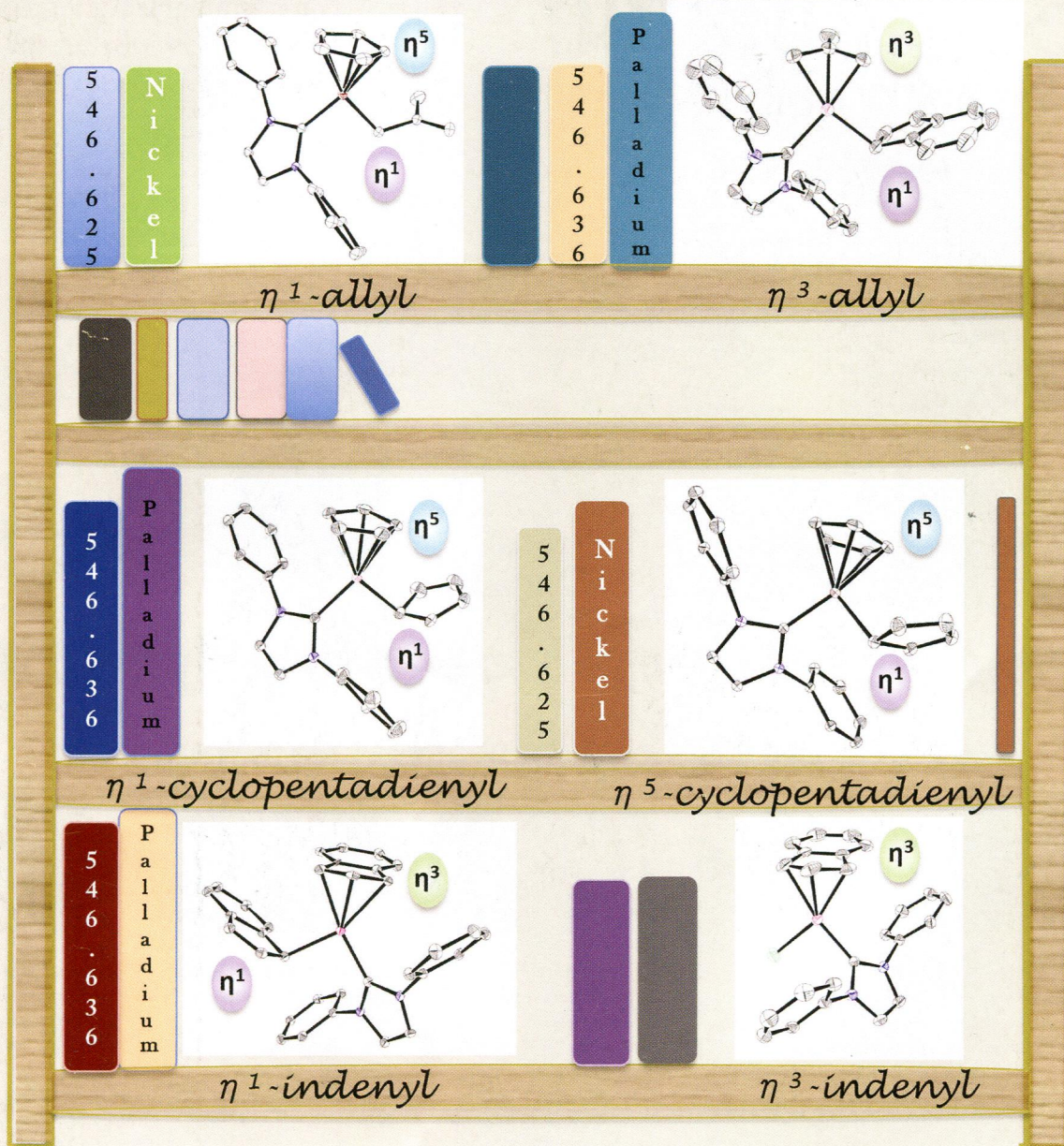


ORGANOMETALLICS

546.62: Group 10 Metals with Varying Ligand Hapticities



ON THE COVER: The cover depicts a newly synthesized family of Ni and Pd compounds supported by combinations of allyl, cyclopentadienyl, and indenyl ligands. The ligands bind with different hapticities depending on the identity of the metal, as well as the other ancillary ligands. The placement of the complexes on the bookshelves represents not only the many hapticities in which these ligands may coordinate but also the change that occurs when the central metal is varied. The numbers depicted on the books are the Dewey Decimal designations for Group 10 Metal Chemistry (546.62), as well as the more specific Palladium (546.636) and Nickel (546.625) complexes that make up this group. See the paper by Hazari et al. on pages 4025–4037.

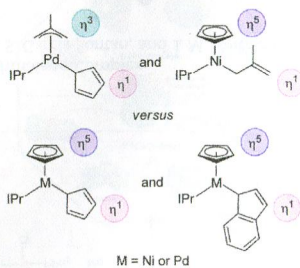
Articles

4025


[dx.doi.org/10.1021/om4002632](https://doi.org/10.1021/om4002632)

Synthesis, Properties, and Reactivity of Palladium and Nickel NHC Complexes Supported by Combinations of Allyl, Cyclopentadienyl, and Indenyl Ligands

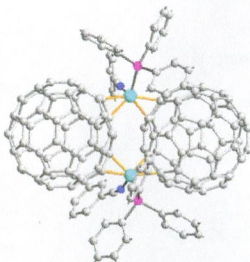
Elizabeth A. Bielinski, Wei Dai, Louise M. Guard, Nilay Hazari,* and Michael K. Takase



4038 5

dx.doi.org/10.1021/om400392c

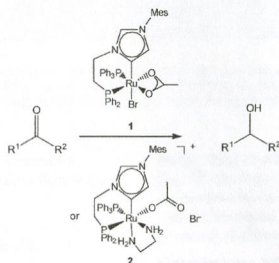
Magnetic Coupling in the Fullerene Dimer $\{Co(Ph_3P)(C_6H_5CN)\}_2(\mu_2-\eta^2\eta^2-C_{60})_2$ with Two Zerovalent Cobalt Atoms as Bridges
 Dmitri V. Konarev,* Sergey I. Troyanov, Yoshiaki Nakano, Ksenya A. Ustimenko, Akihiro Otsuka, Hideki Yamochi, Gunzi Saito, and Rimma N. Lyubovskaya



4042 5

dx.doi.org/10.1021/om400400w

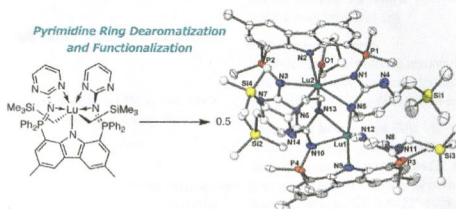
Abnormal N-Heterocyclic Carbene-Phosphine Ruthenium(II) Complexes as Active Catalysts for Transfer Hydrogenation
 Julia Witt, Alexander Pöthig, Fritz E. Kühn,* and Walter Baratta*



4046 5

dx.doi.org/10.1021/om400413e

Organolutetium-Mediated Dearomatization and Functionalization of Pyrimidine Rings
 Kevin R. D. Johnson and Paul G. Hayes*

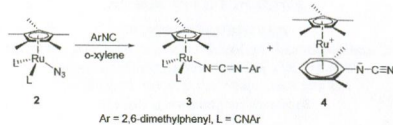


4050 **S**

dx.doi.org/10.1021/om400547r

A Sandwich Zwitterionic Ruthenium Complex Bearing a Cyanamido Group

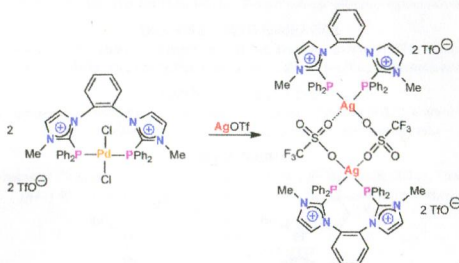
Junfei Li, Wenyong Kuai, Weiping Liu, and Wenjun Zheng*

4054 **S**

dx.doi.org/10.1021/om400602a

Electrostatic Control of Pd²⁺ → Ag⁺ Transmetalation of a Bis-Imidazolophosphine Ligand

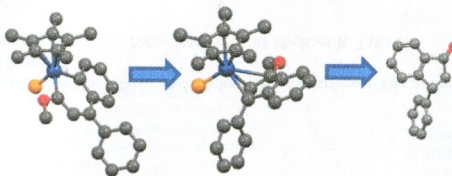
Yves Canac,* Christian Bijani, Carine Duhayon, and Remi Chauvin*

4058 **S**

dx.doi.org/10.1021/om400702b

Formation of Indanone from an Iridanaphthalene Complex

M. Talavera, S. Bolaño,* J. Bravo, J. Castro, S. García-Fontán, and J. M. Hermida-Ramón

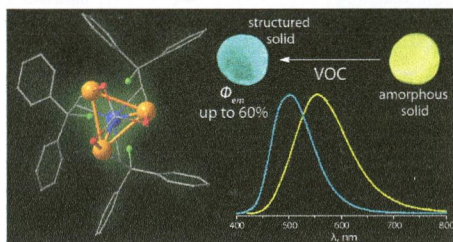


4061 **S**

dx.doi.org/10.1021/om301100v

Toward Luminescence Vapochromism of Tetranuclear Au^I–Cu^I Clusters

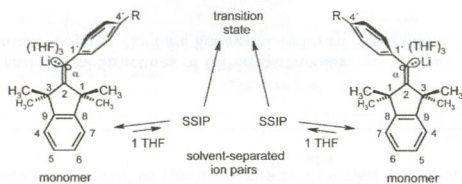
Julia R. Shakirova, Elena V. Grachova,* Alexei S. Melnikov, Vladislav V. Gurzhiy, Sergey P. Tunik,* Matti Haukka, Tapani A. Pakkanen, and Igor O. Koshevoy*

4070 **S**

dx.doi.org/10.1021/om4000852

Pseudomonomolecular, Ionic sp²-Stereo-inversion Mechanism of 1-Aryl-1-alkenyllithiums

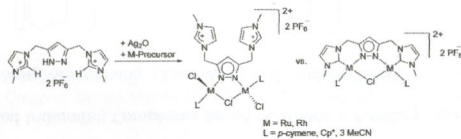
Rudolf Knorr,* Thomas Menke, Claudia Behringer, Kathrin Ferchland, Johann Mehlstäubl, and Ernst Lattke

4082 **S**

dx.doi.org/10.1021/om400106f

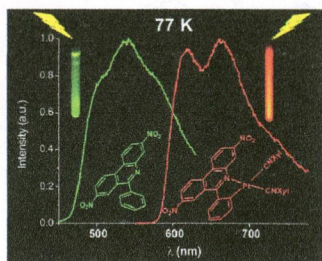
Pyrazolato-Bridged Dinuclear Complexes of Ruthenium(II) and Rhodium(III) with N-Heterocyclic Carbene Ligands: Synthesis, Characterization, and Electrochemical Properties

Stefan A. Reindl, Alexander Pöthig, Markus Drees, Bettina Bechlers, Eberhardt Herdtweck, Wolfgang A. Herrmann,* and Fritz E. Kühn*



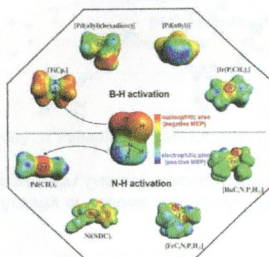
N-Assisted C_{ph}-H Activation in 3,8-Dinitro-6-phenylphenanthridine. New C,N-Cyclometalated Compounds of Platinum(II): Synthesis, Structure, and Luminescence Studies

Violeta Sicilia,* Sara Fuertes, Antonio Martín, and Adrián Palacios



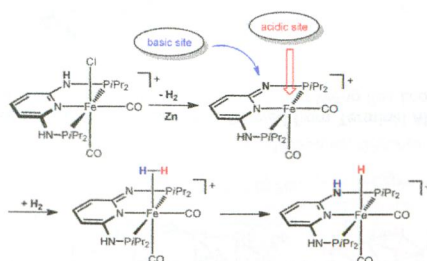
Origin of Binding of Ammonia-Borane to Transition-Metal-Based Catalysts: An Insight from the Charge and Energy Decomposition Method ETS-NOCV

Monika Parafiniuk and Mariusz Paweł Mitoraj*



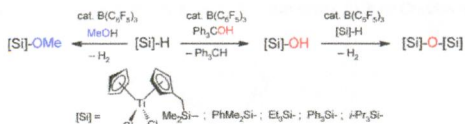
Heterolytic Cleavage of Dihydrogen by an Iron(II) PNP Pincer Complex via Metal-Ligand Cooperation

Bernhard Bichler, Christian Holzhaecker, Berthold Stöger, Michael Puchberger, Luis F. Veiros, and Karl Kirchner*



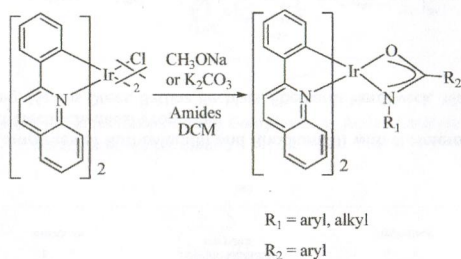
Reactivity of a Titanocene Pendant Si–H Group toward Alcohols. Unexpected Formation of Siloxanes from the Reaction of Hydrosilanes and Ph₃COH Catalyzed by B(C₆F₅)₃

Tomáš Strašák, Jan Sýkora, Martin Lamač, Jiří Kubišta, Michal Horáček, Róbert Gyepes, and Jiří Pinkas*



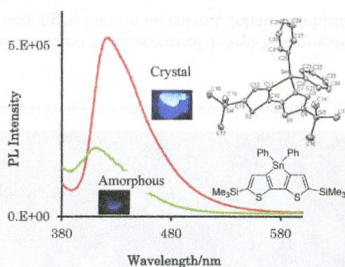
Phosphorescent Cyclometalated Iridium(III) Complexes Based on Amidate Ancillary Ligands: Their Synthesis and Photophysical Properties

Wei Yang, Dawei Wang, Qijun Song, Song Zhang, Quan Wang, and Yuqiang Ding*



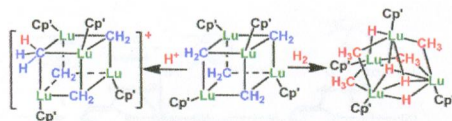
Synthesis, Optical Properties, and Crystal Structures of Dithienostannoles

Daiki Tanaka, Joji Ohshita,* Yousuke Ooyama, Norifumi Kobayashi, Hideyuki Higashimura, Takayuki Nakanishi, and Yasuchika Hasegawa

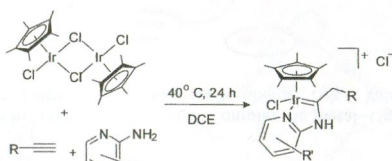


Hydrogenolysis and Protonation of Polymetallic Lutetium Methylidene and Methyl Complexes

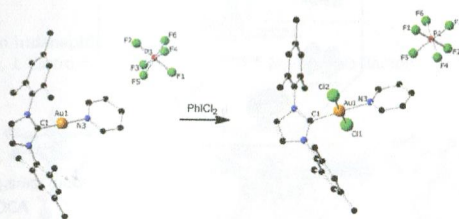
Tingting Li, Masayoshi Nishiura, Jianhua Cheng, Wenxiong Zhang, Yang Li, and Zhaomin Hou*

**Synthesis and Reactivity of Cationic Iridium Aminocarbenes Derived from Terminal Alkynes and 2-Aminopyridines**

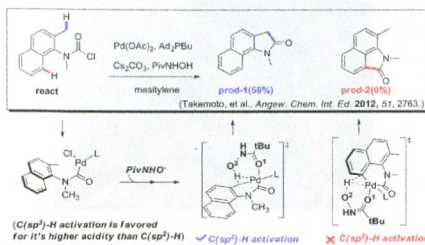
Elumalai Kumaran, Kai Tong Sonia How, Rakesh Ganguly, Yongxin Li, and Weng Kee Leong*

**Synthesis, Characterization, and Catalytic Activity of Cationic NHC Gold(III) Pyridine Complexes**

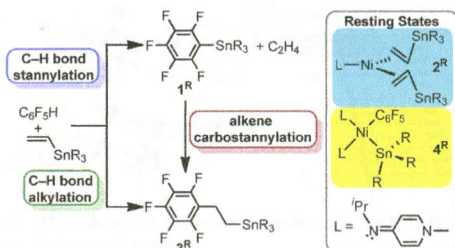
Serena Orbisaglia, Béatrice Jacques, Pierre Braunstein, Damien Hueber, Patrick Pale, Aurélien Blanc,* and Pierre de Frémont*

**Mechanistic Study of Palladium-Catalyzed Chemoselective C(sp³)-H Activation of Carbamoyl Chloride**

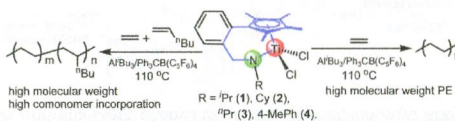
Qi Zhang, Hai-Zhu Yu, and Yao Fu*



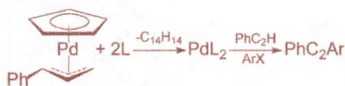
Carbon–Hydrogen Bond Stannylation and Alkylation Catalyzed by Nitrogen-Donor-Supported Nickel Complexes: Intermediates with Ni–Sn Bonds and Catalytic Carbostannylation of Ethylene with Organostannanes
 Meghan E. Doster and Samuel A. Johnson*



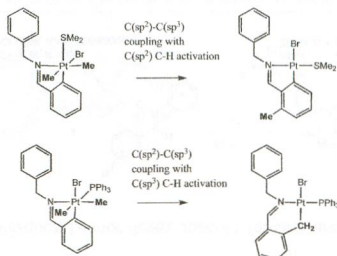
New Titanium(IV) Complexes with 2-Cyclopentadienylbenzylamido Ligands: Synthesis, Characterization, and Catalytic Properties for Ethylene Polymerization and Copolymerization with 1-Hexene
 Xin Tao, Qiaolin Wu, Hang Huo, Wei Gao, and Ying Mu*



η^5 -Cyclopentadienyl- η^3 -1-phenylallylpalladium, an Unusually Effective Catalyst Precursor for Copper-Free and Copper-Assisted Sonogashira Cross-Coupling Reactions Catalyzed by Bis-phosphine Palladium(0) Compounds: The Role of Bis-acetylide Intermediates in the Reduction of a Palladium(II) Catalyst Precursor to a Palladium(0) Catalyst
 Bryan E. Jaksic, Jingsi Jiang, Andrew W. Fraser, and Michael C. Baird*

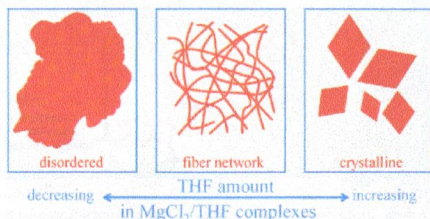


Regioselective C–H Activation Preceded by C_{sp}²–C_{sp}¹ Reductive Elimination from Cyclometalated Platinum(IV) Complexes
 Craig M. Anderson,* Margarita Crespo,* Nicole Kfoury, Michael A. Weinstein, and Joseph M. Tanski



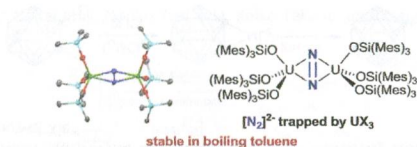
A Single-Crystal Model for MgCl_2 -Electron Donor Support Materials: $[\text{Mg}_3\text{Cl}_5(\text{THF})_4\text{Bu}]_2$ (Bu = *n*-Butyl)

Sami Pirinen, Igor O. Koshevoy, Peter Denifl, and Tuula T. Pakkanen*



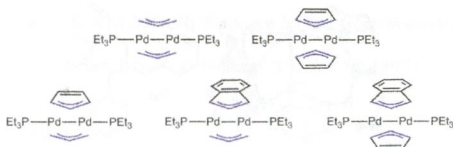
Thermally Stable Uranium Dinitrogen Complex with Siloxide Supporting Ligands

Stephen M. Mansell, Joy H. Farnaby, Anne I. Germeroth, and Polly L. Arnold*



Synthesis, Electronic Structure, and Reactivity of Palladium(I) Dimers with Bridging Allyl, Cyclopentadienyl, and Indenyl Ligands

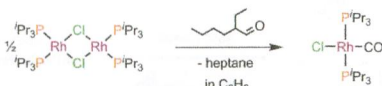
Matthew J. Chalkley, Louise M. Guard, Nilay Hazari,* Peter Hofmann, Damian P. Hruszkewycz, Timothy J. Schmeier, and Michael K. Takase



Assessing the Accuracy of M06-L Organometallic Thermochemistry

Dmitry G. Gusev*

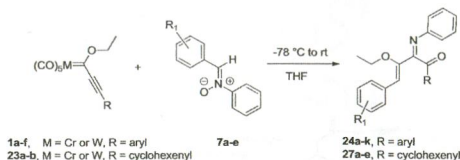
M06-L: good-quality functional for organometallic reactions



M06-L: $\Delta\text{H} = -37.1$; Exp.: $\Delta\text{H} = -36.0 \pm 0.5$ kcal/mol

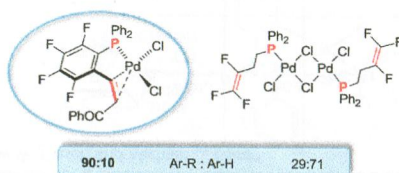
Unprecedented Synthesis of 3-Alkenyl-3-ethoxy-2-iminoketones via 1,3-Dipolar Cycloadditions of Nitrones with Alkynyl Fischer Carbene Complexes

María Inés Flores-Conde, Miguel Angel Vázquez, Leonor Reyes, Joaquín Tamariz, and Francisco Delgado*



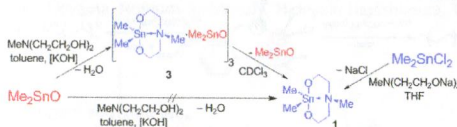
Phosphines with Tethered Electron-Withdrawing Olefins as Ligands for Efficient Pd-Catalyzed Aryl-Alkyl Coupling

Estefanía Gioria, Jesús M. Martínez-Illarduya, Domingo García-Cuadrado, Jesús A. Miguel, Miroslav Genov, and Pablo Espinet*



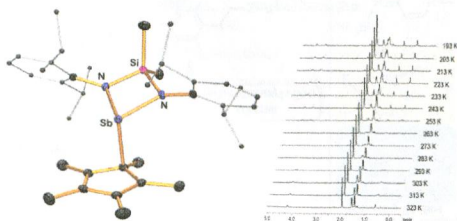
Simplicity Meets Beauty. Trapping Molecular Dimethyltin Oxide in the Novel Organotin Cluster [MeN(CH₂CH₂O)₂SnMe₂Me₂SnO]₃

Michael Gock, Bianca Wiedemann, Christina Dietz, Chenyu Bai, Michael Lutter, Vinusuya Abeyawarathan, and Klaus Jurkschat*



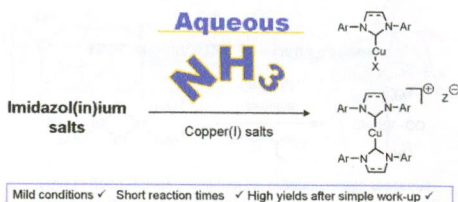
Assigning Hapticity to Cyclopentadienyl Derivatives of Antimony and Bismuth

Benjamin M. Day and Martyn P. Coles*



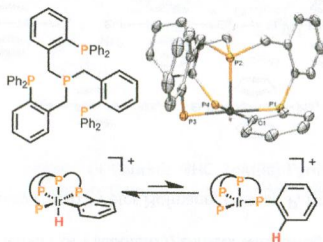
Simplified Preparation of Copper(I) NHCs Using Aqueous Ammonia

Clémentine Gibard, Houssein Ibrahim, Arnaud Gautier, and Federico Cisnetti*



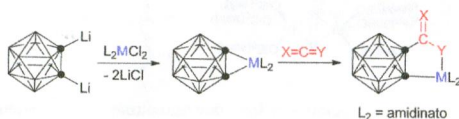
Reductive Elimination at an Ortho-Metalated Iridium(III) Hydride Bearing a Tripodal Tetraphosphorus Ligand

Yann Gloaguen, Lianne M. Jongens, Joost N. H. Reek, Martin Lutz, Bas de Bruin, and Jarl Ivar van der Vlugt*



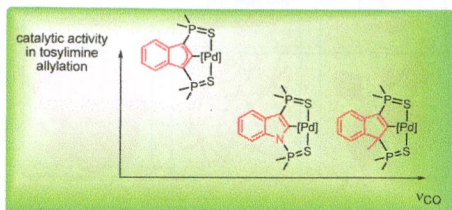
Synthesis of Neutral Group 4 Metal–Carbonyne Complexes and Their Reactivity toward Unsaturated Molecules

Shikuo Ren, Zaozao Qiu, and Zuowei Xie*



Influence of the Ligand Backbone in Pincer Complexes: Indenediide-, Indoyl-, and Indenyl-Based SCS Palladium Complexes

Jérôme Lisena, Julien Monot, Sonia Mallet-Ladeira, Blanca Martin-Vaca,* and Didier Bourissou*



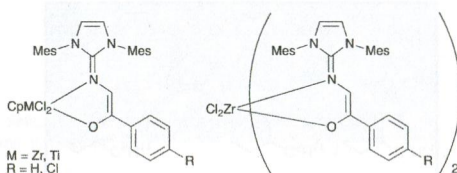
Cyclometalations on the Imidazo[1,2-a][1,8]naphthyridine Framework

Prosenjit Daw, Tapas Ghatak, Henri Doucet, and Jitendra K. Bera*



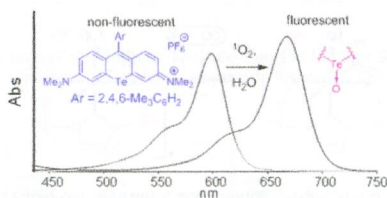
Coordination and Reactivity Study of Titanium and Zirconium Complexes of the First Imidazol-2-imine Ethenolate Ligand

Timothy G. Larocque, Sarim Dastgir, and Gino G. Lavoie*



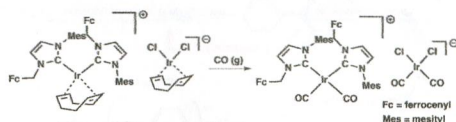
Organotellurium Fluorescence Probes for Redox Reactions: 9-Aryl-3,6-diaminotelluroxanthylum Dyes and Their Telluroxides

Mark W. Kryman, Gregory A. Schamerhorn, Kayi Yung, Bharathwaj Sathyamoorthy, Dinesh K. Sukumaran, Tymish Y. Ohulchansky, Jason B. Benedict,* and Michael R. Detty*



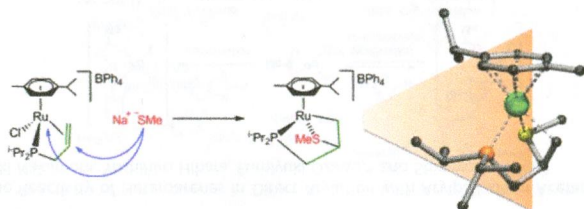
Cationic Iridium Complexes Containing Anionic Iridium Counterions Supported by Redox-Active N-Heterocyclic Carbenes

Kuppuswamy Arumugam, Jinho Chang, Vincent M. Lynch, and Christopher W. Bielawski*



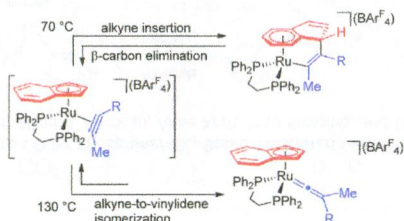
Organoruthenium Complexes Containing New Phosphorus–Carbon and Phosphorus–Carbon–Sulfur Ligands Generated in the Coordination Sphere by Nucleophilic Addition Reactions

Isaac García de la Arada, Josefina Díez, M. Pilar Gamasa, and Elena Lastra*



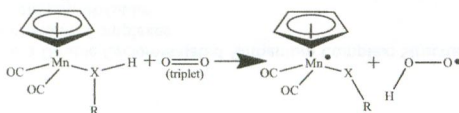
Reactivities of Indenylruthenium Complex toward Internal Alkynes: Formation of Disubstituted Vinylidene Complexes and Indenyl–Alkyne Coupling

Yousuke Ikeda, Yuichiro Mutoh,* Kohei Imai, Noriko Tsuchida, Keiko Takano, and Youichi Ishii*

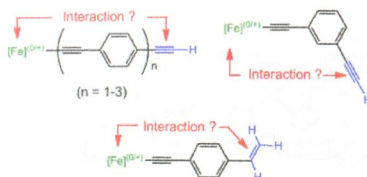


Significant O–H Bond Weakening in $\text{CpMn}(\text{CO})_2(\text{CH}_3\text{OH})$: Evidence for the Generation of the $\text{CpMn}(\text{CO})_2(\text{CH}_3\text{O})$ Radical upon H Atom Abstraction by O_2

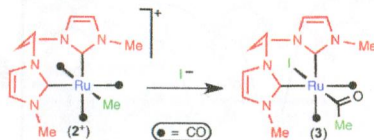
Jun Wei Kee, Tsz Sian Chwee, Xiang Yeow Tan, Richard D. Webster, and Wai Yip Fan*



Synthesis and Characterization of Redox-Active Mononuclear $\text{Fe}(\alpha^2\text{-dippe})(\eta^5\text{-C}_5\text{Me}_5)$ -Terminated π -Conjugated Wires
 Katy Green, Nicolas Gauthier, Hiba Sahounne, Gilles Argouarch, Loïc Toupet, Karine Costuas, Arnaud Bondon, Bruno Fabre,*
 Jean-François Halet,* and Frédéric Paul*

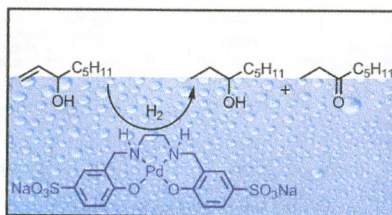


Reactivity of a (Bis-NHC)tricarbonylruthenium(0) Complex with Methyl Triflate and Methyl Iodide. Formation of Methyl- and Acetylruthenium(II) Derivatives: Experimental Results and Mechanistic DFT Calculations
 Javier A. Cabeza,* Marina Damonte, Pablo García-Álvarez, and Enrique Pérez-Carreño



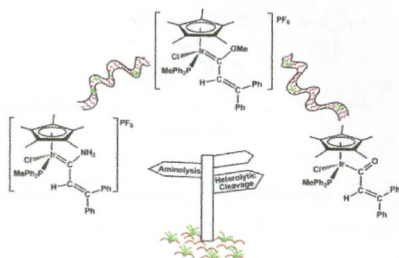
Hydrogenation and Redox Isomerization of Allylic Alcohols Catalyzed by a New Water-Soluble Pd-tetrahydrosalen Complex

Krisztina Voronova,* Mihály Purgel, Antal Udvardy, Attila C. Bényei, Ágnes Kathó, and Ferenc Joó*



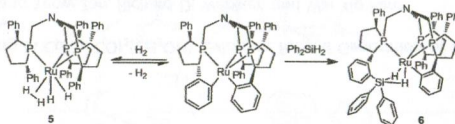
Nucleophilic Attack in Methoxycarbenes: Heterolytic Cleavage of the Carbon (sp^3)–Oxygen Bond versus Aminolysis

M. Talavera, S. Bolaño,* J. Bravo, J. Castro, S. García-Fontán, and J. M. Hermida-Ramón



Hydrogenation and Silylation of a Double-Cyclometalated Ruthenium Complex: Structures and Dynamic Behavior of Hydrido and Hydrosilicate Ruthenium Complexes

Peter Scherl, Hubert Wadepohl, and Lutz H. Gade*



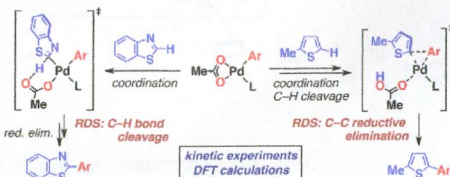
Stoichiometric Reduction of CO_2 to CO by Phosphine/ AlX_3 -Based Frustrated Lewis Pairs

Gabriel Ménard, Thomas M. Gilbert, Jillian A. Hatnean, Anne Kraft, Ingo Krossing, and Douglas W. Stephan*



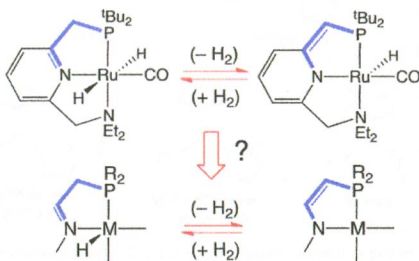
Factors Controlling the Reactivity of Heteroarenes in Direct Arylation with Arylpalladium Acetate Complexes

Masayuki Wakioka, Yuki Nakamura, Yoshihiro Hihara, Fumiyuki Ozawa,* and Shigeyoshi Sakaki



Use of the Imine–Enamine Equilibrium in Cooperative Ligand Design

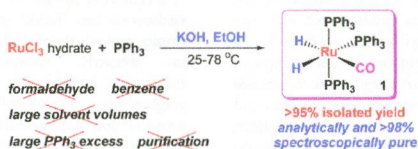
Truman C. Wambach, Jun Myun Ahn, Brian O. Patrick, and Michael D. Fryzuk*



Notes

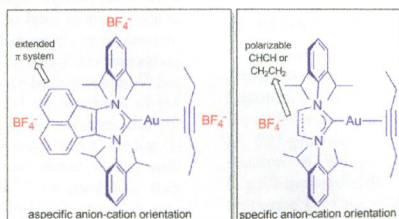
New, Highly Efficient, Simple, Safe, and Scalable Synthesis of $[(\text{PPh}_3)_3\text{Ru}(\text{CO})(\text{H})_2]$

Hamidreza Samouei and Vladimir V. Grushin*



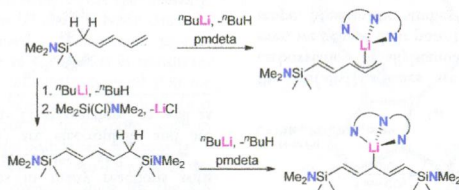
NHC–Gold–Alkyne Complexes: Influence of the Carbene Backbone on the Ion Pair Structure

Gianluca Ciancaleoni, Luca Biasiolo, Giovanni Bistoni, Alceo Macchioni, Francesco Tarantelli, Daniele Zuccaccia,* and Leonardo Belpassi*

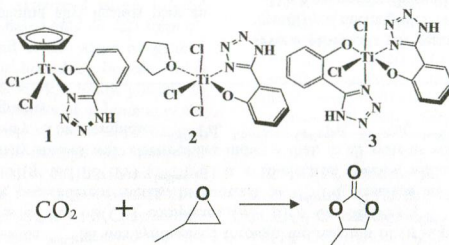


Structural Influences in Lithium Pentadienylsilane Complexes

Benjamin M. Day, Jonathan Clayden, and Richard A. Layfield*

New Titanium Catalysts Containing Tetrazole for Cycloaddition of CO₂ to Epoxides

Min Jeong Go, Kang Mun Lee, Chang Hwa Oh, Yi Young Kang, So Han Kim, Hyoung Ryun Park, Youngjo Kim,* and Junseong Lee*



Additions and Corrections

Correction to Highly Efficient and Selective Chromium(III) Ethylene Trimerization Catalysts with [NON] and [NSN] Heteroscorpionate Ligands

Jun Zhang, Pierre Braunstein,* and T. S. Andy Hor*