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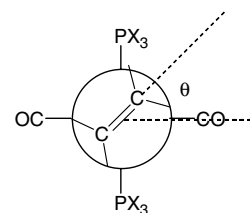
Regular papers

Alireza Ariafard

J. Organomet. Chem. 689 (2004) 2275

DFT studies of structural preference of coordinated ethylene in $W(CO)_3(PX_3)_2(CH_2=CH_2)$ ($X = H, CH_3, F, Cl, Br, \text{ and } I$)

A set of phosphine complexes of the type $W(CO)_3(PX_3)_2(CH_2=CH_2)$ ($X = H, CH_3, F, Cl, Br, \text{ and } I$) were investigated by density functional theory method (BP86) to examine the effect of the substituent X on the orientation of C–C vector of ethylene ligand with respect to one of the metal–ligand bonds as well as the donation and the backdonation in the bonding of phosphine and ethylene ligands.



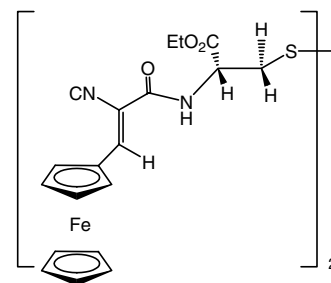
$X = CH_3, H, F, Cl, Br, I$

Sandra Díaz, Asensio González, Concepción López

J. Organomet. Chem. 689 (2004) 2284

Knoevenagel condensation of $[NC-CH_2C(O)-NH-CH(CO_2Et)-S]_2$ with ferrocene-carbaldehyde and the activation of the $\sigma(C-S)$ bond of $[(\eta^5-C_5H_5)Fe(\eta^5-C_5H_4)-CH=C(CN)-C(O)-NH-CH(CO_2Et)-CH_2-S-]_2$ induced by palladium(II)

The synthesis of the optically pure polyamides $[R-CH=C(CN)-C(O)-NH-CH(CO_2Et)-CH_2-S-]_2$ ($R = 4-MeO-C_6H_4, 4-NO_2-C_6H_4$ or $(\eta^5-C_5H_5)Fe(\eta^5-C_5H_4)$) is described. The electrochemical studies as well as the reactivity of the compound with $R =$ ferrocenyl group versus palladium(II) salts are also reported.

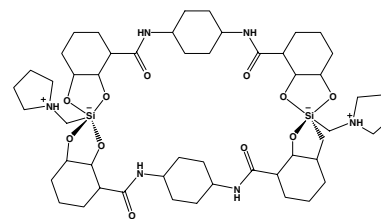


Joseph B. Lambert, Stephanie R. Singer

J. Organomet. Chem. 689 (2004) 2293

Self-assembled macrocycles with pentavalent silicon linkages

Organic substrates containing two catechol (*ortho*-dihydroxybenzene) components at opposite ends self-assemble with a silicon substrate containing three nucleofugic groups under basic conditions to produce macrocycles ranging from monomers to pentamers. Silicon is pentacoordinate, negatively charged, and possessed of one organic monodentate ligand attached via carbon and two catechol bidentate ligands attached via oxygen.

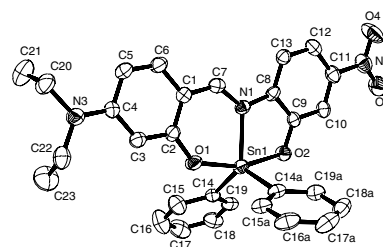


**Horacio Reyes, Concepción García,
Norberto Farfán, Rosa Santillan,
Pascal G. Lacroix, Christine Lepetit,
Keitaro Nakatani**

J. Organomet. Chem. 689 (2004) 2303

Syntheses, crystal structures, and quadratic nonlinear optical properties in four “push–pull” diorganotin derivatives

Four “push–pull” compounds were prepared through a one step reaction. Analysis of the spectroscopic data showed a pentacoordinated tin atom in solution while this atom exhibits a distorted trigonal bipyramidal geometry for the diphenyl derivatives and distorted octahedral for the dibutyl one, in the solid state, as established by X-ray analysis. The DFT computational study shows remarkable differences between the solid and the gas phase structures. The nonlinear optical NLO properties were studied theoretically, as well as with the EFISH technique.

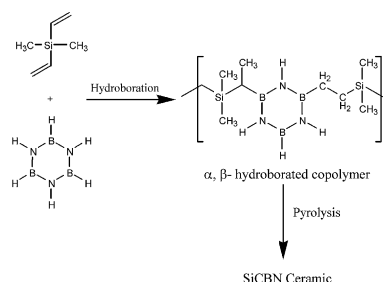


**Jong-Kyu Jeon, Quoc Dat Nghiem,
Dong-Pyo Kim, Jinyoung Lee**

J. Organomet. Chem. 689 (2004) 2311

Olefin hydroboration of borazine with vinylsilanes as precursors of Si–B–C–N ceramics

A processible polymeric precursor for Si–B–C–N ceramics was prepared by a hydroboration reaction between borazine and dimethyldivinylsilane using no catalyst with a synthetic yield 85%.

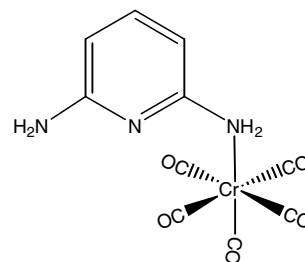


**Izzet Amour Morkan, Kutalmış Güven,
Saim Özkar**

J. Organomet. Chem. 689 (2004) 2319

Pentacarbonyl(2,6-diaminopyridine)chromium(0): synthesis and molecular structure

Photolysis of hexacarbonylchromium(0) in the presence of 2,6-diaminopyridine in toluene solution at 10 °C yields pentacarbonyl(2,6-diaminopyridine)chromium(0), which could be isolated from solution as plate-like crystals and fully characterized by using the single crystal X-ray diffractometry, MS, IR, and NMR spectroscopy. The 2,6-diaminopyridine ligand is bonded to the chromium atom through one of the NH₂ groups.

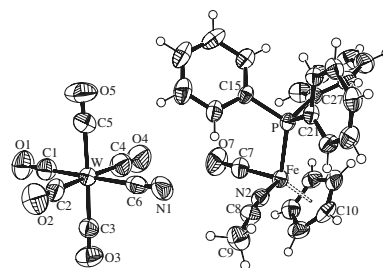


**Antonio Palazzi, Piera Sabatino,
Stefano Stagni, Silvia Bordoni,
Vincenzo G. Albano, Carlo Castellari**

J. Organomet. Chem. 689 (2004) 2324

Coordinating properties of [M(CO)₅(CN)][−] [M = Cr; Mo; W] ligands: formation of ion pairs or dinuclear cyanide-bridged complexes, spectroscopic and X-ray diffraction studies

The coordinating ability of the solvent plays a key role in the reaction of cyanopentacarbonyl anions [M(CO)₅(CN)][−] (M = Cr; Mo; W) with cationic Fe(II) organometallic fragments, which leads either to the formation of ion pairs such as [Cp(CO)(L)Fe(NCCH₃)]⁺[NCM(CO)₅][−], or neutral cyanide-bridged complexes like [Cp(CO)(L)FeNCM(CO)₅]. A comparison of spectroscopic and structural features of the isomeric compounds [Cp(CO)(L)FeNCM(CO)₅] and [Cp(CO)(L)FeCNM(CO)₅] is reported.

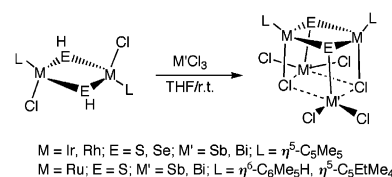


Wen-Yann Yeh, Hidetake Seino,
Takahiko Amitsuka, Shingo Ohba,
Masanobu Hidai, Yasushi Mizobe

J. Organomet. Chem. 689 (2004) 2338

Reactions of hydrosulfido- and hydro-selenido-bridged dinuclear Ir, Rh, and Ru complexes with SbCl_3 and BiCl_3 affording mixed-metal sulfido and selenido clusters containing both noble metals and Group 15 metals

Reactions of the hydrosulfido- or hydro-selenido-bridged dinuclear complexes $[(\text{L})\text{MCl}(\mu\text{-EH})_2\text{M}(\text{L})\text{Cl}]$ ($\text{M} = \text{Ir, Rh, Ru}$; $\text{E} = \text{S, Se}$; $\text{L} = \eta^5\text{-C}_5\text{Me}_5, \eta^5\text{-C}_5\text{EtMe}_4, \eta^6\text{-C}_6\text{Me}_5\text{H}$) with $\text{M}'\text{Cl}_3$ ($\text{M}' = \text{Sb, Bi}$) afforded the mixed-metal chalcogenido clusters containing both the noble metals and the Group 15 metals $[(\text{L})\text{MCl}(\mu\text{-EM}'\text{Cl}_2)_2\text{M}(\text{L})\text{Cl}]$ through dehydrochlorination.

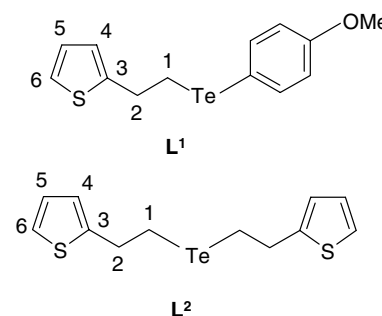


Sumit Bali, Ajai K. Singh, Pankaj Sharma,
R.A. Toscano, J.E. Drake, M.B. Hursthouse,
M.E. Light

J. Organomet. Chem. 689 (2004) 2346

2-[2-(4-Methoxyphenyltelluro)ethyl]thiophene (L^1) bis[2-(2-thienyl)ethyl] telluride (L^2) and their metal complexes; crystal structure of *trans*-dichlorobis{2-(2-(4-methoxyphenyltelluro)ethyl)thiophene-Te}palladium(II) and {bis[2-(2-thienyl)ethyl] telluride}dichloro(*p*-cymene)ruthenium(II)

2-[2-(4-methoxyphenyltelluro)ethyl]thiophene (L^1), bis[2-(2-thienyl)ethyl] telluride (L^2) and their complexes with Ag(I) , Hg(II) , Pd(II) , Pt(II) and Ru(II) have been synthesized and characterized by ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra. The two ligands coordinate only through Te. Single crystal structure of $[\text{PdCl}_2(\text{L}^1)_2]$ (**2**) and $[\text{Ru}(\textit{p}\text{-cymene})\text{Cl}_2(\text{L}^2)]$ (**6**) are solved. The Pd in **2** has square planar geometry and *trans* arrangement of ligands (Pd-Te = 2.5951(7) and 2.5872(7) Å). Unique intermolecular secondary Te...Cl interaction (distance = 3.450/3.449 Å) between neighbouring molecules in **2** results in the formation of a dimer (Pd-Pd = 3.2143(10) Å). In half sandwich compound **6** three coordination sites are occupied by two Cl atoms and Te atom of L^2 (Ru-Te = of 2.6528(9) Å; Ru-Cl = 2.415(2)/2.422(2) Å).

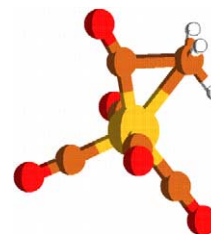


Xianghui Wang, Eric Weitz

J. Organomet. Chem. 689 (2004) 2354

A density functional theory study of alkyl group migration in $\text{RMn}(\text{CO})_5$ complexes

The kinetics of alkyl group migration in $\text{RMn}(\text{CO})_5$ complexes ($\text{R} = \text{CH}_3, \text{C}_2\text{H}_5$ and C_3H_7), isomers of $\text{CH}_3\text{Mn}(\text{CO})_5$, and transition states for interconversion of these species were studied using density functional theory. The activation free energy for this migration reaction was compared with experimental data and provides insights into the important steps in the overall reaction mechanism. The calculated transition state between $\text{CH}_3\text{Mn}(\text{CO})_5$ and the agostic isomer of $\text{CH}_3\text{COMn}(\text{CO})_4$.

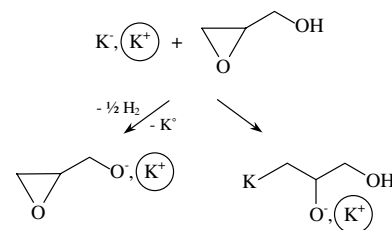


Zbigniew Grobelny, Andrzej Stolarzewicz,
Adalbert Maercker, Stanisław Krompiec,
Janusz Kasperczyk, Józef Rzepa, Holger Frey

J. Organomet. Chem. 689 (2004) 2361

Electron-transfer reduction of selected alcohols with alkali K^- , $\text{K}^+(15\text{-crown-5})_2$ via organopotassium intermediates

Simple alcohols such methanol and propanol are reduced with K^- , $\text{K}^+(15\text{-crown-5})_2$ to appropriate alkoxides. Potassium glycidoxide is the main product obtained in the reaction of **1** with glycidol. The reaction products formed initially can be further destroyed with the excess of **1**. Organopotassium compounds are the intermediates in these processes.

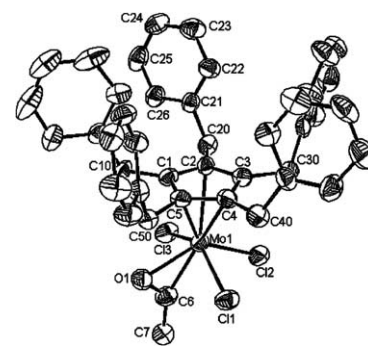


Ana M. Martins, Rita Branquinho,
Jinlan Cui, Alberto R. Dias,
M. Teresa Duarte, José Fernandes,
Sandra S. Rodrigues

J. Organomet. Chem. 689 (2004) 2368

Syntheses and structures of molybdenum and tungsten pentabenzylcyclopentadienyl complexes: new chlorination reactions

$[M(\text{CpBz})(\text{CO})_3\text{CH}_3]$ ($M = \text{Mo}$, **2a**, W , **2b**; $\text{CpBz} = \text{C}_5(\text{CH}_2\text{Ph})_5$) have been prepared and reacted with PCl_5 and $\text{PhI}\cdot\text{Cl}_2$. Depending on the metal and on the chlorinating reagent used $[\text{Mo}(\text{CpBz})(\eta^2\text{-COCH}_3\text{Cl}_3)]$, **3**, $[\text{W}(\text{CpBz})\text{Cl}_4]$, **4**, $[\text{Mo}(\text{CpBz})(\text{CO})_3\text{Cl}]$, **5** and $[\text{Mo}(\text{CpBz})\text{Cl}_4]$, **6** have been obtained. The molecular structures of all compounds are reported.

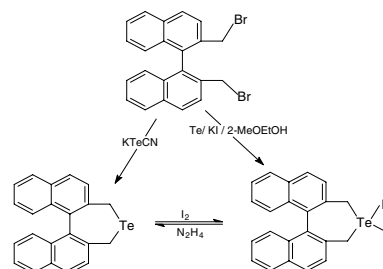


Ali Z. Al-Rubaie, Tarik A. Fahad,
Shaker A.N. Al-Jadaan, Najj A. Aboud

J. Organomet. Chem. 689 (2004) 2377

Synthesis and characterization of 2,7-dihydro-1*H*-dinaphtho[*c,e*]tellurepin: a new heterocyclic telluride

Synthesis of a chiral cyclic telluride (i.e., 2,7-dihydro-1*H*-dinaphtho[*c,e*]tellurepin (**1**)) is reported, together with its dihalo and tellurepinium derivatives. Compound **1** reduced the carbonyl groups in DDQ and TCQ to hydroxyl groups. $[(\text{C}_{22}\text{H}_{16}\text{Te})_2\text{PdCl}_2]$ was prepared by reaction of **1** with $[\text{PdCl}_2(\text{NCPH}_2)]$. All new compounds were characterized by elemental analysis and spectroscopic techniques.

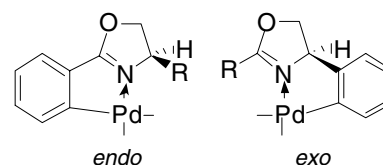


Olga N. Gorunova, Kristopher J. Keuseman,
Bryce M. Goebel, Nadezhda A. Kataeva,
Andrey V. Churakov, Lyudmila G. Kuz'mina,
Valery V. Dunina, Irina P. Smoliakova

J. Organomet. Chem. 689 (2004) 2382

Exo- and *endo*-palladacycles derived from (4*R*)-phenyl-2-oxazolines

The direct *ortho*-palladation of (*R*)-2,4-diphenyl-2-oxazoline and (*R*)-2-methyl-4-phenyl-2-oxazoline afforded an *endo*- and *exo*-palladacycle, respectively. The structures of cyclometallated dimeric complexes and their PPh_3 derivatives were confirmed by spectroscopic methods. The X-ray crystal study of the dimeric complex obtained from (*R*)-2,4-diphenyl-2-oxazoline confirmed the *endo* structure of the palladacycle.

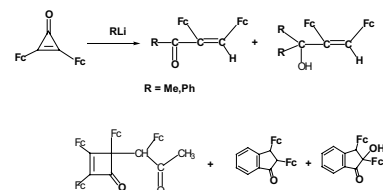


Elena I. Klimova, Tatiana Klimova,
Simón Hernández Ortega,
Maríana Esquivelzeta Rabell,
Lena Ruíz Ramírez, Marcos Martínez García

J. Organomet. Chem. 689 (2004) 2395

Reactions of 2,3-diferrocenylcyclopropanone with methyllithium and phenyllithium

Reactions of 2,3-diferrocenylcyclopropanone with methyllithium and phenyllithium afford products of the nucleophilic opening of the three-membered ring, viz., α , β -unsaturated ketones and allyl alcohols. The insertion product of a methyl(diferrocenyl)vinylcarbenoid into a σ -bond of the starting compound, viz., 2,3,4-triferrocenyl-4-(1-ferrocenyl-2-oxopropyl)cyclobutenone, along with intramolecular *ortho*-alkylation products, viz., 2,3-diferrocenylindanone and 2,3-diferrocenyl-2-hydroxyindanone, were also isolated. X-ray diffraction data for triferrocenylcyclobutenone and 2,3-diferrocenyl-2-hydroxyindanone are presented.

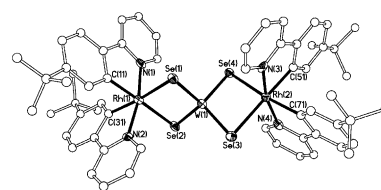


**Man-Kit Lau, Ka-Man Cheung,
Qian-Feng Zhang, Yinglin Song,
Wing-Tak Wong, Ian D. Williams,
Wa-Hung Leung**

J. Organomet. Chem. 689 (2004) 2401

Iridium(III) and rhodium(III) cyclometalated complexes containing sulfur and selenium donor ligands

Treatment of $[M(\text{Buppy})_2\text{Cl}]_2$ with bidentate sulfur ligands $S^{\wedge}S$ afforded the cyclometalated complexes $[M(\text{Buppy})_2(S^{\wedge}S)]$ ($M = \text{Ir}$ or Rh ; $\text{BuppyH} = 2\text{-}(4'\text{-tert-butylphenyl})\text{pyridine}$; $S^{\wedge}S = \text{Et}_2\text{NCS}_2$, $\text{S}_2\text{P}(\text{OMe})_2$, $\text{N}(\text{PPh}_2\text{S})_2$). Interactions of $[M(\text{Buppy})_2\text{Cl}]_2$ with $[\text{WQ}_4]^{2-}$ ($\text{Q} = \text{S}$ or Se) afforded the trinuclear heterometallic complexes $\{[M(\text{Buppy})_2]_2(\mu\text{-WQ}_4)\}$.

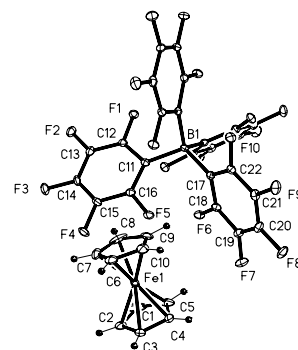


**Abby R. O'Connor, Chip Nataro,
James A. Golen, Arnold L. Rheingold**

J. Organomet. Chem. 689 (2004) 2411

Synthesis and reactivity of $[\text{N}(\text{C}_6\text{H}_4\text{Br})_3]\text{[B}(\text{C}_6\text{F}_5)_4]$: the X-ray crystal structure of $[\text{Fe}(\text{C}_5\text{H}_5)_2]\text{[B}(\text{C}_6\text{F}_5)_4]$

The synthesis and characterization of $[\text{N}(\text{C}_6\text{H}_4\text{Br})_3]\text{[B}(\text{C}_6\text{F}_5)_4]$ and $[\text{Fe}(\text{C}_5\text{H}_5)_2]\text{[B}(\text{C}_6\text{F}_5)_4]$ is presented. The crystal structure of $[\text{Fe}(\text{C}_5\text{H}_5)_2]\text{[B}(\text{C}_6\text{F}_5)_4]$ was determined.

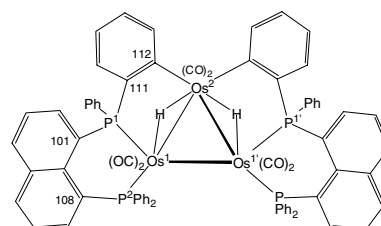


**Michael I. Bruce, Paul A. Humphrey,
Reinhard Schmutzler, Brian W. Skelton,
Allan H. White**

J. Organomet. Chem. 689 (2004) 2415

Reactions of 1,8-bis(diphenylphosphino)naphthalene with $\text{Os}_3(\text{CO})_{12}$: C–H and C–P bond cleavage reactions

Four complexes isolated from reactions between $\text{Os}_3(\text{CO})_{12}$ and 1,8-bis(diphenylphosphino)naphthalene (dppn) contain ligands formed by cleavage of C–H and C–P bonds in the dppn, with *P*-phenyl groups attached by η^1 or η^1 : η^2 modes. Also formed is a complex containing $\text{PPh}_2(\text{C}_{10}\text{H}_7\text{-1})$.



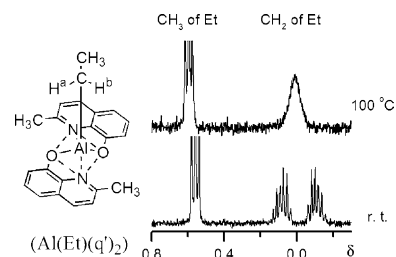
Notes

Takakazu Yamamoto, Takayuki Iijima

J. Organomet. Chem. 689 (2004) 2421

Fluxional behavior of $\text{Al}(\text{Et})(\text{q}')_2$ ($\text{q}' = 2\text{-methyl-8-quinolinolato}$) studied by temperature dependent ^1H NMR spectroscopy

Two $\alpha\text{-CH}_2$ hydrogens of the Et group in $\text{Al}(\text{Et})(\text{q}')_2$ ($\text{q}' = 2\text{-methyl-8-quinolinolato}$) show two ^1H NMR peaks at different positions due to the presence of a chiral center at Al. On raising the temperature, the two peaks collapsed, and coalesced above 100°C .

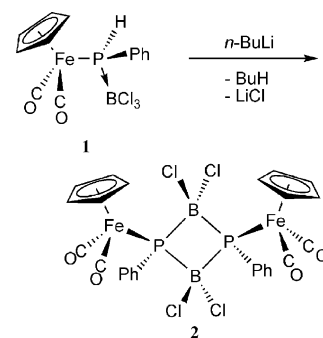


Kazuyuki Kubo, Ikue Kanemitsu,
Eri Murakami, Tsutomu Mizuta,
Hiroshi Nakazawa, Katsuhiko Miyoshi

J. Organomet. Chem. 689 (2004) 2425

Synthesis of a transition-metalated phosphinoborane dimer

$\text{Cp}(\text{CO})_2\text{Fe}\{\text{P}(\text{BCl}_3)\text{HPh}\}$ was treated with $n\text{-BuLi}$ to yield the iron-phosphinoborane dimer, $[\text{Cp}(\text{CO})_2\text{Fe}\{\text{P}(\mu\text{-BCl}_2)\text{Ph}\}]_2$. The dimer has a bent P_2B_2 4-membered ring with two iron complex fragments in equatorial positions.



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