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Contents

Special Issue: Recent Developments in Reactivity of Metal Allyl and Alkyl Complexes

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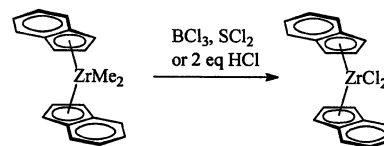
Regular Papers

**Daide Balboni, Isabella Camurati,
Antonio Cascio Ingurgio, Simona Guidotti,
Francesca Focante, Luigi Resconi**

J. Organomet. Chem. 683 (2003) 2

A counterintuitive, yet efficient synthesis of bis(indenyl)zirconium dihalides

Chlorination of $\text{Ind}_2\text{ZrMe}_2$ with BCl_3 , SCl_2 or HCl in Et_2O , produces $\text{Ind}_2\text{ZrCl}_2$ in 90–100% yield. $\text{Ind}_2\text{ZrBr}_2$ and Ind_2ZrI_2 are obtained in high yield from $\text{Ind}_2\text{ZrMe}_2$ and Br_2 or I_2 , respectively. It is found that the σ -ligands of Ind_2ZrX_2 ($X = \text{Me}, \text{Cl}, \text{Br}, \text{I}, \text{OC}_6\text{F}_5$) have no relevant influence on the catalyst activity, nor on the polymer properties, in MAO-activated polymerization of propylene in solution.

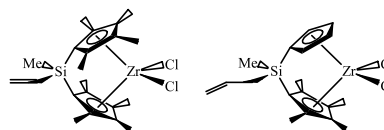


**Antonio Antiñolo, Mariano Fajardo,
Santiago Gómez-Ruiz, Isabel López-Solera,
Antonio Otero, Sanjiv Prashar,
Ana M. Rodríguez**

J. Organomet. Chem. 683 (2003) 11

Group 4 metallocene complexes incorporating vinyl or allyl substituted *ansa* ligands. X-Ray crystal structures of $[\text{Zr}\{\text{Me}(\text{CH}_2=\text{CH})\text{Si}(\eta^5\text{-C}_5\text{Me}_4)_2\}\text{Cl}_2]$, $[\text{Zr}\{\text{Me}(\text{CH}_2=\text{CH}-\text{CH}_2)\text{Si}(\eta^5\text{-C}_5\text{H}_4)_2\}\text{Cl}_2]$ and $[\text{Zr}\{\text{Me}(\text{CH}_2=\text{CHCH}_2)\text{Si}(\eta^5\text{-C}_5\text{Me}_4)(\eta^5\text{-C}_5\text{H}_4)\}\text{Cl}_2]$

The preparation of new *ansa* ligands that have as functional groups vinyl or allyl substituents at the silicon *ansa* bridge and their incorporation in new symmetrical and chiral *ansa*-metallocene complexes of Group 4 metals is described along with their reactivity towards hydrogenation and hydroboration.

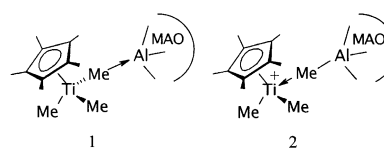


**Konstantin P. Bryliakov,
Nina V. Semikolenova,
Vladimir A. Zakharov, Evgenii P. Talsi**

J. Organomet. Chem. 683 (2003) 23

^{13}C -NMR study of Ti(IV) species formed by Cp^*TiMe_3 and Cp^*TiCl_3 activation with methylaluminoxane (MAO)

Using ^{13}C and ^1H NMR spectroscopy, titanium(IV) species formed in the catalytic systems $\text{Cp}^*\text{TiMe}_3/\text{MAO}$ and $\text{Cp}^*\text{TiCl}_3/\text{MAO}$ ($\text{Cp}^* = \text{C}_5(\text{CH}_3)_5$) were studied at Al/Ti ratios 30–300. Upon activation of Cp^*TiMe_3 and $\text{Cp}^*\text{TiCl}_3/\text{MAO}$ with MAO mainly the 'cation-like' intermediate $\text{Cp}^*\text{Me}_2\text{Ti}^+ \leftarrow \text{Me}^- - \text{Al} = (\text{MAO})$ (**2**) is formed in conditions approaching to those of practical polymerization (Al/Ti ratios > 200).

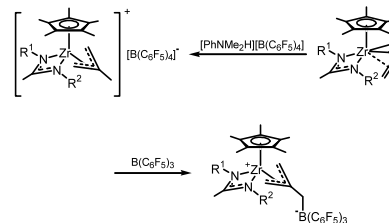


**Denis A. Kissounko, James C. Fettinger,
Lawrence R. Sita**

J. Organomet. Chem. 683 (2003) 29

Synthesis and characterization of cationic and zwitterionic allyl zirconium complexes derived from trimethylenemethane (TMM) cyclopentadienylzirconium acetamidinates

Trimethylenemethane complexes of cyclopentadienylzirconium acetamidinates are viable precursors to cationic and zwitterionic allyl zirconium species through protonation and borane addition, respectively. In the present case, these allyl complexes proved inactive as initiators for the Ziegler-Natta polymerization of ethylene and α -olefins.

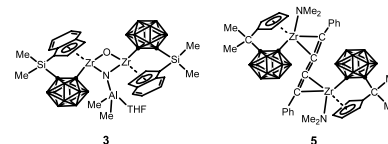


**Yaorong Wang, Haiping Wang,
Hong Wang, Hoi-Shan Chan, Zuwei Xie**

J. Organomet. Chem. 683 (2003) 39

Reactions of $L_2Zr(NMe_2)_2$ with Me_3Al and $PhC\equiv CH$: synthesis and structural characterization of new zirconium carborane complexes [$L_2 = Me_2Si(C_9H_6)(C_2B_{10}H_{10})$ and $Me_2C(C_3H_4)(C_2B_{10}H_{10})$]

$L_2Zr(NMe_2)_2$ can be converted into $L_2ZrMe_2[AlMe_2(NMe_2)]$ and $L_2Zr(NMe_2)(CCPh)$ by reacting with Me_3Al and $PhC\equiv CH$, respectively, leading to the isolation and structural characterization of unexpected zirconium carborane complexes **3** and **5**.

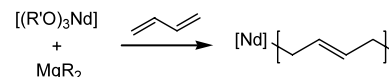


**Jérôme Gromada, Luc le Pichon,
André Mortreux, Frédéric Leising,
Jean-François Carpentier**

J. Organomet. Chem. 683 (2003) 44

Neodymium alk(aryl)oxides–dialkylmagnesium systems for butadiene polymerization and copolymerization with styrene and glycidyl methacrylate

In situ combinations of a neodymium aryloxide(alkoxide) and a dialkylmagnesium promote the *trans*-1,4-stereospecific polymerization of butadiene. Reactions proceed in a pseudo-living fashion, with high initiation efficiency, narrow molecular polydispersity and good control of molecular weights, enabling in turn the efficient diblock copolymerization of butadiene with glycidyl methacrylate.

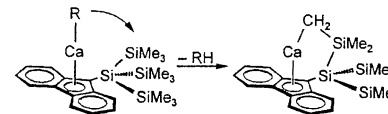


**Florian Feil, Christian Müller,
Sjoerd Harder**

J. Organomet. Chem. 683 (2003) 56

α -Methyl-benzylcalcium complexes: syntheses, structures and reactivity

α -Methyl-benzylcalcium complexes have been prepared. They show similar structures but a higher reactivity than their α - Me_3Si -analogues. Intramolecular C–H activation in a heteroleptic α -methyl-benzylcalcium complex was observed and the product, a calcium complex with a dianionic alkyl/fluorenyl *ansa*-ligand, was characterized by crystal structure determination.

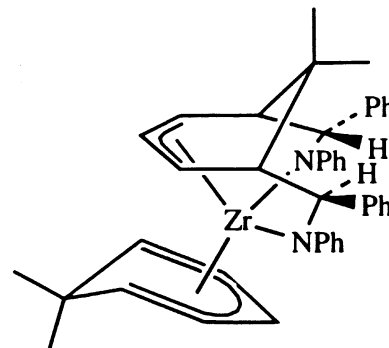


**Rehan Basta, Richard D. Ernst,
Atta M. Arif**

J. Organomet. Chem. 683 (2003) 64

Synthesis and structure of the edge-bridged open zirconocene, $Zr(6,6\text{-dmch})_2(PMe_3)_2$ (dmch = dimethylcyclohexadienyl), and its imine coupling product

An edge-bridged open zirconocene has been isolated as an 18 electron bis(trimethylphosphine) adduct, $Zr(6,6\text{-dmch})_2(PMe_3)_2$. This complex reacts with two equivalents of $PhCH=NPh$, resulting in couplings to both ends of one of the dieny ligands.

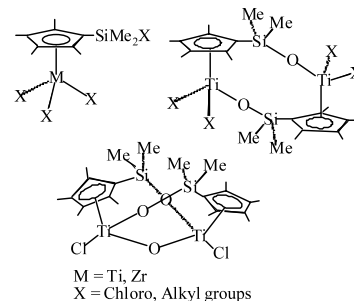


**Olga Buitrago, Gerardo Jiménez,
Tomás Cuenca**

J. Organomet. Chem. 683 (2003) 70

Titanium and zirconium chloro, oxo and alkyl derivatives containing silyl-cyclopentadienyl ligands. Synthesis and characterisation

Trichloro mono-tetramethylcyclopentadienyl complexes $M(\eta^5\text{-C}_5\text{Me}_4\text{SiMe}_2\text{Cl})\text{Cl}_3$ ($M = \text{Ti, Zr}$) are prepared by reaction of $\text{C}_5\text{Me}_4(\text{SiMe}_3)(\text{SiMe}_2\text{Cl})$ with MCl_4 . The titanium compound is hydrolysed to give the dinuclear derivative $\{\text{Ti}[\mu\text{-}(\eta^5\text{-C}_5\text{Me}_4\text{SiMe}_2\text{O}\text{-}\kappa\text{O})]\text{Cl}_2\}_2$ which is converted into $\{\text{Ti}[\mu\text{-}(\eta^5\text{-C}_5\text{Me}_4\text{SiMe}_2\text{O}\text{-}\kappa\text{O})]\text{Cl}_2(\mu\text{-O})\}$ by a subsequent hydrolysis reaction in air. Mononuclear and dinuclear alkyl titanium derivatives are obtained by appropriate alkylating reactions.

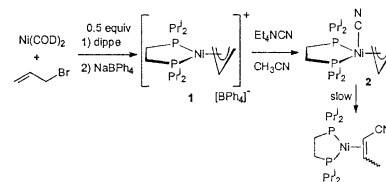


Nicole M. Brunkan, William D. Jones

J. Organomet. Chem. 683 (2003) 77

Preparation, structure, and dynamics of a nickel π -allyl cyanide complex

The complex $(\text{dippe})\text{Ni}(\eta^3\text{-allyl})(\text{CN})$ has been prepared and fully characterized (dippe = bis-(diisopropylphosphino)ethane), including X-ray diffraction studies, as a square pyramidal structure. The complex shows dynamic $^1\text{H-NMR}$ behavior consistent with substantial structural rearrangements upon π to σ allyl interconversion. A comparison is made with $(\text{dippe})\text{Ni}(\eta^3\text{-allyl})\text{Br}$, which also displays a square pyramidal structure.

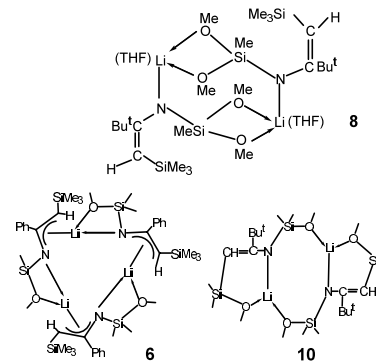


**Peter B. Hitchcock, Michael F. Lappert,
Xue-Hong Wei**

J. Organomet. Chem. 683 (2003) 83

Synthesis and structures of crystalline lithium 1-azaallyls and a 1,3-diazaallyl derived from $\text{Li}\{\text{CH}(\text{SiMe}_3)(\text{SiMe}_{3-n}(\text{OMe})_n)\}$ ($n = 1$ or 2) and $\text{Li}\{\text{CH}(\text{SiMe}_2\text{OMe})_2\}$ and RCN ($R = t\text{Bu, Ph, 2,5-Me}_2\text{C}_6\text{H}_3$, or Ad)

From the appropriate silylmethyl lithium compound and RCN , under ambient conditions, the following crystalline compounds were obtained: $[\text{Li}\{\text{N}(\text{SiMe}_2\text{OMe})\text{C}(t\text{Bu})\text{C}(\text{H})(\text{SiMe}_3)\}_2]$ (**5**), $[\text{Li}\{\text{N}(\text{SiMe}_2\text{OMe})\text{C}(\text{Ph})\text{C}(\text{H})(\text{SiMe}_3)\}_2]$ (**6**), $[\text{Li}\{\text{N}(\text{SiMe}_2\text{OMe})\text{C}(\text{C}_6\text{H}_3\text{Me}_2 - 2,5)\text{NC}(\text{C}_6\text{H}_3\text{Me}_2 - 2,5)\text{C}(\text{H})(\text{SiMe}_3)\}(\text{TMEDA})]$ (**7**), $[\text{Li}\{\text{N}(\text{SiMe}(\text{OMe})_2)\text{C}(t\text{Bu})\text{C}(\text{H})(\text{SiMe}_3)\}_2]$ (**8**), $\text{Li}\{\text{N}(\text{SiMe}(\text{OMe})_2)\text{C}(\text{Ph})\text{C}(\text{H})(\text{SiMe}_3)\}(\text{TMEDA})$ (**9**), and $[\text{Li}\{\text{N}(\text{SiMe}_2\text{OMe})\text{C}(t\text{Bu})\text{C}(\text{H})(\text{SiMe}_2\text{OMe})\}_2]$ (**10**); X-ray structures of each except **9** are reported.

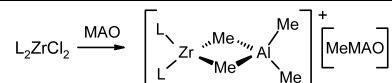


Konstantin P. Bryliakov,
Nina V. Semikolenova,
Dmitrii V. Yudaev, Vladimir A. Zakharov,
Hans H. Brintzinger, Martin Ystenes,
Erling Rytter, Evgenii P. Talsi

J. Organomet. Chem. 683 (2003) 92

¹H-, ¹³C-NMR and ethylene polymerization studies of zirconocene/MAO catalysts: effect of the ligand structure on the formation of active intermediates and polymerization kinetics

Cationic intermediates formed by activation of L₂ZrCl₂ (L₂ are various cyclopentadienyl (Cp), indenyl (Ind) and fluorenyl (Flu) ligands) with MAO in toluene were monitored by ¹H- and ¹³C-NMR at Al/Zr ratios from 50 to 1000. Heterodinuclear [(Cp-R)₂Zr(μ-Me)₂AlMe₂]⁺[Me-MAO]⁻ ion pairs (**III**) dominate in all reaction systems. Correlations between spectroscopic and ethene polymerization data were observed.



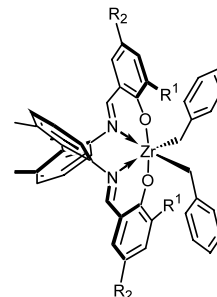
L = various cyclopentadienyl (Cp), indenyl (Ind), fluorenyl (Flu) ligands

Paul D. Knight, Paul N. O'Shaughnessy,
Ian J. Munslow, Brian S. Kimberley,
Peter Scott

J. Organomet. Chem. 683 (2003) 103

Biaryl-bridged Schiff base complexes of zirconium alkyls: synthesis structure and stability

Salicylaldehyde derivatives H₂L of 2,2'-diamino-6,6'-dimethylbiphenyl give isolable alkyls of zirconium [ZrLR₂] (R = CH₂Ph, CH₂Bu^t). Molecular structures confirm their *cis-α* geometry. They decompose via 1,2-migratory insertion of an alkyl group to imine, followed in some instances by a second similar reaction. A brief kinetic study indicates that the rate increases with increased steric demand of R¹.

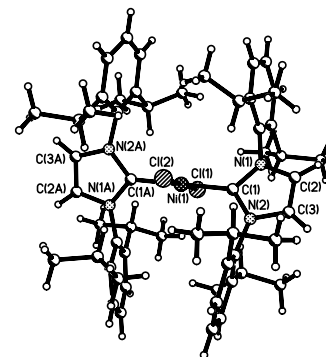


Amanda L. MacKinnon, Michael C. Baird

J. Organomet. Chem. 683 (2003) 114

The synthesis and X-ray structure of *trans*-NiCl₂(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)₂; attempts to polymerize olefins utilizing a nickel(II) complex of a sterically demanding *N*-heterocyclic carbene

The planar compound *trans*-NiCl₂(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)₂, in which the *N*-heterocyclic carbene provides considerable steric hindrance to access to the axial positions of the nickel, is found to dimerize rather than to polymerize ethylene when activated with MAO.

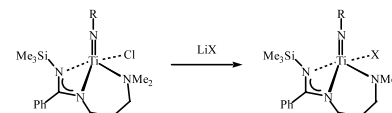


A. Charis R. Croft, Catherine L. Boyd,
Andrew R. Cowley, Philip Mountford

J. Organomet. Chem. 683 (2003) 120

Organometallic and related imidotitanium compounds containing a pendant arm functionalised benzamidinate ligand

Organometallic and related imidotitanium compounds containing a pendant arm functionalised *N*-trimethylsilyl benzamidinate ligand are described.



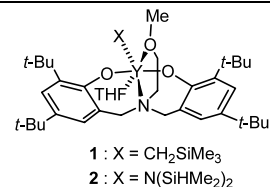
R = ^tBu or 2,6-C₆H₃Me₂; X = Me, Ph, O-2,6-C₆H₃Me₂ or Ni(SiMe₃)₂

**Chen-Xin Cai, Loic Toupet,
Christian W. Lehmann,
Jean-François Carpentier**

J. Organomet. Chem. 683 (2003) 131

Synthesis, structure and reactivity of new yttrium bis(dimethylsilyl)amido and bis(trimethylsilyl)methyl complexes of a tetradentate bis(phenolate) ligand

New alkyl and amido yttrium complexes of a tetradentate bis(phenolate) ligand have been prepared, structurally characterized and investigated as polymerization catalysts.

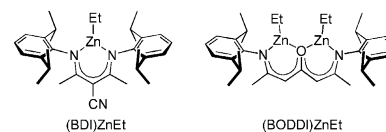


**Scott D. Allen, David R. Moore,
Emil B. Lobkovsky, Geoffrey W. Coates**

J. Organomet. Chem. 683 (2003) 137

Structure and reactivity of mono- and di-nuclear diiminate zinc alkyl complexes

The synthesis, structure and reactivity of five representative β -diiminate (BDI) zinc alkyl complexes and one β -oxo- δ -diiminate (BODDI) zinc alkyl is described.

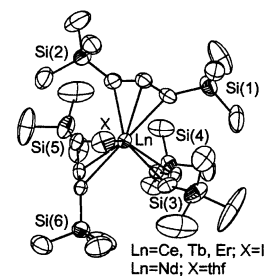


**Christopher J. Kuehl, Cheslan K. Simpson,
Kevin D. John, Alfred P. Sattelberger,
Christin N. Carlson, Timothy P. Hanusa**

J. Organomet. Chem. 683 (2003) 149

Monomeric f-element chemistry with sterically encumbered allyl ligands

A new class of allyl-lanthanide salts of the type [K(thf)₄][(C₃H₃(SiMe₃)₂)₃LnI] (Ln = Ce, Pr, Nd, Gd, Tb, Dy, Er) has been prepared and isolated by reaction of three equivalents of the 1,3-bis(trimethylsilyl)allyl anion with LnI₃. The neutral complex [C₃H₃(SiMe₃)₂]₃Nd(thf) has been isolated from the reaction of the triflate complex Nd(O₃SCF₃)₃ with three equivalents of the 1,3-bis(trimethylsilyl)allyl anion.

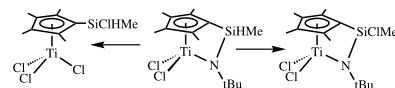


**Ana Belén Vázquez, Pascual Royo,
Eberhardt Herdtweck**

J. Organomet. Chem. 683 (2003) 155

Hydro- and chloro-substituted silyl- and silyl- η^1 -amido- η^5 -tetramethylcyclopentadienyl titanium complexes

A new series of dichloro- and hydrochloro-silyl-Cp titanium [Ti(η^5 -C₅Me₄SiMeXCl)Cl₃] (X = Cl, H) complexes and their methyl derivatives have been isolated and used to prepare the related *ansa*-silyl- η -amido titanium [Ti{ η^5 -C₅Me₄SiMeX(η^1 -N^tBu)}Cl₂] compounds. Alternative reactions at the Si-H and Si-N^tBu-Ti bonds of [Ti{ η^5 -C₅Me₄SiMeH(η^1 -N^tBu)}Cl₂] are reported for various halogenating agents (HCl, TiCl₄, BCl₃).

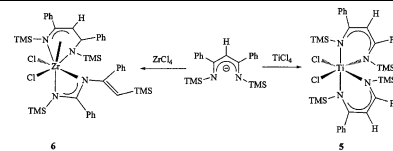


**Ella Shaviv, Mark Botoshansky,
Moris S. Eisen**

J. Organomet. Chem. 683 (2003) 165

β -Diketiminato complexes of Group 4: active complexes for the isomerization of α -olefins and the polymerization of propylene towards elastomeric polypropylene

The β -diketiminato lithium ligand $[\{N(\text{SiMe}_3)\text{C}(\text{Ph})_2\text{CH}\}[\text{Li}]]$ reacted with TiCl_4 and ZrCl_4 forming complexes **5** and **6**. Complex **5** activated by MAO was found to be active in the polymerization of propylene, producing high molecular weight (> 100000) elastomeric polymer, whereas the zirconium complex was found inactive. Complexes **5**, and **6**, were found to be active catalysts, in the presence of MAO (methylalumoxane), for the isomerization of aliphatic olefins (1-octene, allylbenzene), each complex by a different mechanism.

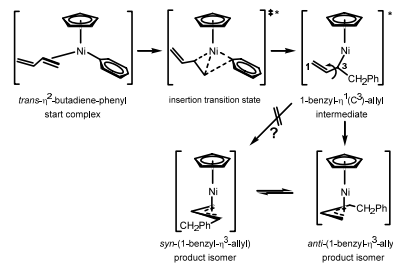


Sven Tobisch, Rudolf Taube

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Theoretical exploration of structure–reactivity relationships in organometallic chemistry: butadiene insertion into the organyl–transition-metal bond and conversion of the allyl–transition-metal fragment in the $[\text{Ni}^{\text{II}}(\eta^5\text{-Cp})(\eta^1\text{-phenyl})(\eta^2\text{-butadiene})]$ complex

A theoretical investigation of the reaction course of the butadiene insertion into the aryl– Ni^{II} bond in the $[\text{Ni}^{\text{II}}(\eta^5\text{-Cp})(\eta^1\text{-phenyl})(\eta^2\text{-butadiene})]$ complex is presented that employed a gradient-corrected DFT method. The first mechanism suggested by Lehmkuhl et al. was refined and supplemented with important details. The critical factors that determine the generation of *anti*- η^3 - and *syn*- η^3 -allyl isomers of the $[\text{Ni}^{\text{II}}(\eta^5\text{-Cp})(1\text{-benzyl-allyl})]$ product have been elucidated. This let us to rationalize the experimentally observed, almost exclusive formation of the *anti*- η^3 -allyl isomer.

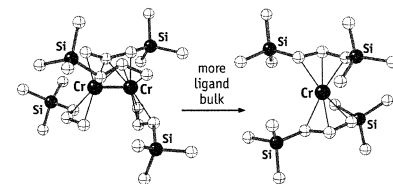


**Christin N. Carlson, J. Dominic Smith,
Timothy P. Hanusa, William W. Brennessel,
Victor G. Young, Jr.**

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Homoleptic allyl complexes of chromium with trimethylsilylated ligands. Formation and molecular structure of $\{[1\text{-}(\text{SiMe}_3)\text{C}_3\text{H}_4]_2\text{Cr}\}_2$, $[1,3\text{-}(\text{SiMe}_3)_2\text{C}_3\text{H}_3]_2\text{Cr}$, and $[1,1',3\text{-}(\text{SiMe}_3)_3\text{C}_3\text{H}_2]_2\text{Cr}$

Use of trimethylsilylated allyl ligands affords a new family of homoleptic chromium complexes. The dimeric $\{[1\text{-}(\text{SiMe}_3)\text{C}_3\text{H}_4]_2\text{Cr}\}_2$ has a structure much like the parent $[(\text{C}_3\text{H}_5)_2\text{Cr}]_2$, but the bis- and *tris*-trimethylsilylated ligands generate monomeric high-spin bis(π -allyl)chromium(II) complexes $[(\text{SiMe}_3)_n\text{C}_3\text{H}_{5-n}]_2\text{Cr}$ that are thermally stable at room temperature even with their extremely low 12-electron counts.

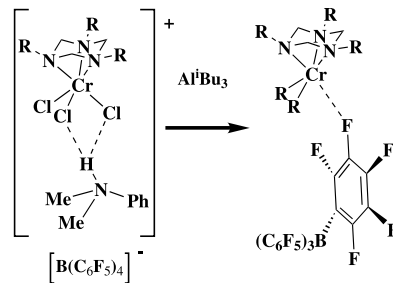


**Randolf D. Köhn, David Smith,
Mary F. Mahon, Martina Prinz,
Shahram Mihan, Gabriele Kociok-Köhn**

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Coordination chemistry of the activation of $[(\text{triazacyclohexane})\text{CrCl}_3]$ with $[\text{PhNMe}_2\text{H}][\text{B}(\text{C}_6\text{F}_5)_4]$ and AlR_3

$[(\text{Triazacyclohexane})\text{CrCl}_3]$ forms 1:1 adducts with $[\text{PhNMe}_2\text{H}][\text{B}(\text{C}_6\text{F}_5)_4]$. Addition of Al^iBu_3 leads to a complex with $[\text{B}(\text{C}_6\text{F}_5)_4]^-$ weakly coordinated to chromium. This complex can trimerise olefins similar to methyl aluminoxane activated complexes. Decomposition of the active complex involves transfer of the triazacyclohexane to aluminium leading to $[(\text{triazacyclohexane})\text{Al}^i\text{Bu}_2][\text{B}(\text{C}_6\text{F}_5)_4]$ and $[(\text{arene})_2\text{Cr}][\text{B}(\text{C}_6\text{F}_5)_4]$ proving that chromium is reduced to the oxidation state +I during the catalysis.

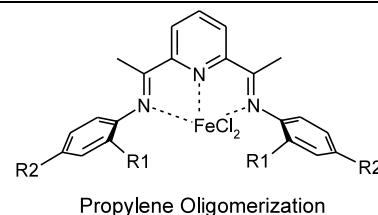


Sebastian Thomas Babik, Gerhard Fink

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Propylene bulk phase oligomerization with bisiminepyridine iron complexes in a calorimeter: mechanistic investigation of 1,2 versus 2,1 propylene insertion

Propylene was oligomerized using iron(II) complexes activated with modified-methylaluminoxane. After analyzing the obtained propylene dimers and trimers a mechanistic pathway for propylene insertion is presented which can distinguish between 1,2 and 2,1 propylene insertions.

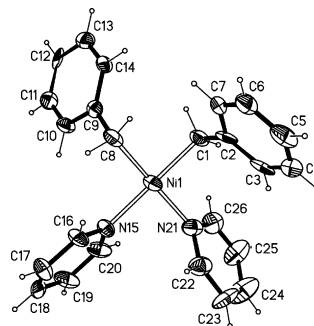


Juan Cámpora, María del Mar Conejo, Kurt Mereiter, Pilar Palma, Carmen Pérez, Manuel L. Reyes, Caridad Ruiz

J. Organomet. Chem. 683 (2003) 220

Synthesis of dialkyl, diaryl and metallacyclic complexes of Ni and Pd containing pyridine, α -diimines and other nitrogen ligands
Crystal structures of the complexes *cis*-NiR₂py₂ (R = benzyl, mesityl)

Dialkyl and metallacyclic complexes of composition *cis*-MR₂Py₂ (M = Ni, Pd; Py = pyridine) have been synthesized. These complexes undergo facile ligand exchange reactions that can be used in the synthesis of organometallic derivatives of chelating nitrogen donors, such as α -diimines or 2-imidoylpyridines.

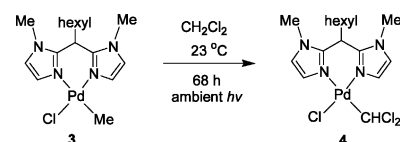


Christopher T. Burns, Han Shen, Richard F. Jordan

J. Organomet. Chem. 683 (2003) 240

Photochemical synthesis of a palladium dichloromethyl complex, {(hexyl)HC(*N*-methylimidazol-2-yl)₂}Pd(CHCl₂)Cl. X-ray molecular structures of {(hexyl)HC(*N*-methylimidazolyl-2-yl)₂}Pd(X)Cl, X = Cl, and CHCl₂

The reaction of (hexyl)HC(mim)₂ (**1**, mim = *N*-methylimidazol-2-yl) with (cod)-PdMeCl in C₆H₆ yields {(hexyl)HC(mim)₂}Pd(Me)Cl (**3**). The photochemical reaction of **3** with CH₂Cl₂ at 23 °C in ambient room light yields {(hexyl)HC(mim)₂}Pd(CHCl₂)Cl (**4**). It is proposed that this reaction proceeds by homolytic scission of the Pd–Me bond of **3**.

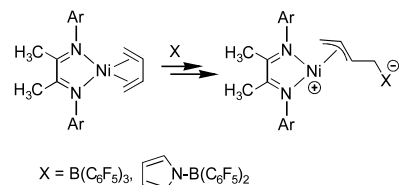


Joachim W. Strauch, Gerald Kehr, Gerhard Erker

J. Organomet. Chem. 683 (2003) 249

Preparation of chelate bis(imine)nickel allyl systems by reaction of their corresponding butadiene complexes with electrophiles

The chelate bis(imine)butadiene nickel complexes **4** add a variety of electrophiles to form the corresponding (π -allyl)nickel complex derivatives. Addition of B(C₆F₅)₃ or (*N*-pyrrolyl)B(C₆F₅)₂ yields neutral dipolar substituted (π -allyl)Ni-type complexes, whereas H⁺-transfer from (2*H*-pyrrolyl)B(C₆F₅)₃ yields a cationic (π -crotyl)Ni derivative. The described (π -allyl)Ni systems polymerize ethene in the presence of triisobutylaluminum.

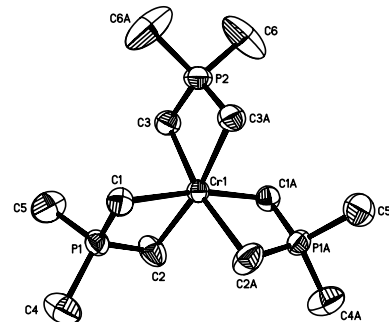


Anke Spannenberg, Perdita Arndt,
Wolfgang Baumann, Uwe Rosenthal

J. Organomet. Chem. 683 (2003) 261

The molecular structure of $\text{Cr}[(\text{CH}_2)_2\text{PMe}_2]_3$: dimethylphosphonium-bis-methylide chromium compounds as inner-phosphonium-alkyl-ate- or 2-phospha-allyl-complexes?

On the basis of the molecular structure of the chromium(III) complex $\text{Cr}[(\text{CH}_2)_2\text{PMe}_2]_3$ (**1a**) and recently described quantum chemical calculations the bonding mode of the chelating dimethylphosphonium-bis-methylide ligand $[(\text{CH}_2)_2\text{PMe}_2]^-$ is discussed either as a part of a more polar inner-phosphonium alkyl-ate complex or as a delocalized 2-phospha-allyl system.



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