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Contents

Regular papers

Irene Veroni, Christodoulos Makedonas, Aliki Rontoyianni, Christiana A. Mitsopoulou

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An experimental and DFT computational study of a novel zerovalent tetracarbonyl tungsten complex of 2-(2'-pyridyl)quinoxaline

The novel complex, $W(CO)_4(2,2'$ -pyridylquinoxaline), has been prepared and structurally characterized. Moreover the extensive solvatochromism of its main transition is investigated by means of DFT and TDDFT calculations and it is interpreted by NMR (1 and 2-D) and UV–Vis spectroscopies.



Makoto Minato, Jian-Guo Ren, Masahiko Kasai, Koji Munakata, Takashi Ito

J. Organomet. Chem. 691 (2006) 282

Synthesis of molybdenocene(IV) and tungstenocene(IV) tropolonato complexes: Its derivative containing calix[4]arene moiety The cationic di- μ -hydroxo dinuclear complexes of molybdenocene and tungstenocene $[Cp_2M(\mu-OH)_2MCp_2]^+$ (Cp = η -C₅H₅; M = Mo or W) react with tropolone to afford tropolonato complexes $[Cp_2M(trop)]^+$ (trop = C₇H₅O₂). The reaction has been extended to the synthesis of calix[4]arene receptor functionalized at the 1,3-positions of the upper rim with two tropolonato-molybdenocene centers.



Damian Plażuk, Janusz Zakrzewski

J. Organomet. Chem. 691 (2006) 287

One-step synthesis of aryl-capped vinylferrocenes from ferrocene and aryl-substituted oxiranes Ferrocene reacts in methanesulfonic acid with aryl-substituted oxiranes to afford aryl-capped vinylferrocenes in moderate yields.



MSA = methanesulfonic acid

Yu Sun, Antje Hienzsch, Jens Grasser, Eberhardt Herdtweck, Werner R. Thiel

J. Organomet. Chem. 691 (2006) 291

Novel phosphine ligands bearing 3(5)pyrazolyl and 4-(2-amino)pyrimidinyl groups: Synthesis and coordination chemistry Novel phosphine ligands bearing pyrazole and pyrimidine functions are obtained in a straight forward reaction from acetylated triphenylphosphines. The coordination chemistry with PdCl₂ is described.



Markus Sailer, Frank Rominger, Thomas J.J. Müller

J. Organomet. Chem. 691 (2006) 299

Ferrocenyl oligophenothiazines as organicorganometallic hybrid electrophores – Synthesis, structure, and electronic properties Oligomeric ferrocene–phenothiazine systems, a novel class of organometallic–organic hybrid electrophores, are easily accessible by Suzuki coupling of iodo ferrocenes and phenothiazinyl pinacolyl boronates. The triad and the pentad with 1,1'-disubstitution on ferrocene adopt preferentially an eclipsed orientation as a consequence of partial intramolecular π stacking. In cyclic voltammetry the central ferrocenyl unit acts as an electronic communicator between phenothiazinyl side chains.



Syed J. Ahmed, Md. Iqbal Hyder, Shariff E. Kabir, Md. Arzu Miah, Antony J. Deeming, Ebbe Nordlander

J. Organomet. Chem. 691 (2006) 309

Dppm-substituted ruthenium clusters with capping sulfido and selenido ligands derived from thiourea, tetramethylthiourea and elemental selenium Sulfur-capped and mixed sulfur/seleniumcapped triruthenium clusters have been synthesised by treatment of $[Ru_3(CO)_{10}(\mu-dppm)]$ with thiourea, tetramethylthiourea or elemental selenium. Bis(dimethylamino)methylidyne ligands are formed in addition to sulfur caps by cleavage of C=S bonds of tetramethylthiourea. The crystal structures of six new compounds are reported.



Izabela Janowska, Janusz Zakrzewski, Keitaro Nakatani, Marcin Palusiak, Marcin Walak, Henryk Scholl

J. Organomet. Chem. 691 (2006) 323

Ferrocenyl D $-\pi$ -A conjugated polyenes with 3-dicyanomethylidene-1-indanone and 1,3-bis (dicyanomethylidene)indane acceptor groups: Synthesis, linear and second-order nonlinear optical properties and electrochemistry

Second-order nonlinear optical chromophores incorporating the ferrocenyl group and 3-dicyanomethylidene-1-indanone-or 1,3-bis(dicyanomethylidene)-indane acceptor groups, connected by a conjugated polyenic bridge of varied length (n = 1-4) have been synthesized. They exhibit large $\mu\beta$ values (up to 8720×10^{-48} esu), measured by the EFISH technique) at 1907 nm.



 $X = O, C(CN)_2$

T.M. Mohan Kumar, B.N. Achar

J. Organomet. Chem. 691 (2006) 331

Synthesis and characterization of lead phthalocyanine and its derivatives

Lead (II) phthalocyanine (PbPc), lead (II) tetranitro phthalocyanine (PbTNP) and lead (II) tetraamino phthalocyanine (PbTAP) are synthesized in pure state. These complexes are characterized using elemental analysis, UV–visible, IR-spectroscopy, X-ray crystallography and thermogravimetry. Electrical conductivity studies are done for all the three complexes in the temperature range from 30 to 200 °C.

Arturo Abreu, S. Jesùs Alas, Hiram I. Beltrán, Rosa Santillan, Norberto Farfán

J. Organomet. Chem. 691 (2006) 337

Synthesis and characterization of boronates derived from non-symmetric amino-bis-phenols

A series of 12 new boronates of the 2-aryldibenzo[d,h]-6-aza-1,3-dioxa-2-boracyclonon ene type were synthesized and characterized by NMR and X-ray diffraction analysis.

Siew Huay Chong, David J. Young, T.S. Andy Hor J. Organomet. Chem. 691 (2006) 349

Combinative use of high-pressure, metaltemplating and sulfur-nucleophilicity towards dithiacyclophane synthesis and its complex intermediates Under high pressure (15 kbar) at r.t., reactions of $[Pt_2(\mu-S)_2(PP)_2]$ $[P-P = 2 \cdot PPh_3;$ $Ph_2P(CH_2)_nPPh_2, n = 2$ (dppe), 3 (dppp)] with α - α' -dichloro-*o*-xylene would progress to a catalytic-like pathway to yield 3,8-dibenzo-1,6-dithiacyclodecane (up to 35%), and a series of mechanistically relevant intermediates and byproducts. This combined use of pressure and sulfur nucleophilicity and the templating effect of a diplatinum offer a unique possibility to prepare macrocyclic dithioether in a one-pot synthesis.



+ РЬО -

180°C

Geir Langli, Christian Rømming, Kjell Undheim

J. Organomet. Chem. 691 (2006) 356

Stereoselective synthesis of an *ansa*-zirconocene in a spirane scaffold A rigid C₂-bridged zirconocene catalyst system with the C₂-bridge embedded in a spirane scaffold has been prepared from 3,4-dihydro-2*H*-fluoren-1(9*H*)-one. The oxo group was converted into a spirocyclobutanone and a fulvene before regio- and stereoselective saturation yielded *cis*-2-(cyclopentadienyl)-1',2',3',4'-tetrahydro-9*H*-spiro[cyclobutane-1,1'fluorene]. Lithiation and zirconation furnished the precatalyst (η^5 -cyclopentadienyl)-spiro [cyclobutane-1,1'-(η^5 -fluorenyl)]zirconium dichloride complex. The structure was confirmed by an X-ray structure analysis.



Michael I. Bruce, Martin Jevric, Brian W. Skelton, Mark E. Smith, Allan H. White, Natasha N. Zaitseva

J. Organomet. Chem. 691 (2006) 361

Syntheses and molecular structures of some phosphine–gold(I) derivatives of 1,3-diynes

The synthesis and spectroscopic and structural characterisation of several phosphine–gold(I) complexes containing various diynyl fragments are described.



Padmamalini Srinivasan, Weng Kee Leong

J. Organomet. Chem. 691 (2006) 371

Ligand substitution in the heterometallic cluster $Cp*IrOs_3(\mu\text{-}H)_2(CO)_{10}$

The ligand substitution reactions of the heterometallic cluster $Cp_*IrOs_3(\mu-H)_2(CO)_{10}$ with phosphines, isonitriles and pyridine under TMNO activation afforded the substitution products $Cp_*IrOs_3(\mu-H)_2(CO)_{10-n}L_n$ (*n* = 1, 2; L = PPh₃, P(OMe)₃, 'BuNC, CyNC or py) in good yields. The solid-state structures and solution structures of these have been investigated.



Eugenio Simón-Manso, Mauricio Valderrama

J. Organomet. Chem. 691 (2006) 380

Group VIII transition metal complexes with the chiral diphosphazane ligand (S)- α - $(Ph_2P)_2N(CHMePh)$: Synthesis and structural characterization The synthesis of the square-planar complex $[Ni(CO)_2 \{\kappa^2 - (PPh_2)_2N(CHMePh)\}]$ (1) and of pseudo-octahedral complexes $[(\eta^n\text{-ring})-MCl\{\kappa^2 - (PPh_2)_2N(CHMePh)\}]BF_4$ $[\eta^n\text{-ring} = \eta^5 - C_5Me_5; M = Rh$ (2), Ir (3). $\eta^6 - C_6Me_6; M = Ru$ (4)] and $[(\eta^5 - C_5H_5)Fe(CO)\{\kappa^2 - (PPh_2)_2N-(CHMePh)\}]BF_4$ (5) have been described. The molecular structures of complexes 2, 3 and 5 have been determined by X-ray diffraction methods. All the crystal structures show the existence of an intramolecular π -stacking interaction between the phenyls of the CHMePh group and the Ph_2P moiety.



Guizhu Chen, Mingli Deng, Chee Keong Don Lee, Weng Kee Leong, Jialin Tan, Chuen Tse Tay

J. Organomet. Chem. 691 (2006) 387

The reaction of $Os_3(\mu-H)(\mu-SbPh_2)(\mu_3,\eta^2-C_6H_4)(CO)_9$ with AsPh₃ afforded the adduct $Os_3(\mu-H)(SbPh_2)(\mu_2,\eta^2-C_6H_4)(CO)_9(AsPh_3)$ and the substitution derivative $Os_3(\mu-H)(SbPh_2)-(\mu_3,\eta^2-C_6H_4)(CO)_8(AsPh_3)$. Reaction with 'BuNC afforded the adduct $Os_3(\mu-H)-(SbPh_2)(\mu_2,\eta^2-C_6H_4)(CO)_9(CN'Bu)$ quantitatively. This adduct isomerised slowly on standing via migration of the isonitrile, while photolysis led to decarbonylation to $Os_3(\mu-H)-(SbPh_2)(\mu_2,\eta^2-C_6H_4)(CO)_8(CN'Bu).$



Cheuk-Lam Ho, Wai-Yeung Wong

J. Organomet. Chem. 691 (2006) 395

Synthesis, structures and photoluminescence behavior of some group 10 metal alkynyl complexes derived from 3-(*N*-carbazolyl)-1propyne A new class of luminescent mononuclear metal complexes of platinum and palladium containing 3-(*N*-carbazolyl)-1-propyne ligands are prepared and characterized. The influence of metal center and its auxiliary groups on the photophysical properties of the carbazole-based organometallic compounds is characterized in detail.





Padmamalini Srinivasan, Weng Kee Leong

J. Organomet. Chem. 691 (2006) 403

The synthesis of heteronuclear clusters containing cyclopentadienyl- or pentamethylcyclopentadienyliridium and ruthenium or osmium The reaction of Cp*Ir(CO)₂ or CpIr(CO)₂ with Ru₃(CO)₁₂, Os₃(μ -H)₂(CO)₁₀ or Os₃(CO)₁₀-(CH₃CN)₂ afforded tetrahedral heteronuclear clusters in good to moderate yields. Solution-state NMR studies show that the hydrides in the iridium–ruthenium clusters are highly fluxional even at low temperatures while those in the iridium–osmium clusters are less so.



Charles A. Johnson II, Benjamin A. Baker, Orion B. Berryman, Lev N. Zakharov, Matthew J. O'Connor, Michael M. Haley

J. Organomet. Chem. 691 (2006) 413

Synthesis and characterization of pyridineand thiophene-based platinacyclynes Seven heterocyclic macrocycles, including the first platinacycles with pyridine and thiophene rings incorporated into the cyclyne system, are reported. Pt-acetylide cyclynes were assembled via tin transmetallation or amine-mediated oxidative addition with stoichiometric $PtCl_2$ -(PEt_3)₂ and CuI.

S1 C9 C10 P1 P2 S2 C2 C1 P1 C21 S2

Robert Kreiter, Judith J. Firet, Michel J.J. Ruts, Martin Lutz, Anthony L. Spek, Robertus J.M. Klein Gebbink, Gerard van Koten

J. Organomet. Chem. 691 (2006) 422

Synthesis, coordination chemistry, and metal complex reactivity of (dimethylamino)methylsubstituted triarylphosphanes; X-ray study on [AuCl(PPh_{3-n}Ar_n)] (Ar = $1-C_6H_3(CH_2NMe_2)_2-$ 3,5, n = 1, 3; Ar = $1-C_6H_4(CH_2NMe_2)-4, n = 3$) Novel 4-mono and 3,5-bis[(dimethylamino)methyl] functionalized triarylphosphanes have been prepared and used for the construction of complexes of the form [AuCl(P)] and [PtCl₂(P)₂]. The solution and solid state behavior of these complexes is very similar to that of the corresponding PPh₃ complexes. The amine functionalities in the gold compounds have been reacted with either acid (HCl, H₃PO₄) to generate ammonium salts or with benzyl bromide to afford benzyl ammonium salts, without the violation of the Au–P bond.



Contents

Joffrey Wolf, Agnès Labande, Jean-Claude Daran, Rinaldo Poli

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Nickel(II) complexes with bifunctional phosphine–imidazolium ligands and their catalytic activity in the Kumada–Corriu coupling reaction Zwitterionic Ni(II) complexes of type NiX₃(NCN⁺), (NCN⁺ = 1-(2-diphenylphosphinoethyl)-3-(2,4,6-trimethylphenyl)imidazolium and X = Cl or Br), have been prepared and characterised by X-ray crystallography. They have been used as catalytic precursors in the Kumada–Corriu coupling reaction between phenylmagnesium chloride and 4-chloroanisole, yielding high catalytic activities.



Margarita Crespo, Mercè Font-Bardía, Xavier Solans

J. Organomet. Chem. 691 (2006) 444

Synthesis, reactivity and crystal structures of platinum (II) and platinum (IV) cyclometallated compounds derived from 2- and 4biphenylimines New [C,N,N'] and [C,N] cyclometallated platinum (II) compounds derived from 2- and 4-biphenylimines are reported along with their reactions with PPh₃ and methyl iodide. The relative position of the two phenyl rings can be related to the steric crowding in the coordination sphere of these compounds.



Fan Zhang, Marc H. Prosenc, Jürgen Heck

J. Organomet. Chem. 691 (2006) 455

Synthesis and characterization of dinuclear monohydro sesquifulvalene complexes with potential NLO properties

The monocationic vinylogue monohydro sesquifulvalene complex *E*-1-(1"-hydroxycarbonylferrocen-1'-yl)-2-{(1"'-6"'- η -cyclohepta-1"',3"', 5"'-trien-1"''-yl) (η^5 -pentamethylcyclopentadienyl) ruthenium(II)}ethene hexafluorophosphate (**5**) was synthesized. After treatment with a base, complex **5** was transformed into the organometallic zwitterion *E*-1-(1"-oxycarbonylferrocen-1'-yl)-2-{(1"'-6"''- η -cyclohepta-1"'', 3"'',5"''-trien-1"''-yl)(η^5 -pentamethylcyclopentadienyl)ruthenium(II)}ethene (**6**).



David Savage, Gwen Malone, Steven R. Alley, John F. Gallagher, Alok Goel, Paula N. Kelly, Helge Mueller-Bunz, Peter T.M. Kenny

J. Organomet. Chem. 691 (2006) 463

The synthesis and structural characterization of *N*-ortho-ferrocenyl benzoyl amino acid esters. The X-ray crystal structure of *N*- $\{ortho-(ferrocenyl)benzoyl\}-L-phenylalanine ethyl ester$

A series of *N*-ortho-ferrocenyl benzoyl amino acid ethyl esters **3–9** have been prepared by coupling ortho-ferrocenyl benzoic acid **2** to the amino acid ethyl esters of glycine, L-alanine, Lleucine, L-phenylalanine, β -alanine, 4-aminobutyric acid and (±)-2-aminobutyric acid using the conventional 1,3-dicyclohexylcarbodiimide, 1-hydroxybenzotriazole protocol. The compounds were fully characterized by a range of NMR spectroscopic techniques and by mass spectrometry (MALDI-MS, ESI-MS). The Xray crystal structure of the L-phenylalanine derivative **6** has been determined.



Junhua Chen, Xiaoqin Zhang, Qiang Feng, Meiming Luo

J. Organomet. Chem. 691 (2006) 470

Novel hexadentate imidazolium salts in the rhodium-catalyzed addition of arylboronic acids to aldehydes

Novel hexadentate imidazolium salts were synthesized. The addition reaction of arylboronic acids to aldehydes is effected conveniently and in high yields by a catalyst system generated in situ from these hexadentate imidazolium salts, [Rh(COD)Cl]₂ and a base.



Concepción López, Ramon Bosque, Sonia Pérez, Anna Roig, Elies Molins, Xavier Solans, Mercè Font-Bardía

J. Organomet. Chem. 691 (2006) 475

Relationships between ⁵⁷Fe NMR, Mössbauer parameters, electrochemical properties and the structures of ferrocenylketimines The study and the theoretical interpretation of the electrochemical properties, 57 Fe NMR and Mössbauer spectroscopic data of $[(\eta^5-C_5H_5)Fe\{(\eta^5-C_5H_4)-C(R^1)=N-R^2\}]$ {R¹ = H, R² = CH₂-CH₂OH (1a), CH(Me)-CH₂OH (1b), CH₂C₆H₅(1c), C₆H₄-2Me (1d), C₆H₄-2SMe (1e) or C₆H₄-2OH (1f) and R¹ = C₆H₅, R² = C₆H₄-2Me (2d)} are reported.



Bao-Hua Zhu, Bin Hu, Hong Hong, Yuan-Qi Yin, Jie Sun

J. Organomet. Chem. 691 (2006) 485

Reactions of linked tetrahedron clusters $[Co_2(CO)_6(\mu-HC_2CH_2O)-]_2R$ with $Rh_2(CO)_4$ -Cl₂ to give mixed-metal linked alkyne-bridged butterfly clusters containing $C_2Co_2Rh_2$ unit Five new Rh–Co mixed-metal linked tetrahedron-octahedron clusters $[Rh_2Co_2(CO)_{10}(\mu_4, \eta^2-HC_2CH_2O-R-OCH_2C_2H-\mu)Co_2(CO)_6]$ and five known linked octahedral clusters $[Rh_2Co_2-(CO)_{10}(\mu_4, \eta^2-HC_2CH_2O-)]_2R$ have been synthesized from reactions of $Rh_2(CO)_4Cl_2$ with $[Co_2(CO)_6(\mu+HC_2CH_2CO)-]_2R$, respectively. The structure of cluster $[Rh_2Co_2(CO)_{10}(\mu_4, \eta^2-HC_2CH_2O-C_6H_4-1, 4-OCH_2C_2H-\mu)Co_2(CO)_6]$ was determined by single-crystal X-ray diffraction analysis.



Paola Ramírez, Raúl Contreras, Mauricio Valderrama, Daphne Boys

J. Organomet. Chem. 691 (2006) 491

Synthesis and reactivity of new trimethylplatinum(IV) complexes containing chiral Schiff bases as ligands: Crystal structure of (OC-6-44-C)-[PtIMe₃{ κ^2 -(*R*)-Ph₂P(C₆H₄)CH= NC*H(Ph)Me-P,N}] The synthesis and characterisation of new neutral complexes in diastereomeric mixtures of formula [PtIMe₃{ κ^2 -Ph₂P(C₆H₄)CH= NC*H(Ph)Me-P,N}] are described. The crystal structure of the diastereoisomer (OC-6-44-C)-[PtIMe₃{ κ^2 -(R)-Ph₂P(C₆H₄)CH=NC*H(Ph) Me-P,N}] is determined by single-crystal X-ray diffraction methods. The treatment of the mixture with pyridine, in the presence of AgBF₄, yields a reductive elimination reaction. The similar reaction with PPh₃ involves a consecutive *ortho*metallation reaction.



Chang-Bin Yu, Yu-Qing Xia, Xiao-Hong Tian, Xiang-Ge Zhou, Guang-Ying Fan, Rui-Xiang Li, Xian-Jun Li, Kim-Chung Tin, Ning-Bew Wong

J. Organomet. Chem. 691 (2006) 499

Syntheses and crystal structures of binuclear ruthenium complexes bearing 1,8'-bis(diphenyl-phosphinomethyl)naphthalene

The reaction of $[\operatorname{RuCl}_2(\eta^6-\operatorname{C}_6\operatorname{H}_6)]_x$ with [1,8bis(diphenylphosphinomethyl)naphthalene] in methanol gave three new complexes, and they showed some unique characters in structure.



Elena I. Klimova, Tatiana Klimova, Leon V. Bakinovsky, Marcos Martínez García

J. Organomet. Chem. 691 (2006) 507

3-Ferrocenyl-1-methyl- and 1-ferrocenyl-3methylcyclopropenes Dehydrobromination of isomeric 3-bromo-1-ferrocenyl-2-methylcyclopropanes afforded 3-ferrocenyl-1-methyl- and 1-ferrocenyl-3-methylcyclopropenes. These undergo smooth opening of the three-membered ring to give 1- and 2-ferrocenylbuta-1,3-dienes and 1- and 2-methyl-1*H*-cyclopentaferrocenes; with 1,3diphenylisobenzofuran they give the classical Diels–Alder adducts.



Wieland Tyrra, Said Aboulkacem, Ingo Pantenburg

J. Organomet. Chem. 691 (2006) 514

Silver compounds in synthetic chemistry. Part 3. 4-Tetrafluoropyridyl silver(I), $AgC_5F_4N - A$ reagent for redox transmetallations with group 12–14 elements

4-Tetrafluoropyridyl silver(I), AgC₅F₄N, has been prepared via the reaction of Me₃SiC₅F₄N and AgF in nearly quantitative yield. Redox transmetallations with group 12–14 elements Zn, Cd, Hg, Ga, In, Sn in propionitrile gave the corresponding 4-tetrafluoropyridyl element compounds. The molecular structures of [PNP][Ag(C₅F₄N)₂], Hg(C₅F₄N)₂, Ga(C₅F₄-N)₃ · EtCN · H₂O, In(C₅F₄N)₃ · 2EtCN and Sn(C₅F₄N)₄ are discussed.



Amitabha Mitra, Melanie J. Harvey, Mary K. Proffitt, Lauren J. DePue, Sean Parkin, David A. Atwood

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Binuclear Salan borate compounds with threecoordinate boron atoms 

Padma Nair, Colin P. White,
Gordon K. Anderson, Nigam P. Rath
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Unsymmetrical complexes containing
linear tetraphosphine ligand DPPEPMReaction of the tetradentate ligand DPPEPM-PP)]
(1, R = Me; 2, R = Ph), $[M(DPPEPM-PP)_2]^-$
 $[MCl_4]$ (3, M = Pd; 4, M = Pt) or [MR
(DPPEPM-PPP)]Cl (6, <math>M = Pt, R = Me; 7,
M = Pt, R = Ph; 8, M = Pd, R = Me). Each
of these has uncoordinated P atoms that can
be utilized in the formation of bi- or trimetallicPPPPPPPPPPP

derivatives.

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Erratum	540



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