

## Contents

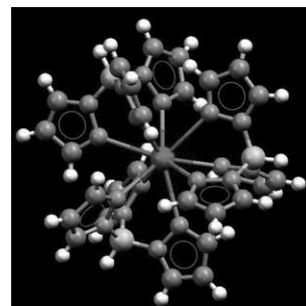
### Regular papers

**Ricardo O. Freire, Nivan B. da Costa Jr.,  
Gerd B. Rocha, Alfredo M. Simas**

*J. Organomet. Chem.* 690 (2005) 4099

Modeling lanthanide coordination compounds: Sparkle/AM1 parameters for praseodymium (III)

The Sparkle/AM1 model, recently defined for Eu(III), Gd(III) and Tb(III) [Inorg. Chem. 44 (2005) 3299] is now extended to Pr(III), using the same parameterization scheme. For 48 complexes, the Sparkle/AM1 unsigned mean error, for all interatomic distances between the Pr(III) ion and the ligand atoms of the first sphere of coordination, is 0.08 Å, again comparable to present day ab-initio/ECP calculations, while being hundreds of times faster.

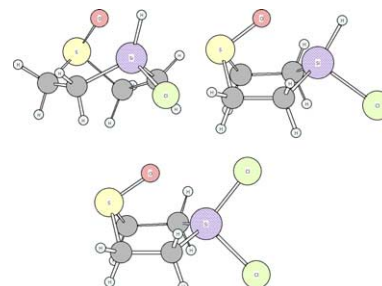


**Fillmore Freeman, Behrooz Entezam,  
Faranak Gomarooni, Timothy S. Welch,  
Bagrat A. Shainyan**

*J. Organomet. Chem.* 690 (2005) 4103

Computational study of conformations and of sulfinyl oxygen-induced pentacoordination at silicon in 4-chloro-4-silathia-cyclohexane 1-oxide and 4,4-dichloro-4-silathia-cyclohexane 1-oxide

Boat and twist conformers of axial chlorosilathiacyclohexane 1-oxides were found to be minima and to be stabilized by transannular coordination of the sulfinyl oxygen with silicon that resulted in trigonal bipyramidal geometry at silicon.

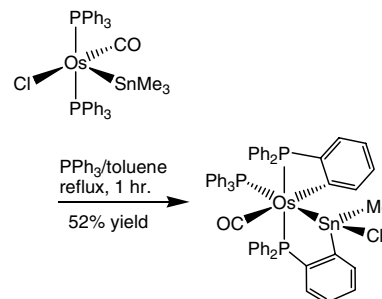


**Guo-Liang Lu, Clifton E.F. Rickard,  
Warren R. Roper, L. James Wright**

*J. Organomet. Chem.* 690 (2005) 4114

Metallacyclic complexes with *ortho*-stannylated triphenylphosphine ligands,  $L_n\text{Os}(\kappa^2(\text{Sn},\text{P})\text{-SnMe}_2\text{C}_6\text{H}_4\text{PPh}_2)$ , derived from thermal reactions of the five-coordinate complex,  $\text{Os}(\text{SnMe}_3)\text{Cl}(\text{CO})(\text{PPh}_3)_2$

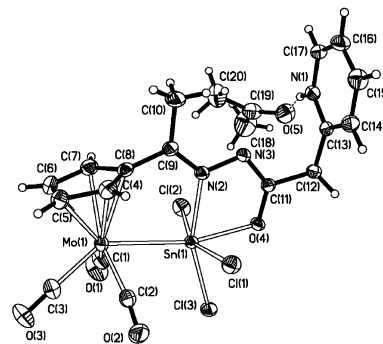
The coordinatively unsaturated trimethylstannyl complex,  $\text{Os}(\text{SnMe}_3)\text{Cl}(\text{CO})(\text{PPh}_3)_2$  undergoes a thermal reaction to form a mixture of  $\text{Os}(\kappa^2(\text{Sn},\text{P})\text{-SnMeClC}_6\text{H}_4\text{PPh}_2)(\kappa^2(\text{C},\text{P})\text{-C}_6\text{H}_4\text{PPh}_2)(\text{CO})(\text{PPh}_3)$  (**1**) and  $\text{Os}(\kappa^2(\text{Sn},\text{P})\text{-SnMe}_2\text{C}_6\text{H}_4\text{PPh}_2)(\kappa^2(\text{C},\text{P})\text{-C}_6\text{H}_4\text{PPh}_2)(\text{CO})(\text{PPh}_3)$  (**2**), each complex containing both *ortho*-stannylated and *ortho*-metallated triphenylphosphine ligands. It is proposed that the *ortho*-stannylation reaction could proceed through the intermediacy of a stannylene complex.



**Liang-Fu Tang, Xue-Mei Zhao,  
Zhi-Hong Zou, Hai-Bin Song, Yu-Ping Zhai**  
*J. Organomet. Chem. 690 (2005) 4124*

Synthesis and crystal structures of cyclodiazastannoxides fused cyclopentadienyl M–Sn (M = Mo, W) bonded organometallic heterocycle

Reaction of  $\text{CH}_3\text{COC}_5\text{H}_4\text{M}(\text{CO})_3\text{SnCl}_3$  (M = Mo or W) with heteroaroylhydrazine in mild conditions yields cyclodiazastannoxides fused cyclopentadienyl M–Sn bonded organometallic heterocycle.

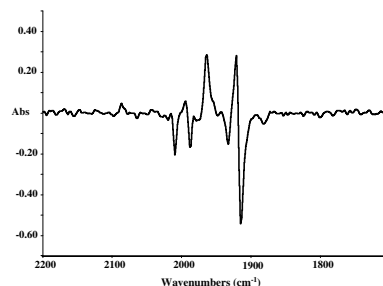


**Thiam Seong Chong, Peng Li,  
Weng Kee Leong, Wai Yip Fan**

*J. Organomet. Chem. 690 (2005) 4132*

TR-FTIR absorption spectroscopy of transition metal carbonyl radicals generated by photodissociation of metal–metal bonds, by halogen abstraction or by radical ligand substitution

Time-resolved FTIR studies of reversible and irreversible processes involving transition metal carbonyl radicals.

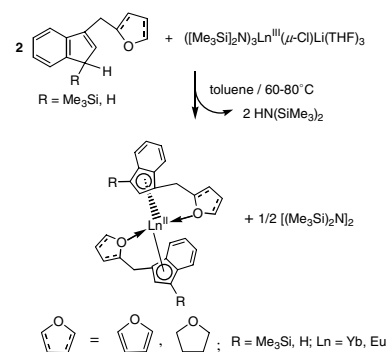


**Yongyong Wu, Shaowu Wang,  
Changtao Qian, Enhong Sheng, Meihua Xie,  
Gaosheng Yang, Qiqing Feng, Lijun Zhang,  
Xinliang Tang**

*J. Organomet. Chem. 690 (2005) 4139*

Homolysis of the Ln–N bond: Synthesis, characterization and catalytic activity of organolanthanide(II) complexes with furfuryl- and tetrahydrofurfuryl-functionalized indenyl ligands

A series of new organolanthanide(II) complexes with general formula  $[\eta^5:\eta^1-(\text{C}_4\text{H}_7\text{OCH}_2\text{-C}_9\text{H}_5\text{R})_2\text{Ln}^{\text{II}}]$  and  $[\eta^5:\eta^1-(\text{C}_4\text{H}_3\text{OCH}_2\text{C}_9\text{H}_5\text{-R})_2\text{Ln}^{\text{II}}]$  (Ln = Yb, Eu; R = Me<sub>3</sub>Si, H) were synthesized and characterized. Studies showed that the complexes with both trimethylsilyl and furfuryl- or tetrahydrofurfuryl functionalized groups on indenyl ligands have high catalytic activities on ring-opening polymerization of  $\epsilon$ -caprolactone.

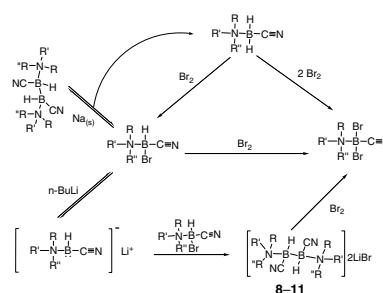


**Khuloud Takroui, Eli Shalom,  
Israel Goldberg, Jehoshua Katzhendler,  
Morris Srebnik**

*J. Organomet. Chem. 690 (2005) 4150*

Diborane (4) derivatives via coupling of amine monobromocyanoboranes: Study of the bromination of amine cyanoborane and molecular structures of the amine dibromocyanoboranes

Novel diborane (4) derivatives of amine cyanoboranes were successfully obtained, **8–11**, as their 2LiBr complexes from the monobromo derivatives of the corresponding amine cyanoboranes, **1–5**. Molecular structures of the trimethylamine dibromocyanoborane, **6**, and the triethylamine dibromocyanoborane, **7**, were determined using X-ray crystallography.

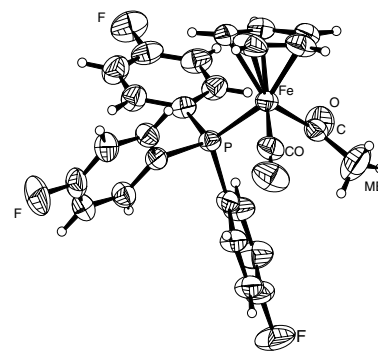


**Ntaoleng M. Makunya, Reinout Meijboom, Alfred Muller, Andreas Roodt**

*J. Organomet. Chem.* 690 (2005) 4159

Tertiary phosphine induced migratory carbonyl insertion in cyclopentadienyl complexes of iron(II)

In this contribution  $[\text{CpFe}(\text{CO})_2\text{Me}]$  is used as a model complex to study migratory CO insertion in the presence of isosteric tertiary phosphine ligands, and illustrates a simple application of this complex as a probe to evaluate steric and electronic properties of phosphine ligands.

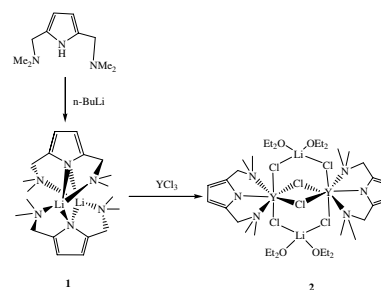


**Pei-Cheng Kuo, Jr-Chiang Chang, Wen-Yi Lee, Hon Man Lee, Jui-Hsien Huang**

*J. Organomet. Chem.* 690 (2005) 4168

Synthesis and characterization of lithium and yttrium complexes containing tridentate pyrrolyl ligands. Single-crystal X-ray structures of  $\{\text{Li}[\text{C}_4\text{H}_2\text{N}(\text{CH}_2\text{NMe}_2)_2, 2, 5]\}_2$  (**1**) and  $\{\text{C}_4\text{H}_2\text{N}(\text{CH}_2\text{NMe}_2)_2, 2, 5\}\text{YCl}_2(\mu\text{-Cl})\cdot\text{Li}(\text{OEt}_2)_2$  (**2**) and ring-opening polymerization of  $\epsilon$ -caprolactone

The lithiated pyrrolyl ligand,  $\{\text{Li}[\text{C}_4\text{H}_2\text{N}(\text{CH}_2\text{NMe}_2)_2, 2, 5]\}_2$  (**1**) was synthesized and structurally characterized. Reaction of **1** with  $\text{YCl}_3$  in the molar ratio 1:1 in diethyl ether at room temperature afforded a di-yttrium di-lithium tetranuclear complex,  $\{\text{C}_4\text{H}_2\text{N}(\text{CH}_2\text{NMe}_2)_2, 2, 5\}\text{YCl}_2(\mu\text{-Cl})\cdot\text{Li}(\text{OEt}_2)_2$  (**2**) in 87% yield. Compounds **1** and **2** were characterized by NMR spectroscopy and single crystal X-ray crystallography. Compound **1** shows high reactivity for the ring-opening polymerization of  $\epsilon$ -caprolactone.

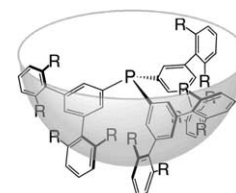


**Yoshiko Ohzu, Kei Goto, Hiroyuki Sato, Takayuki Kawashima**

*J. Organomet. Chem.* 690 (2005) 4175

Syntheses and structures of bowl-shaped triarylphosphines and their palladium(II) complexes

Novel bowl-shaped triarylphosphines, TRMP and TRIP, with large cone angles of  $174^\circ$  and  $206^\circ$ , respectively, were synthesized. The reaction of TRIP with  $\text{PdCl}_2$  produced the first example of a trinuclear palladium(II) chloride phosphine complex,  $[(\text{PdCl}_2)_3\text{-}(\text{TRIP})_2]$ , even when an excess amount of TRIP was employed.



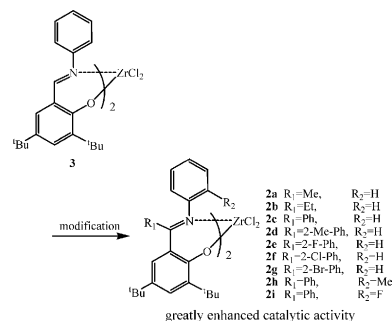
TRMP: R = Me  
TRIP: R = *i*-Pr

**Shangtao Chen, Xiaofan Zhang, Hongwei Ma, Yingying Lu, Zhicheng Zhang, Huayi Li, Zhanxia Lu, Nannan Cui, Youliang Hu**

*J. Organomet. Chem.* 690 (2005) 4184

A series of new zirconium complexes bearing bis(phenoxyketimine) ligands: Synthesis, characterization and ethylene polymerization

Nine new zirconium complexes bearing bis(phenoxyketimine) ligands (**2a–2i**) have been prepared and used for ethylene polymerization. The steric and electronic effects caused by the introduction of substituents on the imine carbon atom ( $\text{R}_1$ ) of the ligand on catalytic properties are discussed in detail.



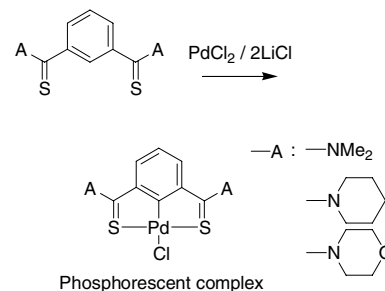
## Notes

Michinori Akaiwa, Takaki Kanbara,  
Hiroki Fukumoto, Takakazu Yamamoto

*J. Organomet. Chem.* 690 (2005) 4192

Luminescent palladium complexes containing thioamide-based SCS pincer ligands

Thioamide-based tridentate ligands, 1,3-benzenedicarbothioamides, were used to afford pincer palladium(II) complexes with  $\eta^3$ -S,C,S type coordination. The complexes exhibit strong emission in a glassy frozen state as well as in the solid state. The decay lifetime of the emission from the complexes is in a range of  $8\text{--}9 \times 10^{-5}$  s, which is indicative of phosphorescent emission.

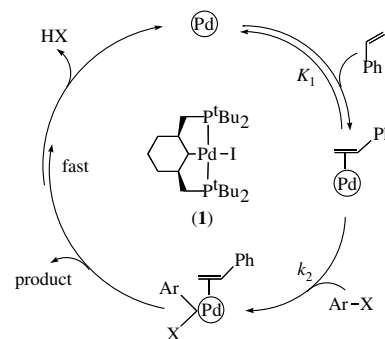


Patrik Nilsson, Ola F. Wendt

*J. Organomet. Chem.* 690 (2005) 4197

Kinetic investigation of a  $\text{PC}(\text{sp}^3)\text{P}$  pincer palladium (II) complex in the Heck reaction

An investigation of the kinetics of the Heck reaction catalysed by (1) has been performed in  $\text{DMF-}d_7$  solution. Based on mercury poisoning experiments a heterogeneous palladium catalyst is proposed. A mechanism consisting of a pre-equilibrium association of the olefin followed by an irreversible reaction with the aryl halide is suggested.

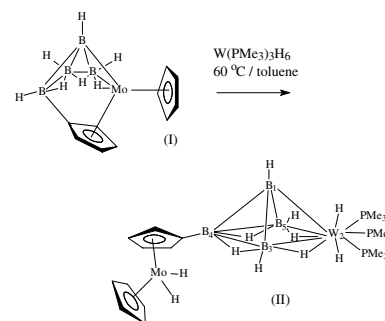


Malcolm L.H. Green, John B. Leach,  
Malcolm A. Kelland

*J. Organomet. Chem.* 690 (2005) 4203

Metal fragment exchange from a molybdaborane to a tungstaborane

Reaction of the molybdaborane *arachno*-2- $[\text{Mo}(\eta\text{-C}_5\text{H}_5)(\eta^5\text{-}\eta^1\text{-C}_5\text{H}_4)\text{B}_4\text{H}_7]$  (I) with the electron-rich molecule  $[\text{W}(\text{PMe}_3)_3\text{H}_6]$  at  $60^\circ\text{C}$  for 12 h in toluene gives the novel tungstaborane *nido*-2- $[\text{W}(\text{PMe}_3)_3\text{H}_2\text{B}_4\text{H}_7\text{-}[\text{Mo}(\eta\text{-C}_5\text{H}_5)(\eta^5\text{-}\eta^1\text{-C}_5\text{H}_4)\text{H}_2]]$  (II) in 60% yield. The reaction is almost quantitative when followed by NMR. This is a rare example of metal fragment exchange within a metallaborane cage.

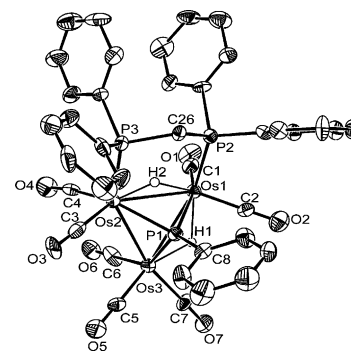


Shamsuddin M. Azad, Kazi A. Azam,  
Shariff E. Kabir, Madhu S. Saha,  
G.M. Golzar Hossain

*J. Organomet. Chem.* 690 (2005) 4206

Addition of primary phosphines to the unsaturated triosmium cluster  $[(\mu\text{-H})\text{Os}_3(\text{CO})_8\{\text{Ph}_2\text{PCH}_2\text{P}(\text{Ph})\text{C}_6\text{H}_4\}]$ : Synthesis of triosmium clusters bearing dppm, phosphido and phosphinidene ligands via P–H bond activation

Treatment of the electronically unsaturated cluster  $[(\mu\text{-H})\text{Os}_3(\text{CO})_8\{\text{Ph}_2\text{PCH}_2\text{P}(\text{Ph})\text{C}_6\text{H}_4\}]$  (**1**) with primary phosphines  $\text{PPhH}_2$  and  $\text{PCyH}_2$  gives the phosphido bridged compounds  $[(\mu\text{-H})\text{Os}_3(\text{CO})_8(\mu\text{-PPhH})(\mu\text{-dppm})]$  (**2**) and  $[(\mu\text{-H})\text{Os}_3(\text{CO})_8(\mu\text{-PCyH})(\mu\text{-dppm})]$  (**3**), respectively, by P–H bond activation of the phosphines and demetallation of the phenyl ring of the diphosphine ligand. Thermolysis of **2** and **3** in refluxing octane at  $128^\circ\text{C}$  results in the formation of the phosphinidene compounds  $[(\mu\text{-H})_2\text{Os}_3(\text{CO})_7(\mu_3\text{-PPh})(\mu\text{-dppm})]$  (**4**) and  $[(\mu\text{-H})_2\text{Os}_3(\text{CO})_7(\mu_3\text{-PCy})(\mu\text{-dppm})]$  (**5**), respectively, by further P–H bond cleavage of the phosphido groups. The molecular structure of **4** has been determined by single crystal X-ray diffraction analysis.



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