

ORGANOMETALLICS

APRIL 14, 2014

VOLUME 33 ISSUE 7

ORGND7 33(7) 1503–1892 (2014)

ISSN 0276-7333

Registered in the U.S. Patent and Trademark Office

© 2014 by the American Chemical Society

ON THE COVER: The background symbolizes the diverse range of questions that organometallic chemists confront in their research, while the magnifying glass represents the efforts of the Roundtable panel to bring clarity and focus to the topics discussed. Read the full Roundtable discussion on pages 1505-1527.

Editor's Page

1503

[dx.doi.org/10.1021/om5003304](https://doi.org/10.1021/om5003304)

Associate Editors Past and Present: A Warm Welcome to Professor Daniel J. Mindiola, and Heartfelt Thanks to Professor Tobin J. Marks
John A. Gladysz



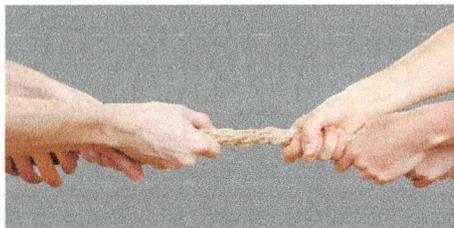
Roundtable

1505

[dx.doi.org/10.1021/om500253z](https://doi.org/10.1021/om500253z)

***Organometallics* Roundtable 2013–2014**

John A. Gladysz,* Robin B. Bedford, Makoto Fujita, François P. Gabbaï, Karen I. Goldberg, Patrick L. Holland, Jaqueline L. Kiplinger, Michael J. Krische, Janis Louie, Connie C. Lu, Jack R. Norton, Marina A. Petrukhina, Tong Ren, Shannon S. Stahl, T. Don Tilley, Charles Edwin Webster, M. Christina White, and Gregory T. Whiteker

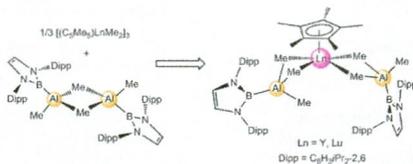


1528 

[dx.doi.org/10.1021/om401163a](https://doi.org/10.1021/om401163a)

Half-Sandwich Rare-Earth-Metal Alkylalumininate Complexes Bearing Peripheral Boryl Ligands

Nicole Dettenrieder, Christoph O. Hoffelder, Lars N. Jende, Cécilia Maichle-Mössmer, and Reiner Anwander*

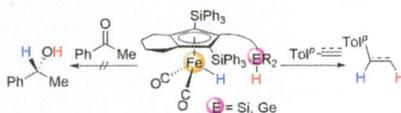


1532 

[dx.doi.org/10.1021/om5000562](https://doi.org/10.1021/om5000562)

Synthesis of Fe–H/Si–H and Fe–H/Ge–H Bifunctional Complexes and Their Catalytic Hydrogenation Reactions toward Nonpolar Unsaturated Organic Molecules

Masahiro Kamitani, Yoshinori Nishiguchi, Ryosuke Tada, Masumi Itazaki, and Hiroshi Nakazawa*

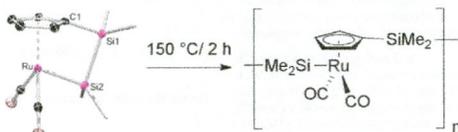


1536 

[dx.doi.org/10.1021/om500111r](https://doi.org/10.1021/om500111r)

Strained *ansa* Half-Sandwich Complexes of Ruthenium and Osmium and a Non-Iron Metallopolymer by Ring-Opening Polymerization

Holger Braunschweig,* Theresa Dellermann, Rian D. Dewhurst, Jan Mies, Krzysztof Radacki, Sascha Stellwag-Konertz, and Alfredo Vargas

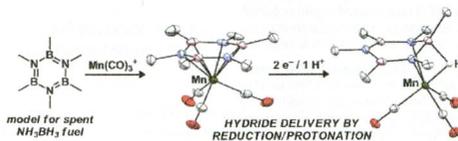


1540 

[dx.doi.org/10.1021/om500157m](https://doi.org/10.1021/om500157m)

Manganese-Mediated Hydride Delivery to a Borazine by Stepwise Reduction and Protonation

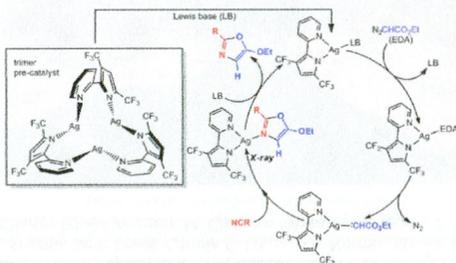
Tyler J. Carter, Justin Y. Wang, and Nathaniel K. Szymczak*



1544 **S**

dx.doi.org/10.1021/om400756t

Mechanistic Understanding of a Silver Pyridylpyrrolide as a Catalyst for 3 + 2 Cyclization of a Nitrile with Diazo Ester
 Jaime A. Flores, Kuntal Pal, Maria E. Carroll, Maren Pink, Jonathan A. Karty, Daniel J. Mindiola,* and Kenneth G. Caulton*

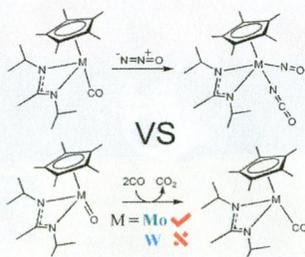


1553 **S**

dx.doi.org/10.1021/om400935f

Mechanism of Carbon Monoxide Induced N–N Bond Cleavage of Nitrous Oxide Mediated by Molybdenum Complexes: A DFT Study

Hujun Xie,* Liu Yang, Xinchun Ye, and Zexing Cao

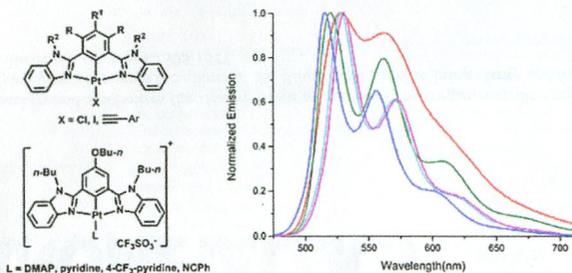


1563 **S**

dx.doi.org/10.1021/om400946n

Neutral and Cationic NCN Pincer Platinum(II) Complexes with 1,3-Bis(benzimidazol-2'-yl)benzene Ligands: Synthesis, Structures, and Their Photophysical Properties

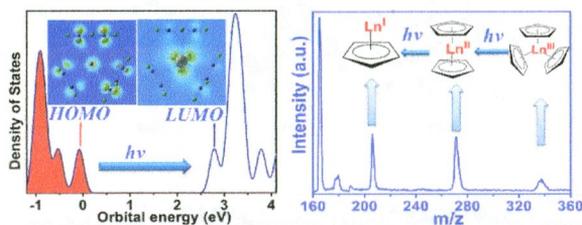
Zhao Wang, Zheming Sun, Xin-Qi Hao, Jun-Long Niu, Donghui Wei, Tao Tu, Jun-Fang Gong,* and Mao-Ping Song*



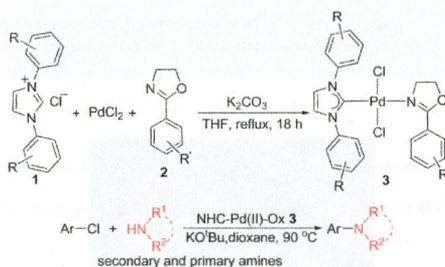
L = DMAP, pyridine, 4-CF₃-pyridine, NCPH

Photofragmentation of Gas-Phase Lanthanide Cyclopentadienyl Complexes: Experimental and Time-Dependent Excited-State Molecular Dynamics

Jiangchao Chen, Andrew M. Hochstatter, Dmitri Kilin, P. Stanley May, Qingguo Meng,* and Mary T. Berry*


N-Heterocyclic Carbene–Palladium(II)–4,5-Dihydrooxazole Complexes: Synthesis and Catalytic Activity toward Amination of Aryl Chlorides

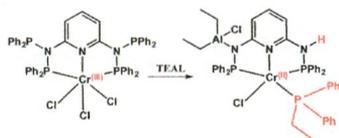
Pei Huang, Yi-Xiang Wang, Hong-Fei Yu, and Jian-Mei Lu*


Synthesis and Biological Evaluation of Organoruthenium Complexes with Azole Antifungal Agents. First Crystal Structure of a Tioconazole Metal Complex

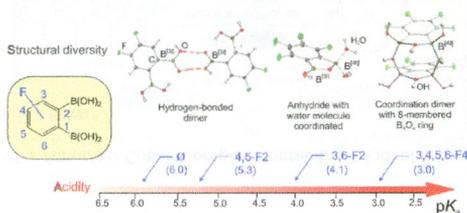
Jakob Kljun, Antony James Scott, Tea Lanišnik Rižner, Jennifer Keiser, and Iztok Turel*



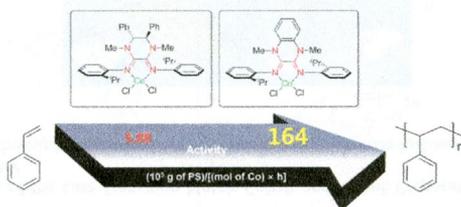
Reactivity with Alkylaluminum of a Chromium Complex of a Pyridine-Containing PNP Ligand: Redox N–P Bond Cleavage
 Ahmed Alzamly, Sandro Gambarotta,* and Ilia Korobkov



Influence of Fluorination and Boronic Group Synergy on the Acidity and Structural Behavior of *o*-Phenylenediboric Acids
 Krzysztof Durka,* Sergiusz Luliński,* Janusz Serwatowski, and Krzysztof Woźniak

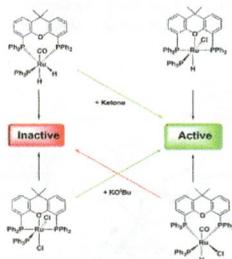


Synthesis of New Bis(amidine)–Cobalt Catalysts and Their Application to Styrene Polymerization
 Wonseok Cho, Hyemin Cho, Chun Sun Lee, Bun Yeoul Lee, Bongjin Moon,* and Jahyo Kang

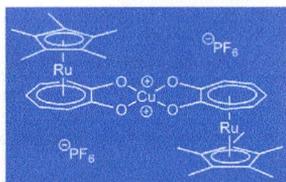


Mechanistic Study on the Ruthenium-Catalyzed Direct Amination of Alcohols

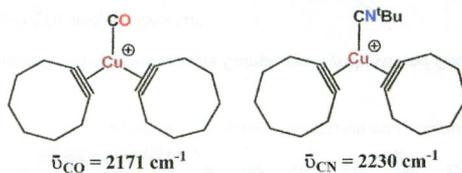
Dennis Pinggen, Martin Lutz, and Dieter Vogt*

 **π -Complexes of Tropolone and Its N-Derivatives: Ambidentate [O,O]/[N,O]/[N,N]-Cycloheptatrienyl Pentamethylcyclopentadienyl Ruthenium Sandwich Complexes**

Michael Pitttracher, Ulla Frisch, Holger Kopacka, Klaus Wurst, Thomas Müller, Luciano Oehninger, Ingo Ott, Evelyn Wuttke, Stefan Scheerer, Rainer F. Winter, and Benno Bildstein*

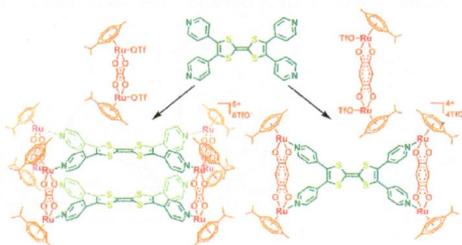
**Coordination and Ligand Substitution Chemistry of Bis(cyclooctyne)copper(I)**

Animesh Das, Chandrakanta Dash, Muhammed Yousufuddin, and H. V. Rasika Dias*

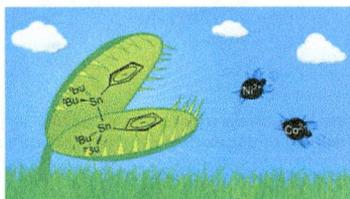


Electron-Rich Arene–Ruthenium Metalla-architectures Incorporating Tetrapyrridyl–Tetrathiafulvene Donor Moieties

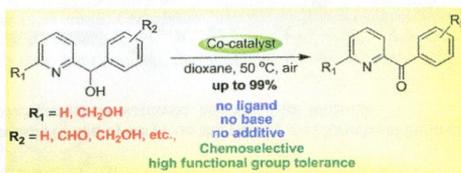
Vaishali Vajpayee, Sébastien Bivaud, Sébastien Goeb, Vincent Croué, Magali Allain, Brian V. Popp, Amine Garci, Bruno Therrien,* and Marc Sallé*

**Tin-Bridged *ansa*-Metallocenes of the Late Transition Metals Cobalt and Nickel: Preparation, Molecular and Electronic Structures, and Redox Chemistry**

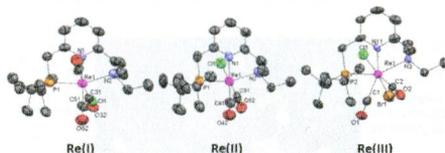
Thomas Arnold, Holger Braunschweig,* Alexander Damme, Christian Hörl, Thomas Kramer, Ivo Krummenacher, and Julian Mager

**Isolation and Characterization of a Trinuclear Cobalt Complex Containing Trigonal-Prismatic Cobalt in Secondary Alcohol Aerobic Oxidation**

I. Karthikeyan, S. K. Alamsetti, and G. Sekar*

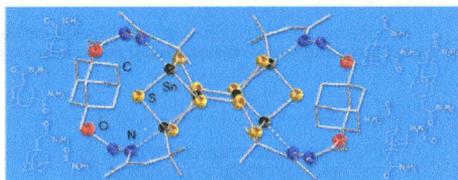


Synthesis, Dynamics, and DFT Studies of Rhenium Dicarboxyl PNN Pincer Complexes in Three Different Oxidation States
Kothanda Rama Pichaandi, Michael G. Mazzotta, John S. Harwood, Phillip E. Fanwick, and Mahdi M. Abu-Omar*



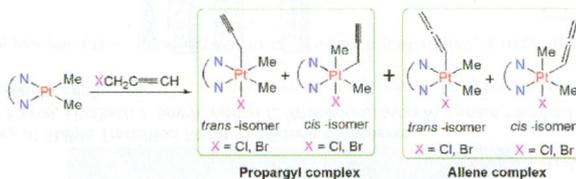
Diamondoid Hydrazones and Hydrazides: Sterically Demanding Ligands for Sn/S Cluster Design

Beatrix E. K. Barth, Boryslav A. Tkachenko, Jens P. Eußner, Peter R. Schreiner, and Stefanie Dehnen*



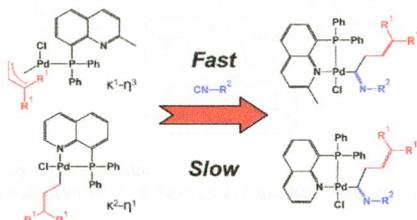
Oxidative Addition of Propargyl Halides, Chloroacetonitrile, and Ethyl Chloroacetate to a Dimethylplatinum(II) Complex: Kinetic and DFT Studies

S. Jafar Hoseini,* Hasan Nasrabadi, Roghayeh Hashemi Fath, Zohreh Moradi, and Mehdi Rashidi*



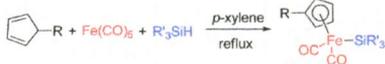
Insertion of Isocyanides across the Pd–C Bond of Phosphinoquinoline Allyl Palladium Complexes Bearing η^1 - and η^3 -Coordinated Allyl Groups. A Synthetic and Mechanistic Study

L. Canovese,* F. Visentin, C. Santo, and V. Bertolasi



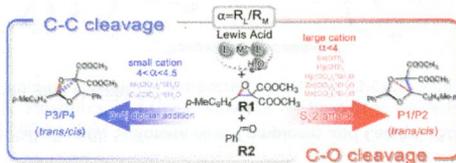
A New Approach to Directly Synthesize $(\eta^5\text{-C}_5\text{H}_4\text{R})\text{Fe}(\text{CO})_2\text{SiR}'_3$ by Reaction of Cyclopentadienes with Pentacarbonyliron and Hydrosilanes

Guangna Gu, Haiou Luo, and Huailin Sun*



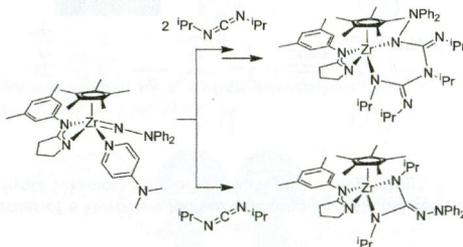
Control of Chemoselectivity by Coordinated Water and Relative Size of Ligands to Metal Cations of Lewis Acid Catalysts for Cycloaddition of an Oxirane Derivative to an Aldehyde: Theoretical and Experimental Study

Ziqi Tian, Yuanjing Xiao, Xiangai Yuan, Zuliang Chen, Junliang Zhang,* and Jing Ma*



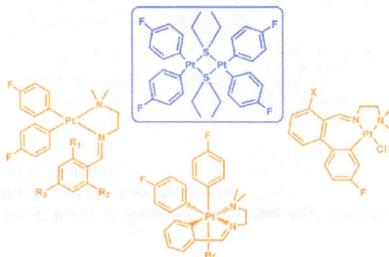
Zirconium and Hafnium Hydrazinediido Half-Sandwich Complexes: Synthesis and Reactivity

Peter D. Schweizer, Hubert Wadepohl, and Lutz H. Gade*



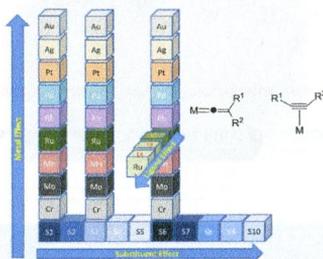
Exploring the Scope of $[\text{Pt}_2(4\text{-FC}_6\text{H}_4)_4(\mu\text{-SEt}_2)_2]$ as a Precursor for New Organometallic Platinum(II) and Platinum(IV) Antitumor Agents

Anna Escolà, Margarita Crespo,* Josefina Quirante,* Roldán Cortés, Anusha Jayaraman, Josefa Badía, Laura Baldomà, Teresa Calvet, Mercè Font-Bardía, and Marta Cascante



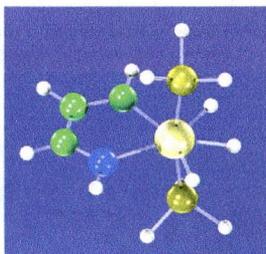
Computational Discovery of Stable Transition-Metal Vinylidene Complexes

Oliver J. S. Pickup, Iman Khazal, Elizabeth J. Smith, Adrian C. Whitwood, Jason M. Lynam,* Keshan Bolaky, Timothy C. King, Benjamin W. Rawe, and Natalie Fey*



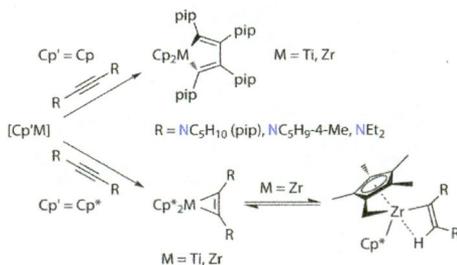
Analysis of the Aromaticity of Five-Membered Heterometallacycles Containing Os, Ru, Rh, and Ir

Rafael Islas,* Jordi Poater, and Miquel Solà*



Titanocene and Zirconocene Complexes with Diaminoacetylenes: Formation of Unusual Metallacycles and Fulvene Complexes

Oscar Arias, Alex R. Petrov, Thomas Bannenberg, Kai Altenburger, Perdita Arndt, Peter G. Jones, Uwe Rosenthal,* and Matthias Tamm*



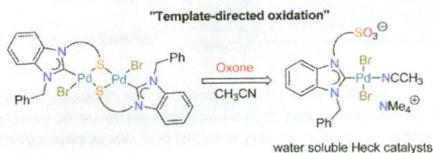
Reactivity and Electronic Properties of a Ferrocene Molecule Bearing an N,C-Chelated BMes₂ Unit

Ying-Li Rao, Tetsuro Kusamoto, Ryota Sakamoto, Hiroshi Nishihara, and Suning Wang*



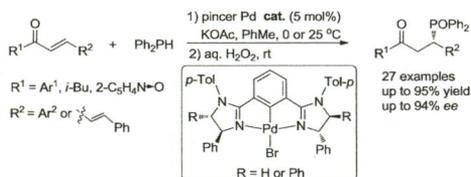
Template-Directed Synthesis of Palladium(II) Sulfonate-NHC Complexes and Catalytic Studies in Aqueous Mizoroki–Heck Reactions

Dan Yuan, Qiaoqiao Teng, and Han Vinh Huynh*



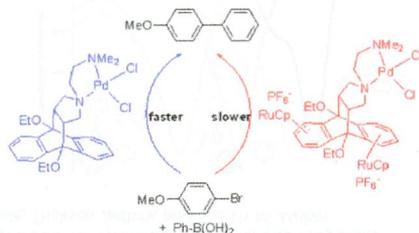
Enantioselective Hydrophosphination of Enones with Diphenylphosphine Catalyzed by Bis(imidazoline) NCN Pincer Palladium(II) Complexes

Xin-Qi Hao, Yong-Wei Zhao, Jing-Jing Yang, Jun-Long Niu, Jun-Fang Gong,* and Mao-Ping Song*



Heteropolymetallic Complexes Linked to a 9,10-Dihydroanthracenyl Frame. Ruthenium as Active Spectator for Palladium Reactivity

Ielyzaveta Bratko, Sonia Mallet-Ladeira, Emmanuelle Teuma, and Montserrat Gómez*



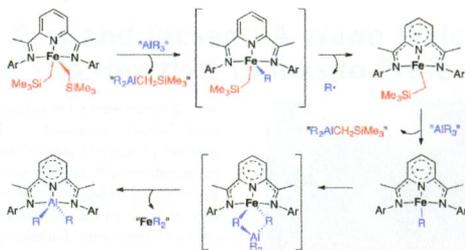
Chelated Assisted Metal-Mediated N–H Bond Activation of β -Lactams: Preparation of Irida-, Rhoda-, Osmia-, and Ruthenatrinems

Luis Casarrubios, Miguel A. Esteruelas,* Carmen Larramona, Jaime G. Muntaner, Montserrat Oliván, Enrique Oñate, and Miguel A. Sierra*



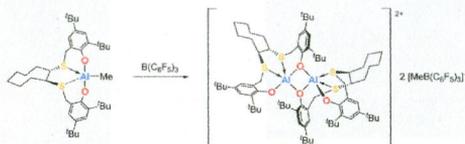
Sequential Reduction and Alkyl Exchange Reactions of Bis(imino)pyridine Dialkyliron(II) with Trimethylaluminum

M. Ángeles Cartes, Antonio Rodríguez-Delgado, Pilar Palma, Eleuterio Álvarez, and Juan Cámpora*



Neutral Methyl and Cationic Aluminum Complexes Supported by a *trans*-1,2-Cyclooctanediyl-Bridged [OSSO]-Type Bis(phenolato) Ligand: Synthesis, Structures, and Use in Catalysis for Propylene Oxide Polymerization

Norio Nakata, Yusuke Saito, and Akihiko Ishii*



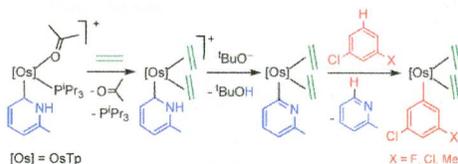
Theoretical Study on the Stability and Aromaticity of Metallasilapentalynes

Xuerui Wang, Congqing Zhu, Haiping Xia,* and Jun Zhu*



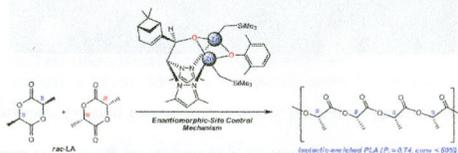
Selective *meta*-C–H Bond Activation of Substituted 1,3-Chlorobenzenes Promoted by an Osmium Pyridyl Complex

Sonia Bajo, Miguel A. Esteruelas,* Ana M. López, and Enrique Oñate



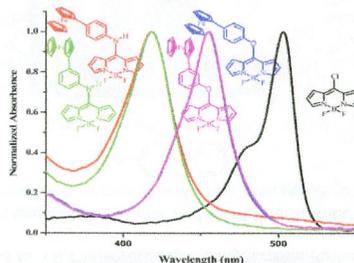
Stereoselective ROP of *rac*-Lactide Mediated by Enantiopure NNO-Scorpionate Zinc Initiators

Manuel Honrado, Antonio Otero,* Juan Fernández-Baeza,* Luis F. Sánchez-Barba,* Andrés Garcés, Agustín Lara-Sánchez, and Ana M. Rodríguez

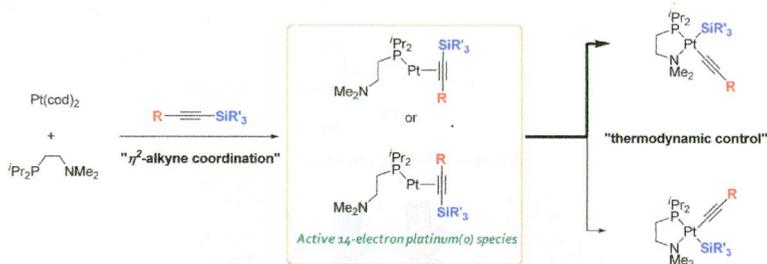


Heteroatom-Connected Ferrocenyl BODIPYs: Synthesis, Structure, and Properties

Rajneesh Misra,* Bhausaheb Dhokale, Thaksen Jadhav, and Shaikh M. Mobin



Experimental and Theoretical Studies on the Platinum-Mediated Selective C(sp)–Si Bond Cleavage of Alkynylsilanes
 Yasuhiro Okuda, Yuya Ishiguro, Seiji Mori, Kiyohiko Nakajima, and Yasushi Nishihara*



Notes

α -Alkylation of Ketones by Trialkylamines under Heterogeneous Pd/C Catalysis

Il Chul Yoon, Tae Gyun Kim, and Chan Sik Cho*

