





Volume 693, issue 10, 1 May 2008



www.elsevier.com/locate/jorganchem

Contents

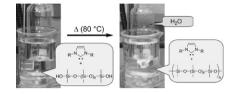
Communications

Sébastien Marrot, Fabien Bonnette, Tsuyoshi Kato, Laurent Saint-Jalmes, Etienne Fleury, Antoine Baceiredo

J. Organomet. Chem. 693 (2008) 1729

N-Heterocyclic carbene-catalyzed dehydration of α , ω -disilanol oligomers

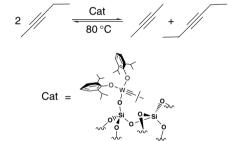
An efficient dehydration of disilanol oligomers, catalyzed by moisture sensitive N-heterocyclic carbenes (NHC), is developed for the first time. This result demonstrates the compatibility of NHCs with the intervention of H_2O in catalytic reactions.



Nicolas Merle, Mostafa Taoufik, Morad Nayer, Anne Baudouin, Erwan Le Roux, Régis M. Gauvin, Frédéric Lefebvre, Jean Thivolle-Cazat, Jean-Marie Basset

J. Organomet. Chem. 693 (2008) 1733

Development of a well-defined silica-supported tungstenocarbyne complex as efficient heterogeneous catalyst for alkyne metathesis The interaction of $[W(\equiv C-tBu)(CH_2-tBu)(OAr)_2]$ (Ar = 2,6- $iPr_2C_6H_3$) (1) with the OH groups of a silica dehydroxylated at 700 °C leads to $[(\equiv SiO)W(OAr)_2(\equiv C-tBu)]$ (2) which was characterized by IR, solid-state NMR and mass balance analysis. This well-defined surface species has been proved to be an efficient catalyst for the metathesis of pent-2-yne.



Regular Papers

Lindsay T. Byrne, Nicole S. Hondow, George A. Koutsantonis, Brian W. Skelton, A. Asgar Torabi, Allan H. White, S. Bruce Wild

J. Organomet. Chem. 693 (2008) 1738

Carbonyl substitution chemistry of some trimetallic transition metal cluster complexes with polyfunctional ligands

The triruthenium cluster $[Ru_3(CO)_{10}(dppm)]$ reacts with a number of multifunctional phosphine ligands to give products consequent on carbonyl substitution and PH activation. Other ligands investigated include $HSCH_2CH_2AsMe(C_6H_4CH_2OMe)$, $HPMe(C_6-H_4(CH_2OMe))$ and its oxide $HP(O)Me(C_6H_4-(CH_2OMe))$.



iv Contents

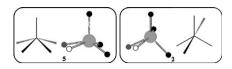
Tushar S. Basu Baul, Archana Mizar, Eleonora Rivarola, Ulli Englert

J. Organomet. Chem. 693 (2008) 1751

Re-visiting of 5-[(E)-2-(aryl)-1-diazenyl]-quinolin-8-ol with tweaking of Sn-Ph groups: Synthesis, spectroscopic characterization and X-ray crystallography

Reactions of sodium 5-[(E)-2-(aryl)-1-diazenyl]quinolin-8-olates (LH, where the aryl group is an R-substituted phenyl ring such that

for L^1H : R = H; L^2H : R = 2'- CH_3 ; L^5H : R = 3'- CH_3 ; L^4H : R = 4'- CCH_3 ; L^5H : R = 4'- CCH_3 and L^6H : R = 4'- CC_2H_5) with Ph_3SnCl in a 1:1 molar ratio yielded complexes of composition Ph_3SnL . The crystal structures of $Ph_3SnL^1 \cdot 0.5C_6H_6$ (1), Ph_3SnL^2 (2), $Ph_3SnL^5 \cdot C_6H_6$ (5) and $Ph_3SnL^6 \cdot 0.5C_6H_6$ (6) were determined. The results of the X-ray studies indicated that the benzene solvated compounds 1, 5 and 6 are distorted square pyramid, with one of the phenyl C atoms in the apex while the ligand arrangement around central Sn atom in 2 is distorted trigonal-bi-pyramidal, with a phenyl C and the oxinato N atoms in axial positions.



Emilie V. Banide, John P. Grealis, Helge Müller-Bunz, Yannick Ortin, Michael Casey, Claudio Mendicute-Fierro, M. Cristina Lagunas, Michael J. McGlinchey

J. Organomet. Chem. 693 (2008) 1759

Chromium, iron, ruthenium and gold complexes of 3,3-(biphenyl-2,2'-diyl)-1-diphenylphosphino-1-phenylallene: A versatile ligand

The allenylphosphine (5), reacts with $(THF)Cr(CO)_5$ and (THT)AuCl to form the complexes (5)- $Cr(CO)_5$ and (5)-AuCl (13), respectively. In contrast, with $Fe_2(CO)_9$ the initially formed (5)- $Fe(CO)_4$, (11), readily loses a carbonyl ligand with concomitant coordination by the adjacent allenyl double bond to yield the η^3 -allenylphosphine- $Fe(CO)_3$ complex (12).

Monika L. Amadoruge, Antonio G. DiPasquale, Arnold L. Rheingold, Charles S. Weinert

J. Organomet. Chem. 693 (2008) 1771

Hydrogermolysis reactions involving the α -germylated nitriles $R_3 GeCH_2 CN~(R=Ph,Pr^i,Bu^i)$ and germanium amides $R_3 GeNMe_2~(R=Pr^i,Bu^i)$ with $Ph_3 GeH$: Substituent-dependent reactivity and crystal structures of $Pr^i{}_3 GeGePh_3$ and $Bu^i{}_3 Ge[NHC(CH_3)CHCN]$

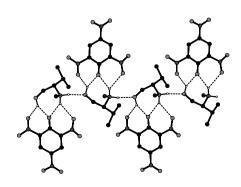
The reactions involving α -germylated nitriles R_3GeCH_2CN (R = Ph, Pr', Bu') and germanium amides R_3GeNMe_2 (R = Pr', Bu') exhibit substituent-dependent reactivity in hydrogermolysis reactions with Ph_3GeH in CH_3CN solution. The crystal structures of $Pr'_3GeGePh_3$ and $Bu'_3Ge[NHC(CH_3)CHCN]$ have been determined.

Petr Štěpnička, Martin Zábranský, Martin Lamač, Ivana Císařová, Petr Němec

J. Organomet. Chem. 693 (2008) 1779

The variability of hydrogen-bonded supramolecular assemblies in crystalline picrates prepared from ferrocenyl-substituted β -aminoalcohols

The readily available ferrocenylated β -aminoalcohols FcCH₂NHCR₂CH₂OH form well-defined crystalline picrates that form supramolecular assemblies via N–H···O and O–H···O bifurcated hydrogen bonds. Whereas the achiral compounds (R₂ = H₂ and Me₂) give rise to closed dimeric assemblies around the crystallographic inversion centres, their chiral counterpart (R₂ = H/i-Pr) forms infinite linear chains (see the picture; the ferrocenyl groups are omitted).

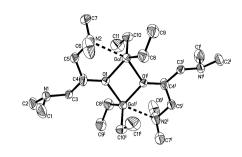


Siama Basharat, Claire J. Carmalt, Robert Palgrave, Sarah A. Barnett, Derek A. Tocher, Hywel O. Davies

J. Organomet. Chem. 693 (2008) 1787

Syntheses, X-ray structures and CVD studies of diorganoalkoxogallanes

Structural studies of the diethylalkoxogallanes, $[Et_2Ga(\mu\text{-OR})]_2$ ($R=CH_2CH_2NMe_2$, $CH(CH_3)$ CH_2NMe_2 , $C(CH_3)_2CH_2OMe$, $CH(CH_2-NMe_2)_2$) incorporating donor-functionalized ligands have shown that these compounds adopt dimeric structures. Thin films of Ga_2O_3 have been deposited on glass by low pressure CVD using some of the compounds or via aerosol assisted CVD from the reaction of Et_3Ga and ROH ($R=CH_2CH_2NMe_2$, $CH(CH_3)CH_2-NMe_2$, $C(CH_3)_2CH_2OMe$, $CH(CH_2NMe_2)_2$) in toluene.

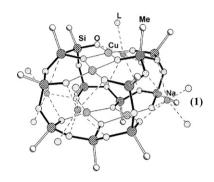


Yulia A. Molodtsova, Konstantin A. Lyssenko, Inesa V. Blagodatskikh, Elena V. Matukhina, Alexander S. Peregudov, Michael I. Buzin, Victor G. Vasil'ev, Dimitris E. Katsoulis, Olga I. Shchegolikhina

J. Organomet. Chem. 693 (2008) 1797

Copper/sodium-directed hydrolytic condensation of methyltriethoxysilane: Self-assembly of polyhedral Cu/Na-methylsiloxane. Synthesis and properties of new stereoregular macrocyclosiloxane

A new crystalline copper/sodium-methylsiloxane $\{Na_4[(MeSi(O)O)_{12}Cu_4]\} \cdot L$ (1) was obtained in a good yield by a hydrolytic condensation of methyltriethoxysilane directed by sodium and copper(II) ions. Compound 1 is a unique source for the synthesis of a new stereoregular organosiloxane macrocycle [MeSi(O)OSiMe₃]₁₂ which is characterized as a Newtonian liquid in a wide temperature region.

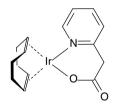


Silke Taubmann, Helmut G. Alt

J. Organomet. Chem. 693 (2008) 1808

Catalytic dehydrogenation of cyclooctane with neutral iridium(I) complexes

A series of new 1,5-cyclooctadiene iridium(I) complexes with chelating ligands has been synthesized. The ligands are naphthoxyimines, carboxylates and alcoholates. The complexes catalyze the homogeneous dehydrogenation of cyclooctane to give cyclooctene and hydrogen without an external hydrogen acceptor up to rates of 75 turnovers. The catalysts are active for at least 48 h at a temperature of 300 °C. The ligand structure has an influence on the activity and selectivity of the corresponding catalysts.



Adelina M. Voutchkova, Dinakar Gnanamgari, Charles E. Jakobsche, Chase Butler, Scott J. Miller, Jonathan Parr, Robert H. Crabtree

J. Organomet. Chem. 693 (2008) 1815

Selective partial reduction of quinolines: Hydrosilylation vs. transfer hydrogenation Two mild catalytic routes for regioselective hydrogenation of the heterocyclic ring of quinoline derivatives are presented. The first route occurs through hydrosilylation using H₃SiPh and is catalyzed by [Rh(nbd)(PPh₃)₂]PF₆ to give 1,2-dihydroquinoline, while the second uses transfer hydrogenation with [Ir(cod)(NHC)PPh₃]BF₄ as catalyst and exclusively produces 1,2,3,4-tetrahydroquinoline.

vi Contents

Xiangji Chen, Yunhang Guo, Qiuyan Zhang, Guiyang Hao, Hongmei Jia, Boli Liu

J. Organomet. Chem. 693 (2008) 1822

Preparation and biological evaluation of ^{99m}Tc-CO-MIBI as myocardial perfusion imaging agent

The inter-transformations between [99mTc(CO)₃(H₂O)(MIBI)₂]⁺, [99mTc(CO)₃(MIBI)₃]⁺, and [99mTc(CO)₂(MIBI)₄]⁺ were investigated. The biodistribution results showed that [99mTc(CO)₃(MIBI)₃]⁺ had the most favorable characteristics for cardiac imaging. The structure characterization on their corresponding rhenium complexes indicated that there were differences between 99mTc-CO-MIBI and Re-CO-MIBI in preparation and hydrophobic characteristics.

Yanjun Chen, Peng Hao, Weiwei Zuo, Kun Gao, Wen-Hua Sun

J. Organomet. Chem. 693 (2008) 1829

2-(1-Isopropyl-2-benzimidazolyl)-6-(1-aryliminoethyl)pyridyl transition metal (Fe, Co, and Ni) dichlorides: Syntheses, characterizations and their catalytic behaviors toward ethylene reactivity

A series of 2-(1-isopropyl-2-benzimidazolyl)-6-(1-aryliminoethyl)pyridyl metal complexes [iron(II) (1a-6a), cobalt(II) (1b-6b) and nickel(II) (1c-6c)] were synthesized and fully

characterized by elemental and spectroscopic analyses. Single-crystal X-ray diffraction analyses of five coordinated complexes ${\bf 5a}$, ${\bf 3b}$, ${\bf 5b}$, ${\bf 1c}$ and ${\bf 2c}$ reveal ${\bf 5a}$ and ${\bf 5b}$ as distorted trigonal-bipyramidal geometry, and ${\bf 3b}$, ${\bf 1c}$ and ${\bf 2c}$ as distorted square pyramidal geometry. All complexes performed ethylene oligomerization with the assistance of various organoaluminums. The iron complexes displayed good activity in the presence of MAO and MMAO. Upon activated by Et₂AlCl, the cobalt analogues showed moderate ethylene reactivity, while the nickel analogues exhibited relatively higher activity.

Pathik Maji, Wei Wang, Andrew E. Greene, Yves Gimbert

J. Organomet. Chem. 693 (2008) 1841

Studies directed toward the synthesis of chiral tungsten and molybdenum carbonyl complexes

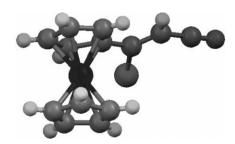
Limiting the number of coordination sites in hexacoordinated monometallic complexes with two bidentate ligands and having chirality on one or both of the ligands could offer an effective strategy for achieving enantioselective Pauson–Khand reactions. Synthetic efforts to prepare such complexes are reported.

Rolfe H. Herber, Israel Nowik, Jeffrey O. Grosland, Ryan G. Hadt, Victor N. Nemykin

J. Organomet. Chem. 693 (2008) 1850

Metal atom dynamics in organometallics: Cyano ferrocenes

Temperature-dependent ⁵⁷Fe Mössbauer spectroscopy has been used to elucidate the hyperfine interactions and dynamics of the metal atom in a series of cyano ferrocenes and the results compared to DFT calculations of the complexes.



Contents vii

Lara-Isabel Rodríguez, Oriol Rossell, Miquel Seco, Arantxa Orejón, Anna M. Masdeu-Bultó

J. Organomet. Chem. 693 (2008) 1857

Palladocarbosilane dendrimers as catalysts for the asymmetric hydrovinylation of styrene in supercritical carbon dioxide *P*-Stereogenic phosphine-containing carbosilane dendrimers with $PdCl(\eta^3-2-MeC_3H_4)$ units grafted on the periphery have been tested in the asymmetric hydrovinylation of styrene in $scCO_2$ media.

Dend = carbosilane dendrimer; R = 2-biphenylyl

James D. Farwell, Peter B. Hitchcock, Michael F. Lappert, Gerrit A. Luinstra, Andrey V. Protchenko, Xue-Hong Wei

J. Organomet. Chem. 693 (2008) 1861

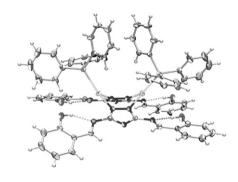
Synthesis and structures of some sterically hindered zinc complexes containing 6-membered Z_{nNCCCN} and Z_{nOCCCN} rings

The synthesis and structures of six crystalline zinc β -diketiminates and 2-(piperazinyl-*N*-methyl)-4,6-di-*tert*-butylphenoxides, including **2** and **8**, potential candidates for copolymerisation of epoxides and carbon dioxide, are reported.

G. Attilio Ardizzoia, Stefano Brenna, Fulvio Castelli, Simona Galli, Chiara Marelli, Angelo Maspero

J. Organomet. Chem. 693 (2008) 1870

New copper(I) and silver(I) triazolatocomplexes: Synthesis, reactivity and catalytic activity in olefin cyclopropanation The synthesis of Cu(I) and Ag(I) complexes containing triazolate ligands (H_3L^1) and H_3L^2 is described. The copper derivatives showed interesting reactivity towards CO and ethyl diazoacetate, while the structure of $[Ag(H_2L^1)(PPh_3)]_2$, is also reported. Moreover, high *trans*-diastereoselectivities were attained in olefin cyclopropanations catalyzed by one of the isolated Cu(I) species.



María B. Faraoni, Darío C. Gerbino, Julio C. Podestá

J. Organomet. Chem. 693 (2008) 1877

Palladium-catalyzed stereoselective hydrostannation of substituted propargyl alcohols with trineophyltin hydride The palladium-catalyzed hydrostannation of ten propargyl alcohols with trineophyltin hydride (1) in THF leads to stannylated allyl alcohols following a *syn* addition stereochemistry, in good to excellent yields and with high stereoselectivity. The regioselectivity might be ascribed to the steric bulk of the *proximal* substituents rather than to electronic effects.

$$\begin{array}{c|c} & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

viii Contents

Anton M. Prokhorov, Pavel A. Slepukhin, Dmitry N. Kozhevnikov

J. Organomet. Chem. 693 (2008) 1886

CuCl₂ induced reactions of 6-ethynyl- and 6-cyano-5-aryl-2,2'-bipyridines with various N- and O-nucleophiles in comparison with the reactions of relative 1,2,4-triazines

Stable towards nucleophilic attack 5-aryl-6-cyano-2,2'-bipyridines react easily with water, methanol, ethanolamine in the presence of copper(II) chloride yielding complexes containing carboxylates, carboximidates or carboxamidines. Relative 5-cyano- as well 5-ethynyl-3-pyridyl-1,2,4-triazines are more active in the CuCl₂ induced reactions due to higher electron-withdrawing properties of this heterocycle.

Mahmut Ulusoy, Onur Şahin, Orhan Büyükgüngör, Bekir Çetinkaya

J. Organomet. Chem. 693 (2008) 1895

Imidazolium salicylaldimine frameworks for the preparation of tridentate *N*-heterocyclic carbene ligands

Sterically hindered salicylaldimine functionalized imidazolium salts 2 have been prepared. The structures of the synthesized compounds were determined by spectroscopic techniques.

The reaction of these salts containing arylmethyl-N chain (aryl: phenyl (2a), 2,4,6-trimethylphenyl (2b), 2,3,4,5,6-pentamethylphenyl (2c)) with Pd(OAc)₂ in boiling toluene afforded Pd(II) complexes 3 in high yields. The X-ray structure of 1-[3-(3,5-di-tert-butyl-2-ox-ophenyl)propyliminato]-3-(2,4,6-trimethylbenzyl)imidazol-2-ylidenebromopalladium(II) (3b) has been determined. The Suzuki–Miyaura reaction was used to investigate their activity as catalysts either prepared in situ or from well-defined complexes. They are very efficient when activated arylbromides are used as substrates.

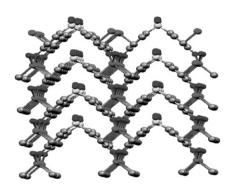
Robabeh Bashiri, Kamran Akhbari, Ali Morsali, Matthias Zeller

J. Organomet. Chem. 693 (2008) 1903

A three-dimensional Ag^I coordination polymer constructed via η^2 Ag-C bonds: Thermal, fluorescence, structural and solution studies

A 3D polymer built with the assistance of η^2 Ag–C bonds, [Ag₂(μ_8 -SB)] (1) [H₂SB = 4-[(4-

hydroxyphenyl)sulfonyl]-1-benzenol], has been synthesized and characterized and its structure was determined by X-ray crystallography. In addition to the coordination to the O atoms of SB^{2-} the Ag atoms also form strong η^2 Ag–C bonds, resulting in the formation of an AgO_2C_2 environment. The thermal stabilities of 1 and of its thallium(I) analogue, [Tl₄(μ_8 -SB)₂] (2), were studied by thermal gravimetric (TG) and differential thermal analyses (DTA). The ligand and compounds 1–2 are luminescent in the solution state, with emission maxima at 380, 353 and 468 nm, respectively.



Sergey A. Belov, Roman S. Kirsanov, Dmitrii P. Krut'ko, Dmitrii A. Lemenovskii, Andrei V. Churakov, Judith A.K. Howard

J. Organomet. Chem. 693 (2008) 1912

Novel sandwich complexes of zirconium $[C_9H_5(SiMe_3)_2](C_5Me_4R)ZrCl_2$ ($R=CH_3$, $CH_2CH_2NMe_2$): Synthesis and reduction behavior

Novel Zr complexes (Ind^{Si2})ZrCl₃ and (Ind^{Si2})(C₅Me₄R)ZrCl₂ (R = CH₃ (1), CH₂-CH₂NMe₂ (2)) (Ind^{Si2} = C₉H₅(SiMe₃)₂) were prepared. Formation of [η^5 : η^2 (C,N)-C₅Me₄CH₂CH₂N(Me)CH₂](Ind^{Si2})ZrH by reduction of **2** was proved by NMR data. Crystal structures of **1** and product of hydrolysis of **2** ([C₅Me₄CH₂CH₂NMe₂]ZrCl₂)₂O were established by X-ray diffraction.

$$\begin{array}{c} \text{N(CH}_3)_2 \\ \text{Me}_3 \text{Si} \\ \text{Me}_3 \text{Si} \end{array} \begin{array}{c} \text{N(CH}_3)_2 \\ \text{Mg/Hg, THF} \\ \text{20 °C, 5 days} \end{array} \begin{array}{c} \text{Me}_3 \text{Si} \\ \text{Me}_3 \text{Si} \end{array} \begin{array}{c} \text{ZC} \\ \text{Me}_3 \text{Si} \\ \text{Me}_3 \text{Si} \end{array}$$

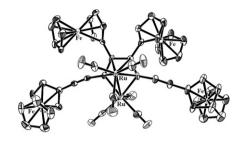
Contents ix

Pradeep Mathur, Atanu Das, Saurav Chatterjee, Shaikh M. Mobin

J. Organomet. Chem. 693 (2008) 1919

Coupling reaction between the uncoordinated acetylenic bond of $[Ru_3(CO)_{10}\{\mu_3-FcC_2C\equiv CFc\}]$ and $FcC\equiv CC\equiv CFc$ to form $[Ru_2(CO)_6\{C_4Fc_2(C\equiv CFc)_2\}_2]$, $[Ru_2(CO)_6[\mu_1^1:\eta^1:\eta^2:\eta^2-\{FcC\equiv CCC(Fc)-C(O)-C(Fc)CC\equiv CFc\}]$ and $[Ru_2(CO)_6[\mu_1^1:\eta^1:\eta^2:\eta^2-\{FcC\equiv CCC(Fc)-C(O)-C(-C\equiv CFc)C(Fc)\}]$

A coupling reaction between the uncoordinated acetylenic bond of [Ru₃-(CO)₁₀{ μ_3 -FcC₂C=CFc}] (1) and FcC=CC=CFc occurs to form the ruthenacyclopentadiene complex [Ru₂(CO)₆{C₄Fc₂(C=CFc)₂}] (2), and two isomers of the diruthenacycloheptadienone complex, [Ru₂(CO)₆[μ - η ¹: η ¹: η ²: η ²-{FcC=CCC(Fc)-C(O)-C(Fc)CC=CFc}] (3) and [Ru₂(CO)₆[μ - η ¹: η ¹: η ²: η ²-{FcC=CCC(Fc)-C(O)-C(-C=CFc)C(Fc)}] (4).



Erpeng Zhang, Hongwei Hou, Huayun Han, Yaoting Fan

J. Organomet. Chem. 693 (2008) 1927

Syntheses, crystal structures of a series of copper(II) complexes and their catalytic activities in the green oxidative coupling of 2,6-dimethylphenol

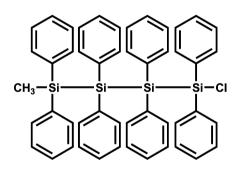
A series of copper(II) complexes have been prepared according to appropriate synthetic strategies with the aim of exploiting new catalysts. A green aqueous-medium catalysis process of the oxidative coupling of DMP has been explored by using these complexes as catalysts.

Simon J. Holder, Mariliz Achilleos

J. Organomet. Chem. 693 (2008) 1938

An oligosilane initiator for the Wurtz-type polymerisation of dichloromethylphenylsilane

1-Chloro-4-methyl-1,1,2,2,3,3,4,4-octaphenyl-tetrasilane was employed as an initiator in the Wurtz-type reductive coupling polymerisations of dichloromethylphenylsilane with sodium in toluene at 65 °C. Yields of polymethylphenylsilane were in the range 32–35% which is almost double the yield obtained by otherwise identical reactions in the absence of the initiator (16–19%).



Notes

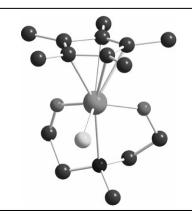
Younjin Hong, Sang-Deok Mun, Junseong Lee, Youngkyu Do, Youngjo Kim

J. Organomet. Chem. 693 (2008) 1945

Synthesis, characterization, and catalytic activities in syndiospecific polymerization of styrene for half-sandwich titanium complexes with non-Cp tridentate dianionic ligands $MeN(CH_2CR_2O^-)_2$

New half-titanocenes, $Cp^*TiCl[(OCR_2CH_2)-NMe(CH_2CR_2^{'}O)]$ [R,R' = H (1), R,R' = Me,

H, (2), R,R' = Me (3)], were prepared from Cp^*TiCl_3 (4) with the corresponding alcohols in the presence of triethylamine. X-ray analysis shows that 1 has slightly distorted trigonal bipyramidal geometry around Ti. These complexes exhibited moderate catalytic activities for syndiospecific styrene polymerization in the presence of MAO and the activity increased in the order: 2 > 1 > 4 > 3 (at 50 °C), 1 > 2 > 4 > 3 (at 70 °C and 90 °C).



x Contents

Alfredo M. Simas, Ricardo O. Freire, Gerd B. Rocha

J. Organomet. Chem. 693 (2008) 1952

Lanthanide coordination compounds modeling: Sparkle/PM3 parameters for dysprosium (III), holmium (III) and erbium (III)

The Sparkle/PM3 is extended to dysprosium (III), holmium (III) and erbium (III) ions. The parameterization procedure was the same used

to obtain Sparkle/AM1 parameters for each of these three lanthanide ions. The Sparkle/PM3 unsigned mean error for all interatomic distances between the trivalent lanthanide ion and the ligand atoms of the first sphere of coordination is similar to the Sparkle/AM1 ones, indicating they are comparable parameterizations. Moreover, their accuracy is similar to what can be obtained by present-day ab initio effective core potential calculations on such lanthanide complexes. Hence, the choice of which model to use remains with the researcher who must evaluate the impact of either AM1 or PM3 on the quantum chemical description of the organic ligands.

