin Song, Hongwei Hou, Yaoting Fan

J. Organomet. Chem. 693 (2008) 2624

Syntheses and characterization of ferrocenylthiocarboxylate-containing coordination compounds for nonlinear optics

Four metal-organic coordination compounds containing ferrocenylthiocarboxylate components have been prepared in

Francesco Babudri, Antonio Cardone, Tiziana Cassano, Gianluca M. Farinola, Francesco Naso, Raffaele Tommasi

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Synthesis and optical properties of a poly(2',5'-dioctyloxy-4,4',4''-terphenylene-vinylene) with high content of (Z) vinylene units

 $W(CO)_3(C \equiv C - C_6H_5)$ (13), were prepared. The phenyl group in 5 is oriented perpendicularly to the Cp with an eclipsed conformation. The orientation is rationalized and complemented by molecular orbital calculation. The opposite correlation was observed on the chemical shift assignments of C(2)-C(5) on Cp ring in compounds of $[(\eta^5-C_5H_4)-COOCH_3]Cr(NO)_2X$ and $[(\eta^5-C_5H_4)-COOCH_3]W(CO)_3X$, using HetCOR NMR spectroscopy. The electron density distribution in the cyclopentadienyl ring is dis-cussed on the basis of ¹³C NMR data and compared with the calculations via density functional **B3LYP** correlation-exchange method.



search of good nonlinear optical materials. Hg-containing compound 4 exhibits very strong third-order NLO absorptive and refractive effects. The NLO absorptive coefficient α_2 value (2.11×10⁻¹⁰ m W⁻¹) is larger than those of all the reported ferrocenylcarboxylate-containing coordination compounds and comparable to the well-performing Hg-containing complexes. Additionally, we further analyzed their NLO behaviors through studying electrochemical properties of the four compounds.



Poly(2',5'-dioctyloxy-4,4',4"-terphenylenevinylene) with (Z) configuration of the vinylene double bonds was prepared by Suzuki–Miyaura polymerization of (Z)-4,4'diiodostilbene and 2,5-dioctyloxy-1,4-benzenediboronic acid.



Notes

Natalia N. Sergeeva, Vanesa López Pablo, Mathias O. Senge

J. Organomet. Chem. 693 (2008) 2637

Synthesis of porphyryl boronates with (un)saturated side-chains

Cross-metathesis and addition reactions allow the rapid generation of porphyrin synthons with mono and bis-substituted unsaturated boronyl residues.



 $[PPN][Ir(CO)_4] + [C_3Ph_3][B$

Pek Ke Chan, Weng Kee Leong

J. Organomet. Chem. 693 (2008) 2641

Reaction of $[M(CO)_4]^-$ (M = Ir, Rh) with cyclopropenyl tetrafluoroborate – Ring opening and coupling of cyclopropenyl ligands to form dinuclear metal complexes

Reaction of [PPN][Ir(CO)₄] with $[C_3Ph_3][BF_4]$ resulted in ring opening to afford the dinuclear species Ir₂-(CO)₄(μ , η^1 : η^2 -C₃Ph₃)(μ , η^2 : η^3 -C₃Ph₃) and Ir₂(CO)₄(μ , η^4 : η^4 -C₆Ph₆), the latter also involving coupling of the resulting acyclic, propenyl ligands.



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