

Contents

Publisher's Note: New Regional Editor xviii

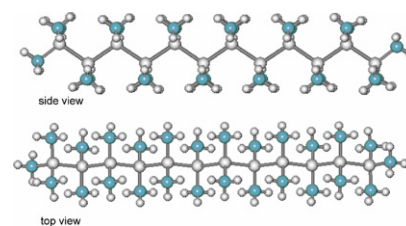
Regular papers

**Hiroshi Kawabata, Shigekazu Ohmori,
Kazumi Matsushige, Hiroto Tachikawa**

J. Organomet. Chem. 691 (2006) 5525

The electronic structures of all *trans* form of permethyl-oligosilane radical cation with longer chain: A density functional theory study

DFT calculations have been carried out for neutral, radical cation and dication of permethyl-oligosilane, $\text{Si}_n(\text{CH}_3)_{2n+2}$ ($n = 4-30$), to elucidate the electronic structures at ground and low-lying excited states. The spin distribution in the oligosilanes was determined. Also, IR-band of radical cation was assigned on the basis of theoretical calculations.

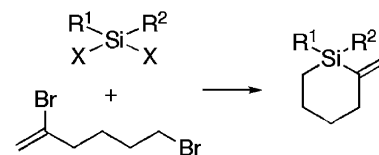


Silvia Díez-González, Luis Blanco

J. Organomet. Chem. 691 (2006) 5531

Synthesis of 2-methylidene-1-silacyclohexanes from 2,6-dibromohex-1-ene and polyhalosilanes

Various 2-methylidene-1-silacyclohexanes were prepared by straightforward syntheses from readily available polychloro- or polyfluorosilanes, magnesium and 2,6-dibromohex-1-ene using Barbier-type conditions or a previously synthesized Grignard reagent. Good yields were obtained considering the low stability of the products in the reaction conditions.

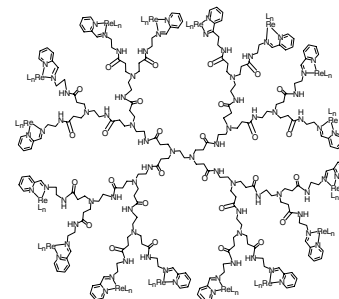


Xinxin Zhao, Yaw-Kai Yan, Chit-Kay Chu

J. Organomet. Chem. 691 (2006) 5540

Synthesis and characterization of polyamidoamine dendrimers surface-functionalized with bromotricarbonylpyridyliminerhenium(I) units

First and second generation PAMAM dendrimers were modified through condensation reactions to give pyridylimine Schiff base ligands. G0, G1 and G2 pyridylimine PAMAM dendrimers were reacted with $[\text{ReBr}(\text{CO})_3]$ to give terminally modified dendrimers having four, eight and 16 rhenium tricarbonyl moieties at the terminals, respectively.



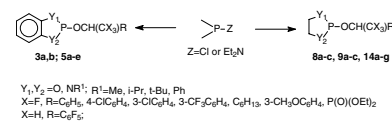
$\text{ReL}_n = \text{ReBr}(\text{CO})_3$

Oleg Artyushin, Irina Odinets, Evgenii Goryunov, Ivan Fedyanin, Konstantin Lyssenko, Tatyana Mastryukova, Gerd-Volker Röschenthaler, Tamás Kégl, György Keglevich, László Kollár

J. Organomet. Chem. 691 (2006) 5547

α -Fluorinated cyclic amidophosphite ligands. Their synthesis, Rh complexes and catalytic activity in the hydroformylation of styrene

The synthetic routes to both benzoannellated (**3a,b**, **5a–e**) and monocyclic (**8a–c**, **9a–c**, **14a–g**) (amido)phosphate ligands with fluorine containing substituents were elaborated. Their Rh(I) complexes formed *in situ* demonstrate high activity in the hydroformylation of styrene along with selectivity in respect to branched aldehyde. The “structure–activity” relationship was estimated using quantum-chemical calculations.

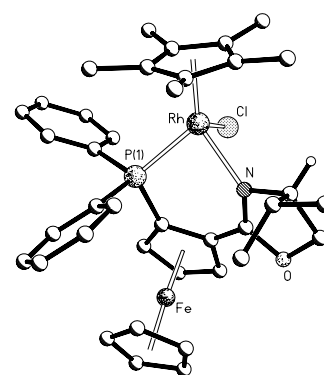


Daniel Carmona, Roberto Medrano, Isabel T. Dobrinovich, Fernando J. Lahoz, Joaquina Ferrer, Luis A. Oro

J. Organomet. Chem. 691 (2006) 5560

Synthesis and structure of chiral-at-metal complexes with the ligand (*S*)-2-[(*S_p*)-2-(diphenylphosphino)ferrocenyl]-4-isopropylloxazoline

Half-sandwich complexes of formula [(η^5 -ring)MCl]PF₆ [L = (*S*)-2-[(*S_p*)-2-(diphenylphosphino)ferrocenyl]-4-isopropylloxazoline; (η^5 -ring)M = (η^5 -C₅Me₅)Rh; (η^5 -C₅Me₅)Ir; (η^6 -*p*-MeC₆H₄*i*Pr)Ru; (η^6 -*p*-MeC₆H₄*i*Pr)Os] have been prepared and characterised. The related solvate complexes [(η^5 -C₅Me₅)ML (Me₂CO)]²⁺ (M = Rh, Ir) are active catalysts for the Diels–Alder reaction between methacrolein and cyclopentadiene.

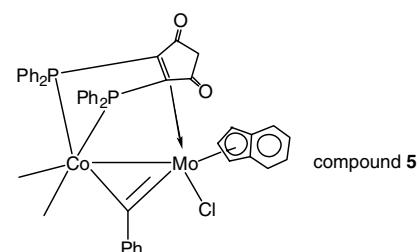


William H. Watson, Bhaskar Poola, Michael G. Richmond

J. Organomet. Chem. 691 (2006) 5567

Ligand substitution in the tetrahedrane clusters RCCO₂Mo(η^5 -indenyl)(CO)₈ with 4,5-bis(diphenylphosphino)-4-cyclopenten-1,3-dione (bpcd): Influence of the carbyne and indenyl ligands on the stability of the substitution products and X-ray diffraction structures of HCCO₂Mo(η^5 -indenyl)(CO)₆(μ -bpcd) and CoMo(η^5 -indenyl)(μ -CPh)(CO)₂(μ -bpcd)Cl

Thermolysis of the mixed-metal cluster HCCO₂Mo(η^5 -indenyl)(CO)₈ (**1**) with the diphosphine ligand 4,5-bis(diphenylphosphino)-4-cyclopenten-1,3-dione (bpcd) in DCM or DCE solvents yields the bpcd-bridged cluster HCCO₂Mo(η^5 -indenyl)(CO)₆(μ -bpcd) (**2**). The related benzylidyne-capped cluster PhCCO₂Mo(η^5 -indenyl)(CO)₈ (**3**) reacts with bpcd under analogous conditions to give the unstable cluster Co₂MoCp(η^5 -indenyl)(CO)₅[μ_2 , η^2 , η^1 -C(Ph)C=C(PPh₂)C(O)CH₂C(O)](μ -PPh₂) (**4**) and the carbyne-bridged compound CoMo(η^5 -indenyl)(μ -CPh)(CO)₂(μ -bpcd)Cl (**5**). These compounds have been fully characterized in solution by IR and NMR spectroscopies, and by X-ray crystallography in the case of compounds **2** and **5**.

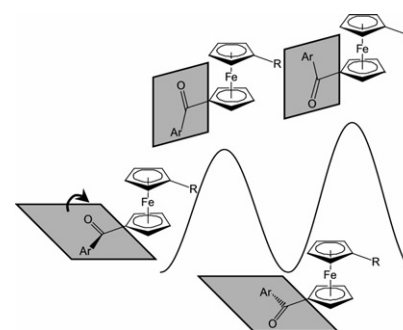


Katja Heinze, Manuela Beckmann

J. Organomet. Chem. 691 (2006) 5576

Dynamic behaviour of 1,*n*'-disubstituted ferrocenes

1,*n*'-Disubstituted ferrocenes with ketone/phthalimido (**2**) and ketone/amine substituents (**3**) were synthesised and fully characterised. The molecular structure of **2** was confirmed by X-ray crystal structure determination. The dynamic behaviour was experimentally studied in solution and theoretically by DFT calculations. The thermal stability of the ketone/amine derivative **3** was investigated using thermal analyses.

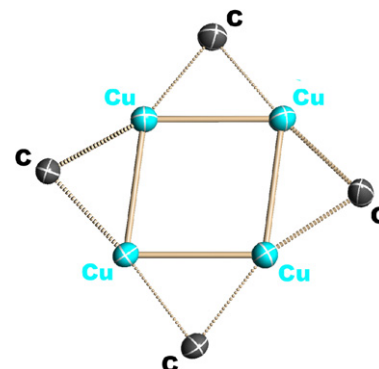


René T. Boéré, Jason D. Jason D. Masuda, Peter Tran

J. Organomet. Chem. 691 (2006) 5585

Synthesis, crystal structure and DFT calculations on 2,6-diisopropylphenylcopper; its use in the preparation of dichloro-2,6-diisopropylphenylphosphine

In the crystal, the molecules consist of a planar trapezoid of Cu atoms in which each edge is bridged by the *ipso* carbon atoms of the perpendicularly disposed 2,6-diisopropylphenyl groups. These C atoms are displaced above (left, right) and below (top, bottom) the plane defined by the Cu atoms.

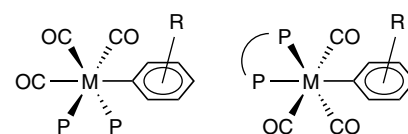


Gabriele Albertin, Stefano Antoniutti, Jesús Castro, Stefano Carniato, Soledad García-Fontán

J. Organomet. Chem. 691 (2006) 5692

Preparation and protonation reactions of aryl complexes of manganese and rhenium

The preparation of aryl complexes $M(\eta^1\text{-Ar})(\text{CO})_n\text{P}_{5-n}$ of manganese and rhenium is presented. The structural parameters of the $\text{Re}(\eta^1\text{-C}_6\text{H}_5)(\text{CO})_5[\text{Ph}_2\text{PO}(\text{CH}_2)_2\text{OPPh}_2]$ derivative was also determined. The protonation of the aryl complexes with Brønsted acid was studied and led to free hydrocarbons and the unsaturated $[\text{M}(\text{CO})_n\text{P}_{5-n}]^+$ cations.



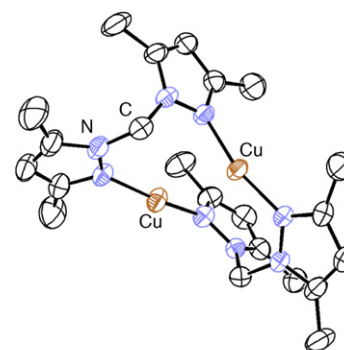
M = Mn, Re
P, P-P = phosphites

Adriano Boni, Guido Pampaloni, Riccardo Peloso, Daniele Belletti, Claudia Graiff, Antonio Tiripicchio

J. Organomet. Chem. 691 (2006) 5602

Synthesis of copper(I) bis(3,5-dimethylpyrazolyl)methane olefin complexes and their reactivity towards carbon monoxide

New copper(I) bis(3,5-dimethylpyrazolyl)methane complexes have been prepared, the carbonylation reactions of new olefin derivatives of general formula $[\text{Cu}[\text{CH}_2(3,5\text{-Me}_2\text{Pz})_2](\text{olefin})]\text{TfO}$ have been studied and the parameters of the equilibria for the displacement of the coordinated olefin by carbon monoxide – $\{\text{Cu}[\text{CH}_2(3,5\text{-Me}_2\text{Pz})_2](\text{olefin})\} + \text{TfO} + \text{CO} \rightleftharpoons \{\text{Cu}[\text{CH}_2(3,5\text{-Me}_2\text{Pz})_2](\text{CO})\} + \text{TfO} + \text{olefin}$ – have been determined.



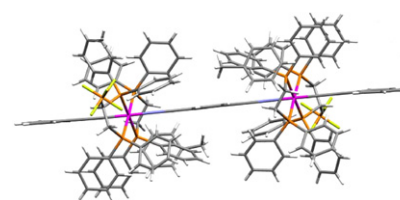
$\{\text{Cu}_2[\mu\text{-CH}_2(3,5\text{-Me}_2\text{Pz})_2]\}^{2+}$

Jean-Luc Fillaut, Neerja Nagpal Dua, Florence Geneste, Loïc Toupet, Sourisak Sinbandhit

J. Organomet. Chem. 691 (2006) 5610

Nitrile ligands for controlled synthesis of alkynyl-ruthenium based homo and hetero bimetallic systems

Wire like mono- and poly-nuclear molecules based on alkynyl ruthenium complexes. Extended rigid rod systems of nanometric size with multilevel electron transfers whose core unit is based on alkynyl ruthenium complexes are readily accessed. Their electronic dual character is exemplified through electrochemical studies.

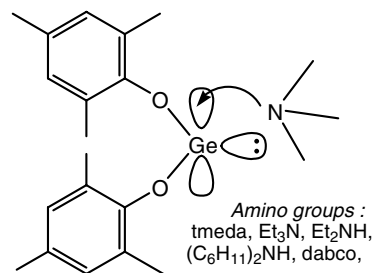


**Eric Bonnefille, Stéphane Mazières,
Nancy El Hawi, Heinz Gornitzka,
Claude Couret**

J. Organomet. Chem. 691 (2006) 5619

Synthesis and chemistry of aryloxygermylene-amine complexes

The synthesis and characterization of dimesityloxygermylene-amine and chloromesityloxygermylene-amine complexes is presented. The versatile reactivity of $(\text{MesO})_2\text{Ge-tmeda}$ is reported, especially the cycloaddition with 2,3-dimethyl-1,3-butadiene and dimethyl acetylenedicarboxylate. Mesityloxy groups are revealed to be good ligands for this chemistry and have good potential for further look.

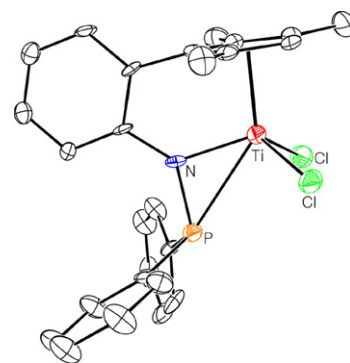


**Chun Ji Wu, Sang Hoon Lee, Hoseop Yun,
Bun Yeoul Lee**

J. Organomet. Chem. 691 (2006) 5626

Synthesis and structures of *o*-phenylene-bridged Cp/phosphinoamide titanium complexes

o-Phenylene-bridged Me_2Cp or Me_3Cp /phosphinoamide titanium and zirconium complexes were prepared and the structures of some complexes were determined by X-ray crystallography. They show negligible activity in ethylene polymerization.

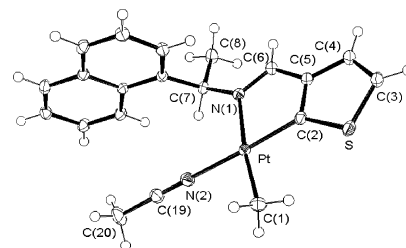


**Craig Anderson, Margarita Crespo,
James Morris, Joseph M. Tanski**

J. Organomet. Chem. 691 (2006) 5635

Reactivity of cyclometallated platinum complexes with chiral ligands

Methyl platinum complexes with orthometalated imine ligands reacted with chiral ligands to produce new complexes with two chiral centers with different electronic and steric properties. Their reactions with methyl iodide were then studied.

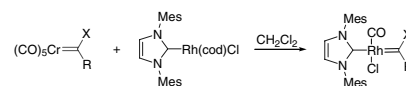


**José Barluenga, Rubén Vicente, Luis A. López,
Miguel Tomás**

J. Organomet. Chem. 691 (2006) 5642

Chromium(0)–rhodium(I) metal exchange: Synthesis and X-ray structure of new Fischer (NHC)carbene complexes of rhodium(I)

A new type of metal carbene complex of group 9, specifically NHC/Fischer biscarbene complexes of rhodium(I), is synthesized and fully characterized. Preliminary results on their thermal stability and reactivity toward alkynes and allenes are also reported.

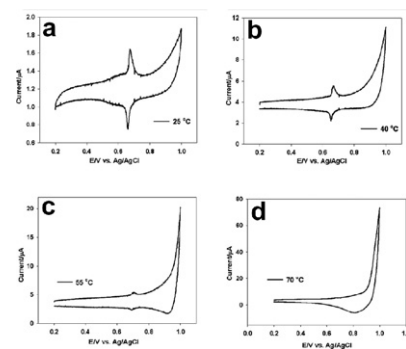


M.M. Rahman, I.C. Jeon

J. Organomet. Chem. 691 (2006) 5648

Thermal effect on the voltammogram of 7-ferrocenecarboxyloxy-1-heptanethiol self-assembled monolayer

The loss of ferrocene via nucleophilic attack at various temperatures and resulted that there is an accelerated loss of ferrocene from the chain termini (disappearing of redox peaks) due to increase of temperatures, and the capacitance of the layer in its reduced state and a positive shift in the $E_{1/2}$ value are observed. A comparison between temperature (activated) data and the effects of multiple scans recorded at room temperature suggests that there is a re-orientation, induced at slightly elevated temperatures, which is associated with the ferrocene ester linkage at the chain terminus and which apparently renders ferrocene more susceptible to nucleophilic attack.

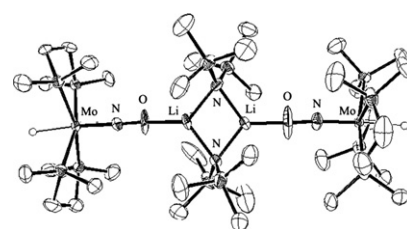


Fupei Liang, Helmut W. Schmale, Heinz Berke

J. Organomet. Chem. 691 (2006) 5655

μ -Coordination chemistry of NO ligands: Adducts of *trans*-Mo(dmpc)₂(H)(NO) with lithium salts

Electron rich complexes like *trans*-Mo(dmpc)₂(H)(NO) possess a potent O_{NO} donor atom coordinating strongly to the lithium ions of Li[HBEt₃], LiBH₄ and Li[N(SiMe₃)₂]. μ -NO coordination is observed in cyclic structures or coordination polymers.

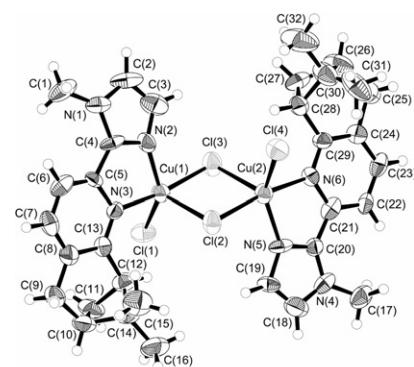


Pang-Fei Teng, Chui-Shan Tsang, Ho-Lun Yeung, Wing-Leung Wong, Wing-Tak Wong, Hoi-Lun Kwong

J. Organomet. Chem. 691 (2006) 5664

Syntheses of *C*₁-symmetric bidentate ligands having pyridyl and 1,3-Thiazolyl, 1-methylimidazolyl or pyrazinyl donor groups for enantioselective palladium-catalyzed allylic substitution and copper-catalyzed cyclopropanation

Chiral bidentate ligands, which possess 1,3-thiazolyl, 1-methylimidazolyl or pyrazinyl and one pyridyl group, were prepared. X-ray crystal structure analysis of a copper(II) complex having 1-methylimidazolyl group indicated that it is a μ -chloro bridge dimer. The Pd(II) and Cu(II) complexes were active catalysts in the asymmetric allylic substitution and cyclopropanation respectively.

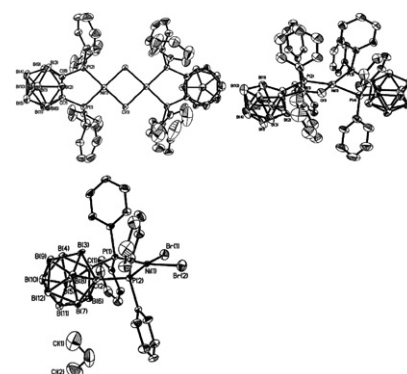


Jianmin Dou, Daopeng Zhang, Dacheng Li, Daqi Wang

J. Organomet. Chem. 691 (2006) 5673

Synthesis and characterization of three nickel(II) carborane complexes containing *nido*- or *closo*-carborane diphosphine ligand

Three nickel(II) carborane complexes, [Ni₂(μ -Cl)₂{7,8-(PPH₂)₂-7,8-C₂B₉H₁₀}₂] (1), [Ni{7-(OPPPh₂)-8-(PPH₂)-7,8-C₂B₉H₁₀}]{7,8-(PPH₂)₂-7,8-C₂B₉H₁₀}] (2) and [NiBr₂{1,2-(PPH₂)₂-1,2-C₂B₁₀H₁₀}] · CH₂Cl₂ (3), have been synthesized by the reactions of 1,2-bis(diphenylphosphino)-1,2-dicarbocloso-dodecaborane with NiCl₂ · 6H₂O and NiBr₂ · 6H₂O in ethanol under different conditions, respectively. For cluster 1, it could also be obtained under the solvothermal condition. All the three clusters were characterized by elemental analysis, FT-IR, ¹H and ¹³C NMR spectroscopy and X-ray structure determination.

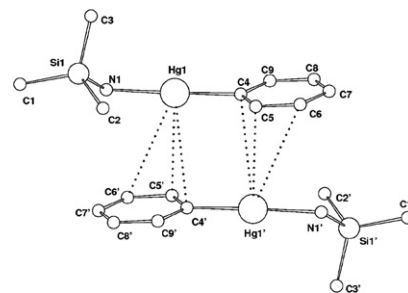


**Yann Sarazin, Joseph A. Wright,
Manfred Bochmann**

J. Organomet. Chem. 691 (2006) 5680

Synthesis and crystal structure of $[C_6H_5Hg(H_2NSiMe_3)][H_2N\{B(C_6F_5)_3\}_2]$, a phenyl–mercury(II) cation stabilised by a non-coordinating counter-anion

The new heteroleptic mercury(II) complex $PhHgN(SiMe_3)_2$ reacts with the cationic Brønsted acid $[H(OEt)_2][H_2N\{B(C_6F_5)_3\}_2]$ to yield $[C_6H_5Hg(H_2NSiMe_3)][H_2N\{B(C_6F_5)_3\}_2]$. The phenyl–mercury(II) cation exhibits Hg(II)–arene intermolecular π -bonding.

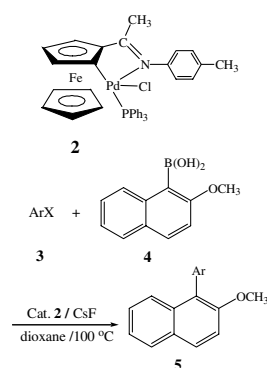


Hong Li, Yangjie Wu, Weibo Yan

J. Organomet. Chem. 691 (2006) 5688

An efficient catalyst for the synthesis of *ortho*-substituted biaryls by the Suzuki cross-coupling: Triphenylphosphine adduct of cyclopalladated ferrocenyline

The air and moisture stable triphenylphosphine adduct of cyclopalladated ferrocenyline **2** has been successfully used in palladium-catalyzed Suzuki cross-coupling for the synthesis of *ortho*-substituted biaryls in air. In the presence of 0.05 mol% of **2** as catalyst and 3 equivalent of CsF as base in dioxane at $100^\circ C$, *ortho*-substituted biaryls were synthesized with moderate to high yields in the reactions of 2-methoxy-1-naphthylboronic acid with aryl halides, and 14 new *ortho*-substituted biaryls were obtained and characterized.

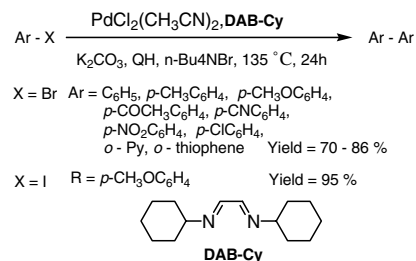


Ning Ma, Zheng Duan, Yangjie Wu

J. Organomet. Chem. 691 (2006) 5697

DAB-Cy as an inexpensive and effective ligand for palladium-catalyzed homocoupling reaction of aryl halides

A novel catalytic system of $PdCl_2(CH_3CN)_2$ with *N,N'*-dicyclohexyl-1,4-diazabutadiene (DAB-Cy) ligand was successfully used in reductive coupling of aryl halides.

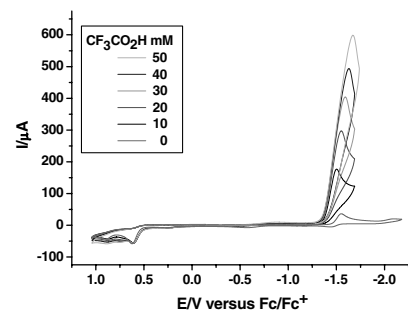


**Li-Cheng Song, Jian-Hua Ge, Xu-Feng Liu,
Li-Qun Zhao, Qing-Mei Hu**

J. Organomet. Chem. 691 (2006) 5701

Synthesis, structure and electrochemical properties of *N*-substituted diiron azadithiolates as active site models of Fe-only hydrogenases

Six new *N*-substituted ADT-type models $[(\mu-SCH_2)_2NR]Fe_2(CO)_6$ (**5**, R = CH_2CO_2Et ; **6**, $C_6H_4C(O)Me-p$; **7**, $C_6H_4CO_2Me-p$; **8**, C_6H_4SCN-p), $[(\mu-SCH_2)_2NC(O)CH_2C_{10}H_7-2]Fe_2(CO)_6$ (**9**) and 1,4- $[Fe_2(CO)_6(\mu-SCH_2)_2NC(O)]_2C_6H_4$ (**10**), as well as four new *N,N*-bis(chloromethyl)amines $RN(CH_2Cl)_2$ (**1**, R = CH_2CO_2Et ; **2**, $C_6H_4C(O)Me-p$; **3**, $C_6H_4CO_2Me-p$; **4**, C_6H_4SCN-p) were synthesized and characterized. Crystal structures of **5-7** and **9** along with the proton reduction to H_2 catalyzed by **7** are described.

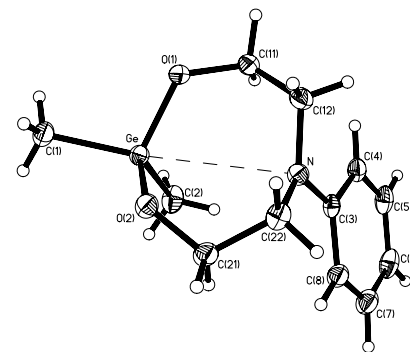


Elmira Kh. Lermontova, Anastasia A. Selina, Sergey S. Karlov, Andrei V. Churakov, Judith A.K. Howard, Yuri F. Oprunenko, Mikhail Yu. Antipin, Jörg Sundermeyer, Galina S. Zaitseva

J. Organomet. Chem. 691 (2006) 5710

The transannular interaction germanium–nitrogen in germocanes: The influence of substituents

The combined X-ray diffraction and NMR studies of the germocane structures allowed to state the relationships between the strength of the Ge ← N interaction and the nature of substituents in different positions of ocane skeleton. The determining factor is the nature of substituents at the Ge atom.

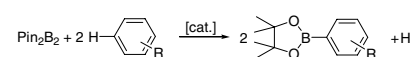


Guido D. Frey, Christoph F. Rentzsch, Denise von Preysing, Tobias Scherg, Michael Mühlhofer, Eberhardt Herdtweck, Wolfgang A. Herrmann

J. Organomet. Chem. 691 (2006) 5725

Rhodium and iridium complexes of *N*-heterocyclic carbenes: Structural investigations and their catalytic properties in the borylation reaction

Bridged and unbridged *N*-heterocyclic carbene (NHC) ligands are metalated with [Ir/Rh(COD)₂Cl]₂ to give rhodium(I/III) and iridium(I) mono- and biscarbene substituted complexes. For the first time, bis(carbene) substituted iridium complexes were used as catalysts in the synthesis of arylboronic acids starting from pinacolborane and arene derivatives.

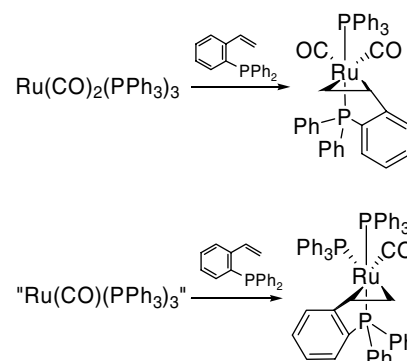


Eiichiro Mizushima, Naoto Chatani, Fumitoshi Kakiuchi

J. Organomet. Chem. 691 (2006) 5739

Synthesis of [Ru(CO)₂(PPh₃)(SP)] and [Ru(CO)(PPh₃)₂(SP)] and their catalytic activities for the hydroamination of phenylacetylene

The reaction of [Ru(CO)₂(PPh₃)₃] with *o*-styryldiphenylphosphine (SP) gave [Ru(CO)₂(PPh₃)(SP)] in high yield and the reaction of “Ru(CO)(PPh₃)₃” with SP afforded [Ru(CO)(PPh₃)₂(SP)] in moderate yield. When catalytic activities of several ruthenium complexes or the hydroamination of phenylacetylene with anilines were examined, Ru(CO)₂(PPh₃)(SP) showed the excellent catalytic activity.

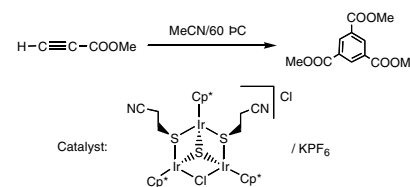


Akihiro Saito, Hidetake Seino, Hidenobu Kajitani, Fusao Takagi, Akihito Yashiro, Takeshi Ohnishi, Yasushi Mizobe

J. Organomet. Chem. 691 (2006) 5746

Synthesis of sulfido- and thiolato-bridged Ir₃ cluster and its reactions with alkyne and isocyanide including highly regioselective cyclotrimerization of methyl propiolate

Triiridium cluster [(Cp^{*}Ir)₃(μ₃-S)(μ₂-SCH₂CH₂CN)₂(μ₂-Cl)]Cl (**4**) was treated with XyNC (Xy = 2,6-Me₂C₆H₃) in the presence of KPF₆ at 60 °C to give a mixture of a mononuclear complex [Cp^{*}Ir(SCH₂CH₂CN)(CN-Xy)] [PF₆] and a dinuclear complex [(Cp^{*}Ir(CNXY))₂(μ-S)(μ-SCH₂CH₂CN)] [PF₆], whereas the reaction of **4** with methyl propiolate in the presence of KPF₆ at 60 °C resulted in the formation of a cyclic trimer of the alkyne 1,3,5-C₆H₃(COOMe)₃.

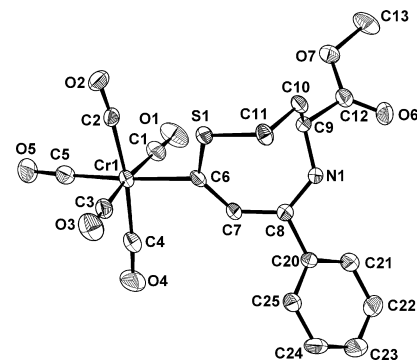


**Normen Szesni, Christiane Hohberger,
Gehad Genidy Mohamed, Nicolai Burzlaff,
Bernhard Weibert, Helmut Fischer**

J. Organomet. Chem. 691 (2006) 5753

Synthesis of heterocyclic carbene ligands via 1,2,3-diheterocyclization of allenylidene complexes with dinucleophiles

Novel heterocyclic carbene ligands are accessible via diheterocyclization from π -donor-substituted allenylidene pentacarbonyl complexes and dinucleophiles, $\text{HX}-\text{Y}-\text{NH}_2$ ($\text{X}=\text{NH}, \text{S}$). The reactions proceed by initial substitution of one group at C_γ of the allenylidene ligand by NH_2 followed by addition of XH to the $\text{C}_\alpha-\text{C}_\beta$ bond. The spacer Y determines the size of the ring.

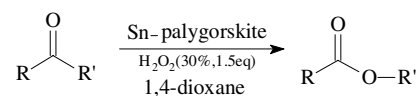


**Ziqiang Lei, Qinghua Zhang, Rongmin Wang,
Guofu Ma, Chengguo Jia**

J. Organomet. Chem. 691 (2006) 5767

Clean and selective Baeyer–Villiger oxidation of ketones with hydrogen peroxide catalyzed by Sn-palygorskite

An environmentally benign and selective Baeyer–Villiger oxidation system is introduced. Palygorskite-supported Sn complexes were prepared by a simple procedure. Cyclic ketones and acyclic ketones were oxidized by hydrogen peroxide in a reaction catalyzed by palygorskite-supported Sn complexes, affording corresponding lactones or esters with selectivity for the product of 90–99%. The influence of the solvents, reaction temperature, the amount of catalyst used and the reaction time on the catalytic activity and product selectivity were investigated in detail. The catalyst is cheap, easy to be prepared in large scale and can be recycled.

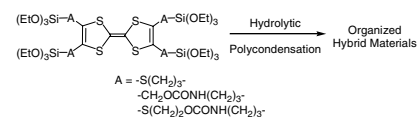


**Nathalie Bellec, Frédéric Lerouge,
Olivier Jeannin, Geneviève Cerveau,
Robert J.P. Corriu, Dominique Lorcy**

J. Organomet. Chem. 691 (2006) 5774

Auto-organization modulation of tetra-substituted tetrathiafulvalenes (TTF) in silica based hybrid materials

Anisotropic organization of electroactive organic bridging moieties in hybrid materials obtained by sol–gel chemistry is function of the interaction forces induced by the spacer between the TTF core and the four triethoxysilane groups. The silica-based hybrid solids are highly polycondensed and present different scales of organization (nanometric and micrometric).

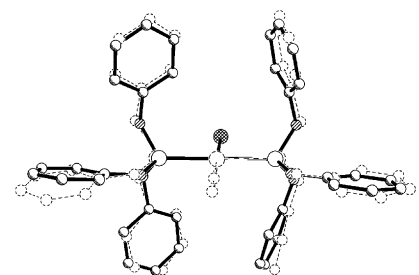


**Alfred Muller, Reinout Meijboom,
Andreas Roodt**

J. Organomet. Chem. 691 (2006) 5782

A crystallographic and DFT study on Vaska-type $\text{trans}[\text{Rh}(\text{CO})\text{Cl}(\text{PR}_3)_2]$ complexes containing flexible ligands: The molecular structure of $\text{trans}[\text{Rh}(\text{CO})\text{Cl}\{\text{P}(\text{OC}_6\text{H}_5)_3\}_2]$

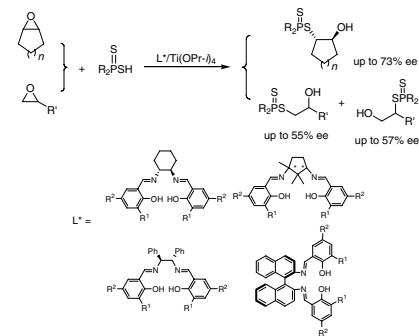
An investigation into the effect of the flexibility of substituents on the disorder of the $\text{Cl}-\text{Rh}-\text{CO}$ moiety in Vaska-type $\text{trans}[\text{Rh}(\text{CO})\text{Cl}(\text{PR}_3)_2]$ complexes is presented. The influence of the packing of the complexes with $\text{PR}_3 = \text{P}(\text{CH}_2\text{C}_6\text{H}_5)_3$, $\text{P}(\text{OC}_6\text{H}_5)_3$, $\text{P}(\text{O}-2\text{-MeC}_6\text{H}_4)_3$ and $\text{P}(\text{O}-2,6\text{-Me}_2\text{C}_6\text{H}_3)_3$ was evaluated by comparing the X-ray structures with the results of DFT calculations on these complexes. An overlay of the calculated and found structures shows the main differences to be in the orientation of the phenyl substituents. Reasonable agreement between the calculated and molecular structures was found.



**Zhenghong Zhou, Zhaoming Li,
Wang Quanyong, Bing Liu, Kangying Li,
Guofeng Zhao, Qilin Zhou, Chuchi Tang**
J. Organomet. Chem. 691 (2006) 5790

(Salen)Ti(IV) complex catalyzed asymmetric ring-opening of epoxides using dithiophosphorus acid as the nucleophile

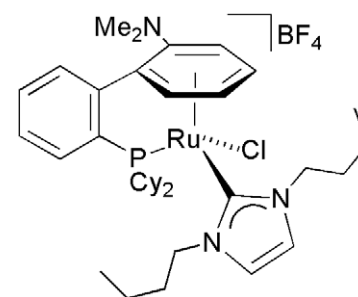
The enantioselective ring-opening of *meso* epoxides with dithiophosphorus acids catalyzed by a (salen)Ti(IV) complex formed *in situ* upon the treatment of Ti(OPr-*i*)₄ and chiral Schiff base was realized. The resulting products were obtained with low to good enantioselectivities (up to 73% ee). Moderate enantioselectivity was obtained for the (salen)Ti(IV) complex catalyzed ring-opening of racemic mono-substituted epoxides. High regioselectivity was observed for the alkyl substituted epoxides, whereas poor regioselectivity was obtained for the aryl substituted ones.



Jack W. Faller, Philip P. Fontaine
J. Organomet. Chem. 691 (2006) 5798

Synthesis and characterization of a planar chiral and chiral-at-metal ruthenium *N*-heterocyclic carbene complex

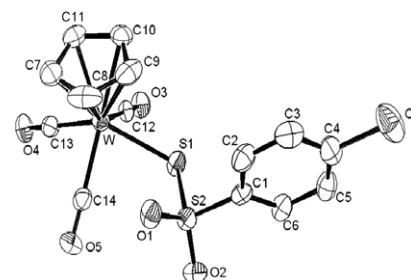
The stereoselective conversion of the neutral planar chiral arene-tethered complex [Ru(η^6 : η^1 -Me₂NC₆H₄C₆H₄PCy₂)Cl₂ (**1**), into [Ru(η^6 : η^1 -Me₂NC₆H₄C₆H₄PCy₂)(1,3-dibutylimidazol-2-ylidene)Cl]BF₄ (**2**) *via* silver transmetalation is described. Two fluxional processes were observed in **2**. The dication derived from **2** was used to catalyze the asymmetric Diels-Alder reaction of methacrolein and cyclopentadiene.



**Mohammad El-khateeb, Helmar Görls,
Wolfgang Weigand**
J. Organomet. Chem. 691 (2006) 5804

Cyclopentadienyl tungsten complexes with thiocarboxylate and thiosulfonate ligands: Structures of CpW(CO)₃SCOPh and CpW(CO)₃SSO₂-4-C₆H₄Cl

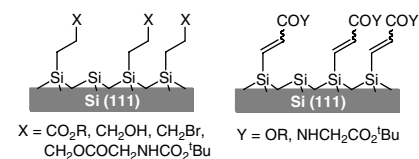
Treatment of CpW(CO)₃SH with RCOCl or RSO₂Cl affords CpW(CO)₃SCOR (**1**) [R = Me (**a**), CH₂Cl (**b**), Ph (**c**), 4-C₆H₄NO₂ (**d**)] and CpW(CO)₃SSO₂R (**2**) [R = Me (**a**), Ph (**b**), 4-C₆H₄Cl (**c**), 4-C₆H₄NO₂ (**d**)], respectively. Compounds **1** and **2** were characterized by elemental analyses, IR and ¹H NMR spectroscopy. The solid state structures of **1c** and **2c** were determined by an X-ray crystal structure analysis.



Yang Liu, Shoko Yamazaki, Suguru Izuhara
J. Organomet. Chem. 691 (2006) 5809

Modification and chemical transformation of Si(1 1 1) surface

A Si(1 1 1)-H surface was reacted with activated alkenes under mild conditions to give modified surfaces with terminal functional groups. Further chemical transformation of the modified surfaces was reported. Coverage ratios of ester modified surfaces were estimated by combination of surface reduction and gas chromatography analysis.

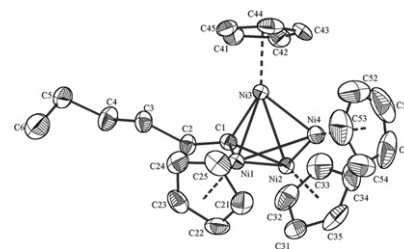


**Piotr Buchalski, Marek Cypryk,
Janusz Lipkowski, Stanisław Pasynekiewicz,
Antoni Pietrzykowski**

J. Organomet. Chem. 691 (2006) 5825

Novel tetrahedral tetranickel cluster with
alkylidyne ligand (NiCp)₄(μ₃-CR)

A novel tetrahedral (μ₃-alkylidyne)tetranickel cluster (NiCp)₄(μ₃-C(CH₂)₄CH₃) was obtained in the reaction of nickelocene with potassium and 1-hexene. The compound, characterised by means of MS and X-ray diffraction analysis, possessed 63 valence electrons, three more than the expected “magic number” for such type of clusters. It is paramagnetic with the magnetic moment 3.54 μ_B. This corresponds to three unpaired electrons per molecule and has been confirmed by DFT calculations. The alkylidyne carbon atom is located on one face of the nickel tetrahedron.

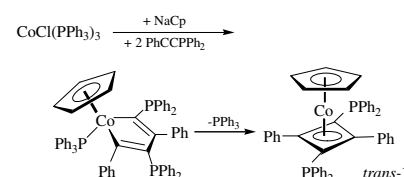


**Chin-Pei Chang, Roman G. Kultyshev,
Fung-E Hong**

J. Organomet. Chem. 691 (2006) 5831

Reaction of CpCo(PPh₃)₂ with
diphenylphosphinoalkynes: Syntheses and
X-ray structures of 1,3-cyclobutadiene-
substituted CpCoCb diphosphine and
2,5-cobaltacyclopentadiene
diphosphine
dioxide

A potentially bidentate cobalt-containing
phosphine, [(η⁵-C₅H₅)Co(η⁴-1,3-
(PPh₂)₂C₄Ph₂)] (*trans*-1), was prepared and its
capacity as phosphine ligand in the Suzuki
coupling reactions in the presence of Pd(OAc)₂
was evaluated.

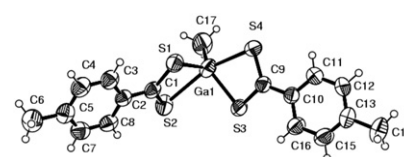


**Shamik Ghoshal, Vimal K. Jain,
Dimple P. Dutta, Prasad P. Phadnis,
Munirathinam Nethaji**

J. Organomet. Chem. 691 (2006) 5838

Gallium and indium dithiocarboxylates:
Synthesis, spectroscopic characterization and
structure of [MeGa(S₂Ctol)₂]

Several gallium and indium dithiocarboxylate
complexes of the type [Me_nM(S₂CR)_{3-n}]
(M = Ga, In; n = 0, 1, 2; R = phenyl (Ph), *p*-
tolyl (tol), mesityl (Mes)) have been synthe-
sized and characterized by spectroscopic
methods. Structure of [MeGa(S₂Ctol)₂] has
been established by X-ray crystallography.
The complex [Me₂InS₂Ctol] underwent a two-
step thermal decomposition leading to the
formation of tetragonal β-In₂S₃.

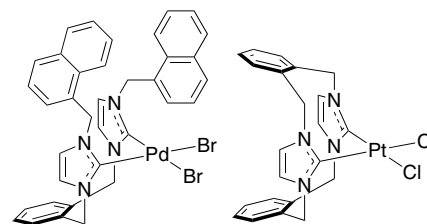


**Murray V. Baker, David H. Brown,
Peter V. Simpson, Brian W. Skelton,
Allan H. White, Charlotte C. Williams**

J. Organomet. Chem. 691 (2006) 5845

Palladium, rhodium and platinum complexes
of *ortho*-xylyl-linked bis-*N*-heterocyclic
carbenes: Synthesis, structure and catalytic
activity

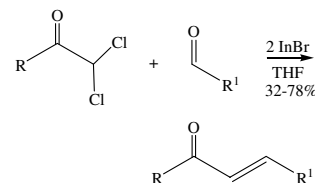
New Pd(II), Pt(II) and Rh(I) complexes that
contain two NHC units linked by an *ortho*-
xylyl group are described and structurally and
spectroscopically characterised. The catalytic
activity of the Pd(II) complexes in Heck and
Suzuki cross-coupling reactions has been ex-
amined to investigate any effects of the struc-
tural changes in the NHC-ligand framework.



Clovis Peppe, Rafael Pavão das Chagas*J. Organomet. Chem.* 691 (2006) 5856

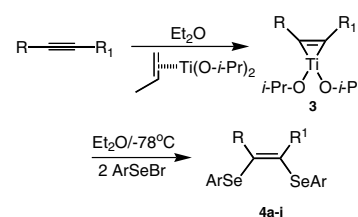
Indium(I) bromide-promoted stereoselective preparation of (*E*)- α,β -unsaturated ketones via sequential intermolecular aldol-type coupling/elimination reactions of α,α -dichloroketones with aldehydes

Indium(I) bromide promotes the reaction of α,α -dichloroketones with aldehydes to produce (*E*)- α,β -unsaturated ketones, exclusively. The transformation occurs via two sequential reactions, an aldol-type coupling between the two carbonylic reagents followed by an elimination process.

**Claudio C. Silveira, Rodrigo Cella, Adriano S. Vieira***J. Organomet. Chem.* 691 (2006) 5861

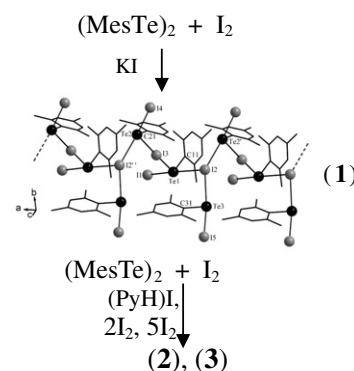
Stereoselective synthesis of vinylic (*Z*)-*vic*-bis(arylchalcogenides)

Alkyne-titanium complexes **3**, readily prepared *in situ* by the reaction of alkynes with $\text{Ti}(\text{O-}i\text{-Pr})_4/2$ *i*-PrMgCl, react with chalcogen electrophilic species under mild conditions to provide the corresponding addition products **4** in fair to good yields. The obtained vinylic *vic*-bis(arylchalcogenides) are useful synthetic intermediates for introducing vinyl functions into organic molecules.

**Eliandro Faoro, Gelson Manzoni de Oliveira, Ernesto Schulz Lang***J. Organomet. Chem.* 691 (2006) 5867

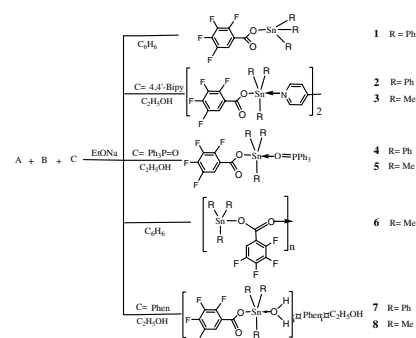
Uncommon assembling of organotellurium iodides: Synthesis and X-ray characterization of $[\text{mesTeI}(\mu\text{-I})_2(\text{TeImes})_2]_n$, $(\text{C}_5\text{H}_6\text{N})_4[\text{mesTeI}_2]_2(\text{I}_3)_2$ and $\{(\text{C}_5\text{H}_6\text{N})_3[(\text{mesTeI}_3)(\mu\text{-I}^-)(\text{TeI}_3\text{mes})](\text{I}_3)_2\}_n$ (mes = 2,4,6-trimethylphenyl)

$(\text{MesTe})_2$ (mes = mesityl) reacts with I_2 in the presence of KI to give $[\text{mesTeI}(\mu\text{-I})_2(\text{TeImes})_2]_n$ (**1**). If $(\text{PyH})\text{I}$ and two/five equivalents of I_2 are added to the mixture $(\text{mesTe})_2/\text{iodine}$, $(\text{C}_5\text{H}_6\text{N})_4[\text{mesTeI}_2]_2(\text{I}_3)_2$ (**2**) and $\{(\text{C}_5\text{H}_6\text{N})_3[(\text{mesTeI}_3)(\mu\text{-I}^-)(\text{TeI}_3\text{mes})](\text{I}_3)_2\}_n$ (**3**) are produced. Complex **2** form single dimers, **1** and **3** assemble polymeric chains. In compound **1** tellurium occurs as Te^{II} and Te^{IV} . Charge Transfer (CT) systems are associated to the I_3^- ions and **3** probably encloses also an inner CT system.

**Chunlin Ma, Junshan Sun, Rufen Zhang***J. Organomet. Chem.* 691 (2006) 5873

Self-assembly of triorganotin(IV) moieties with 2,3,4,5-tetrafluorobenzoic acid and 4,4'-bipy, triphenylphosphine oxide or phen: Syntheses, characterizations and supramolecular structures

A series of triorganotin(IV) complexes with 2,3,4,5-tetrafluorobenzoic acid and mixed-ligands of the types: $\text{R}_3\text{Sn}(\text{O}_2\text{CC}_6\text{HF}_4)_m \cdot \text{L}$ ($m = 1, \text{L} = 0, \text{R} = \text{Ph}$ **1**; $m = 1, \text{L} = \text{Ph}_3\text{PO}$, $\text{R} = \text{Ph}$ **4**, Me **5**), $[\text{R}_3\text{Sn}(\text{O}_2\text{CC}_6\text{HF}_4)_m]_n \cdot \text{L}$ ($m = 2, \text{L} = 4,4'$ -bipy, $\text{R} = \text{Ph}$ **2**, Me **3**; $m = n, \text{L} = 0, \text{R} = \text{Me}$ **6**), and $[\text{R}_3\text{Sn}(\text{O}_2\text{CC}_6\text{HF}_4) \cdot (\text{H}_2\text{O})]_m \cdot \text{L} \cdot \text{C}_2\text{H}_5\text{OH}$ ($m = 2, \text{L} = \text{Phen}$, $\text{R} = \text{Ph}$ **7**, Me **8**), (4,4'-bipy = 4,4'-bipyridyl; Phen = 1,10-phenanthroline), have been synthesized by the reaction of triorganotin chloride and 2,3,4,5-tetrafluorobenzoic acid in the presence of mixed-ligands: 4,4'-bipy, triphenylphosphine oxide, or phen. All complexes were characterized by elemental analysis, IR, ^1H , ^{13}C , ^{119}Sn NMR spectroscopy analysis. Except for **5** and **8**, all the complexes were also characterized by X-ray crystallography.



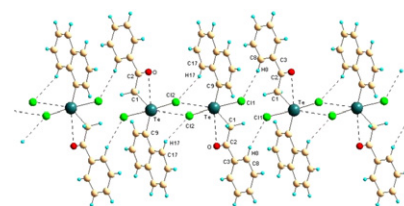
A=2,3,4,5-Tetrafluorobenzoic acid; B= Triorganotin(IV) chlorides

Ashok K.S. Chauhan, Anamika, Arun Kumar, Ramesh C. Srivastava, R.J. Butcher, Andrew Duthie

J. Organomet. Chem. 691 (2006) 5887

1-Naphthyl- and mesityltellurium(IV, II) derivatives of small bite chelating organic ligands: Effect of steric bulk and intramolecular secondary bonding interaction on molecular geometry and supramolecular association

Influence of sterically demanding 1-naphthyl or mesityl ligand and a small bite chelating ligand capable of 1,4-Te \cdots O intramolecular interaction on the crystal structure of unsymmetric diorganotellurium(IV) compounds was studied. The stronger steric repulsion of the mesityl group in comparison to lone pair–bond pair repulsion widens the equatorial C–Te–C angle in the diorganotellurium dichloride. Extensive Te \cdots Cl bond interactions present in the case of the 1-naphthyl derivative, 1Aa are inhibited in the mesityl derivative due to larger steric requirement.

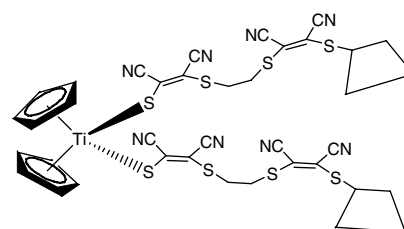


Zhenda Lu, Changsheng Lu, Xiaoming Ren, Qingjin Meng

J. Organomet. Chem. 691 (2006) 5895

New metallocene-bridged cyclodextrin dimer: A stable derivative of the antitumor drug titanocene dichloride and its potent cytotoxicity against human breast cancer (MCF-7) cells

A novel cyclodextrin dimer bridged with titanocene moiety has been synthesized and characterized. The introduction of the cyclodextrin into the titanocene compound remarkably increased its soluble and stable ability in water and the new compound demonstrated much higher cytotoxicity against human breast cancer cells than titanocene dichloride.

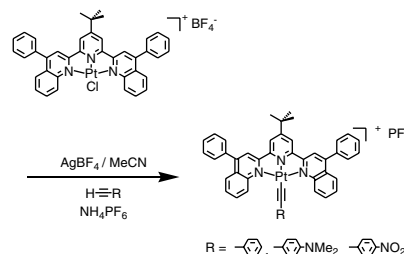


Chul Baik, Won-Sik Han, Youngjin Kang, Sang Ook Kang, Jaejung Ko

J. Organomet. Chem. 691 (2006) 5900

Synthesis and photophysical properties of luminescent platinum(II) complexes with terdentate polypyridine ligands: [Pt(bpqb)X] and [Pt(tbbppy)X](PF₆) (bpqb-H = 1,3-bis(4'-phenyl-2'-quinoliny) benzene; tbbppy = 4-*tert*-butyl-1,3-bis(4'-phenyl-2'-quinoliny) pyridine; X = Cl, C \equiv CC₆H₅, C \equiv CC₆H₄NMe₂, C \equiv CC₆H₄NO₂)

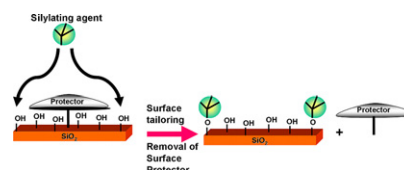
A series of square planar Pt(II) complexes (**1–8**) have been synthesized and characterized. Most of complexes display room temperature photoluminescence. The emission energies are sensitive to the acetylide ligands with different substituents on the phenyl ring.



Alireza Badiei, Laurent Bonneviot, Nicolas Crowther, Ghodsi Mohammadi Ziarani
J. Organomet. Chem. 691 (2006) 5911

Surface tailoring control in micelle templated silica

Surface tailoring control was studied using new concept surface-protector (SP) group that can cover a part of surface. In micelle templated silica (MTS), cationic surfactant had the role of SP group. The SP groups prevent to surface tailoring by silylating agents. Thus the uncovered surface will be silylated, and then the SP group will be removed. It was demonstrated that controlled silylation may yield hydrophilic islands of very small size within the channel of MTS.

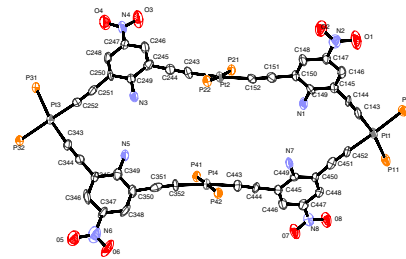


**Ilaria Fratoddi, Maurizio Delfini,
Fabio Sciubba, Michael B. Hursthouse,
Helen R. Ogilvie, Maria V. Russo**

J. Organomet. Chem. 691 (2006) 5920

Intermolecular stacking of a tetranuclear cyclic Pt(II) complex: NMR characterization and X-ray crystal structure of *cis-trans-cis-trans* tetra[μ -2,6-diethynyl-4-nitroaniline-bis(tri(*p*-tolyl)phosphine)platinum(II)]

A cyclic complex containing four Pt(II) centers bridging four 2,6-diethynyl-4-nitroaniline spacers was obtained. X-ray crystal structure showed the formation of alternate of *cis* and *trans* Pt centers in a twisted cyclic structure. NOESY and ROESY studies gave support to the presence of intermolecular stacking interactions among adjacent cycles.

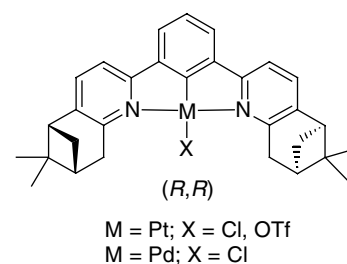


**Myeong Sik Yoon, Rengan Ramesh,
Jeongryul Kim, Dowook Ryu, Kyo Han Ahn**

J. Organomet. Chem. 691 (2006) 5927

Chiral Pt(II)/Pd(II) pincer complexes that show C–H···Cl hydrogen bonding: Synthesis and applications to catalytic asymmetric aldol and silylcyanation reactions

Chiral pyridine-based Pt(II)/Pd(II) pincer complexes are synthesized, which show C–H···Cl hydrogen bonding both in solution and solid states. Catalytic efficiency was evaluated with the triflate pincer complex in asymmetric aldol and silylcyanation reactions.

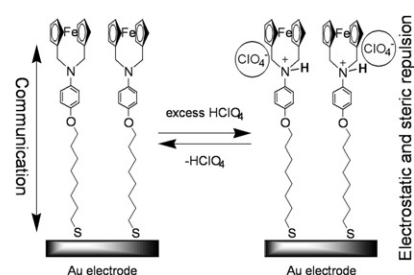


**Masaki Horie, Tatsuaki Sakano,
Kohtaro Osakada**

J. Organomet. Chem. 691 (2006) 5935

Preparation and electrochemical properties of SAM of alkanethiols functionalized with 2-aza[3]ferrocenophane on gold electrode

Thiols functionalized with *N*-aryl[3]azaferrocenophane formulated as HS-(CH₂)_n-N(CH₂Cp)₂Fe (**1–4**; *n* = 6, 8, 10, 12) and disulfide obtained by oxidation of **4** (**5**) were synthesized. Self-assembled monolayers (SAMs) of these thiols and disulfide on gold electrode were prepared and electrochemical properties were investigated by cyclic voltammetry in neutral and acidic solution.

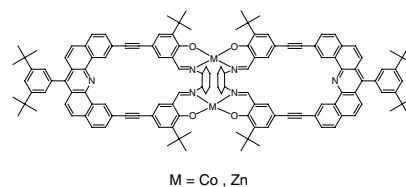


**Duckhyun Kim, Il Jung, Kyu Ho Song,
Sang Ook Kang, Jaejung Ko**

J. Organomet. Chem. 691 (2006) 5946

Self-assembly of rectangles via building units bearing salen and oxazoline ligands

Building units with two parallel coordination sites such as salen and oxazoline units have been synthesized. The spacer-chelators readily self-assembled with metal acetates such as Zn²⁺ and Co²⁺ to form molecular rectangles. The overall dimensions of the rectangles are 6.2 Å × 23.5 Å.

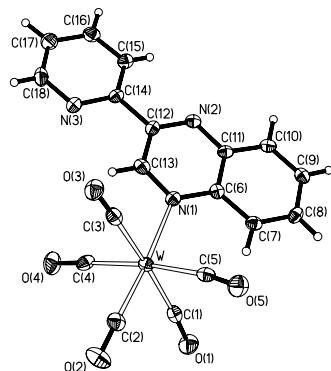


**Irene Veroni, Christiana A. Mitsopoulou,
Fernando J. Lahoz**

J. Organomet. Chem. 691 (2006) 5955

Isolation, X-ray structure and properties of an unusual pentacarbonyl(2,2'-pyridyl-quinoxaline) tungsten complex

The synthesis, spectroscopical and structural characterization of 2-(2'-pyridyl)quinoxaline-pentacarbonyl tungsten (**1**) are reported. 2-(2'-Pyridyl)quinoxaline is mono-coordinated in an unexpected way resulting in new potential complexes. The reaction of **1** with toluene under mild conditions afford, after an isomerization of the ligand the related tetracarbonyl tungsten complex.

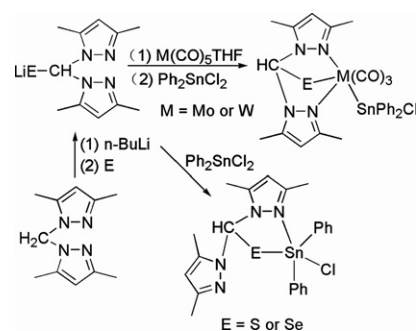


Run-Yu Tan, Hai-Bin Song, Liang-Fu Tang

J. Organomet. Chem. 691 (2006) 5964

The modification of bis(pyrazol-1-yl)methanes by chalcogen (S and Se) and their related reactions with organotin chloride and $M(\text{CO})_5\text{THF}$ ($M = \text{Mo}$ and W)

The modification of bis(pyrazol-1-yl)methanes by sulfur or selenium on the methine carbon atom has been successfully carried out by the reaction of the bis(pyrazol-1-yl)methide anions with elemental sulfur or selenium, and their related reactions with organotin chloride and $M(\text{CO})_5\text{THF}$ ($M = \text{Mo}$ and W) have also been studied.

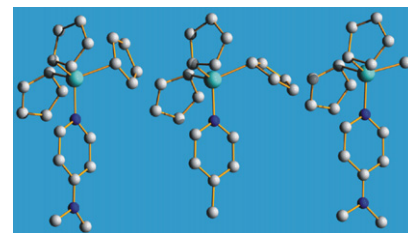


**Kinga Leszczyńska, Izabela Madura,
Antoni R. Kunicki, Janusz Zachara**

J. Organomet. Chem. 691 (2006) 5970

Cyclopentadienylaluminum donor-acceptor complexes – Molecular and supramolecular structure

Lewis acid–base complexes of cyclopentadienylaluminum derivatives $\text{Me}_x\text{Cp}_{3-x}\text{Al}$ ($x = 0-2$) and trimethylaluminum with 4-dimethylaminopyridine and 4-methylpyridine, were structurally characterized. The change of Cp–Al bond character from $\eta^1(\pi)$ to $\eta^1(\sigma)$ was found to reasonable correlate with the aromaticity of Cp^- ligand described by HOMA index. The presence of $\text{CH} \cdots \pi$ interactions leads to the formation of 2-D supramolecular networks and impacts on the coordination sphere of aluminum and the conformation of Cp ring.



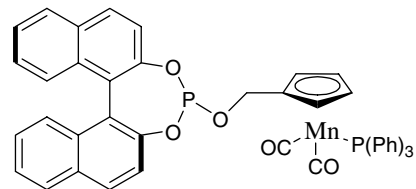
Notes

**Sergey E. Lyubimov, Vadim A. Davankov,
Nikolay M. Loim, Lyudmila N. Popova,
Pavel V. Petrovskii, Petr M. Valetskii,
Konstantin N. Gavrilov**

J. Organomet. Chem. 691 (2006) 5980

Cymantrene-derived monodentate phosphites: New ligands for Rh-catalyzed enantioselective hydrogenation

Novel chiral monodentate phosphite ligands bearing cymantrene fragment have been prepared. Phosphite **4** with PPh_3 , instead of CO-ligand, in cymantrene moiety provided higher enantioselectivity than its unsubstituted analogue **3** in hydrogenation of (*Z*)-methyl-2-acetamido-3-phenylacrylate.

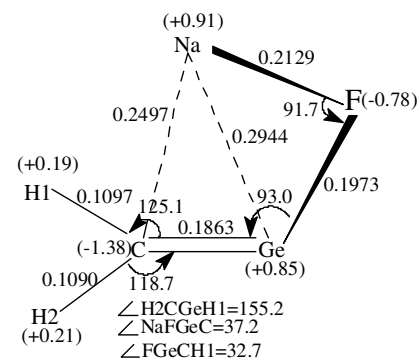


Wen-Zuo Li, Jian-Bo Cheng, Bao-An Gong,
Cui-Ping Xiao

J. Organomet. Chem. 691 (2006) 5984

DFT study on the unsaturated germylenoid
 $\text{H}_2\text{C}=\text{GeNaF}$

Equilibrium structures and isomerization reactions of the unsaturated germylenoid $\text{H}_2\text{C}=\text{GeNaF}$ were calculated at the B3LYP/6-311+G(d,p) level.



Elizabeth D. Blue, T. Brent Gunnoe,
Jeffrey L. Petersen, Paul D. Boyle

J. Organomet. Chem. 691 (2006) 5988

Protonation of *N*-heterocyclic carbene ligand coordinated to copper(I): Coordination mode of imidazolium cation as a function of counterion as determined by solid-state structures

Reactions of $(\text{IPr})\text{Cu}(\text{X})$ ($\text{X} = \text{Cl}$ or OTf , $\text{IPr} = 1,3\text{-bis}(2,6\text{-diisopropylphenyl})\text{imidazol-2-ylidene}$) complexes with HOTf or HCl results in protonation of C2 of IPr to form an imidazolium cation. The coordination mode of the imidazolium depends upon the counterions. Complexes $[(\text{IPrH})\text{Cu}(\text{OTf})(\mu\text{-OTf})_2]$ and $[(\text{IPrH})][\text{CuCl}_2]$ have been fully characterized including solid-state structures.

