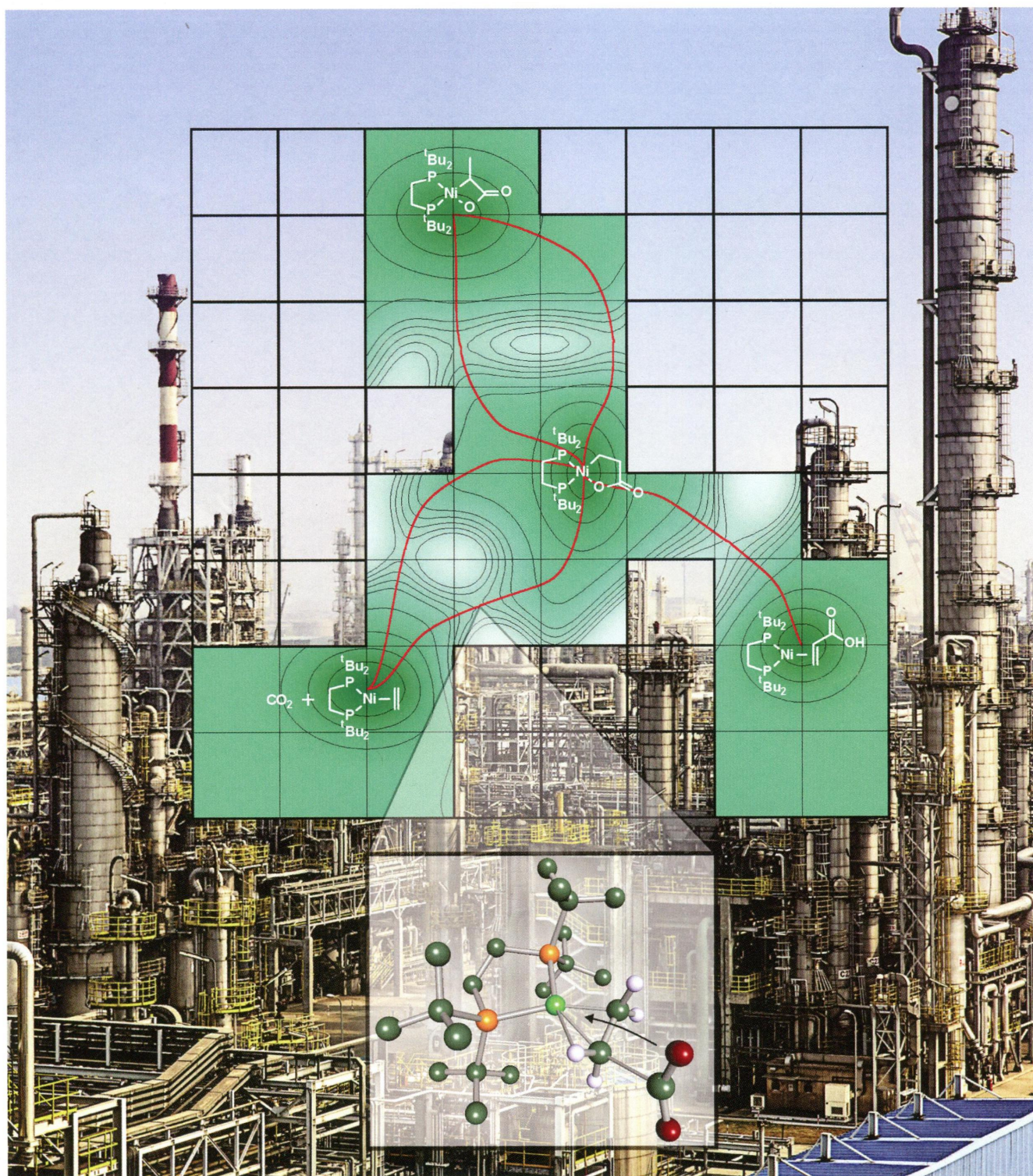


# ORGANOMETALLICS



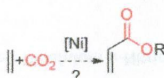
**ON THE COVER:** Exploring the Ni-mediated coupling of CO<sub>2</sub> and ethylene: Despite recent progress in the synthesis of acrylates from carbon dioxide and ethylene, the underlying mechanisms still require investigation. Theoretical calculations of the reaction mechanism yield minima and transition states and the connecting reaction paths. Yet, most of the multidimensional potential energy surface is not explicitly known. This situation is illustrated by the map, where remaining blank spaces, known intermediates, and investigated paths are shown. The depicted transition state for nickelalactone formation is in competition with the mechanism known from the literature. See the paper by Hofmann et al. on pages 3657–3668.

## Articles

 3657 **S**
[dx.doi.org/10.1021/om500151h](https://doi.org/10.1021/om500151h)

### Acrylate Formation from CO<sub>2</sub> and Ethylene Mediated by Nickel Complexes: A Theoretical Study

Philipp N. Plessow, Ansgar Schäfer, Michael Limbach, and Peter Hofmann\*

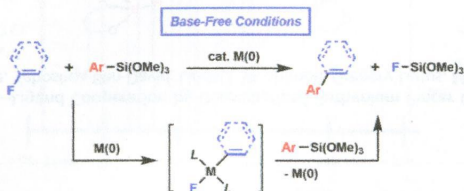


## Communications

 3669 **S**
[dx.doi.org/10.1021/om5005513](https://doi.org/10.1021/om5005513)

### Base-Free Hiyama Coupling Reaction via a Group 10 Metal Fluoride Intermediate Generated by C–F Bond Activation

Hiroki Saijo, Hironobu Sakaguchi, Masato Ohashi, and Sensuke Ogoshi\*

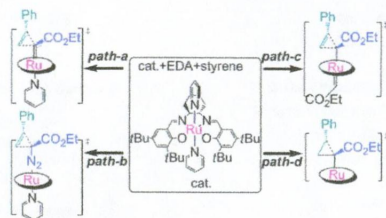


3673 **S**

dx.doi.org/10.1021/om400956z

## Theoretical Studies on the Mechanism, Enantioselectivity, and Axial Ligand Effect of a Ru(salen)-Catalyzed Asymmetric Cyclopropanation Reaction

Ting Shi, Yu Luo, Xiao-Lei Wang, Shaoyong Lu, Yi-Lei Zhao,\* and Jian Zhang\*

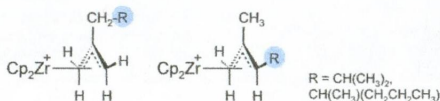


3683

dx.doi.org/10.1021/om400972u

Synthesis, Structures, and Dynamic Features of  $d^0$  Zirconocene–Allyl Complexes

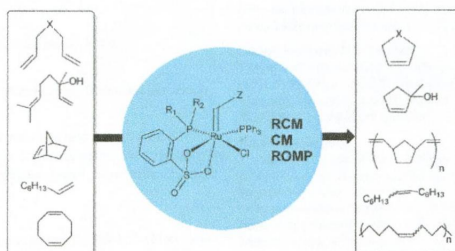
Mihaela Vatamanu

3695 **S**

dx.doi.org/10.1021/om500212x

## 18-Electron Ruthenium Phosphine Sulfonate Catalysts for Olefin Metathesis

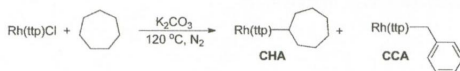
Oumar Bashir, Laurence Piche, and Jerome P. Claverie\*

3702 **S**

dx.doi.org/10.1021/om500313g

 $K_2CO_3$ -Promoted Consecutive Carbon–Hydrogen and Carbon–Carbon Bond Activation of Cycloheptane with Rhodium(III) Porphyrin Complexes: Formation of Rhodium Porphyrin Cycloheptyl and Benzyl

Kin Shing Chan\* and Yun Wai Chan



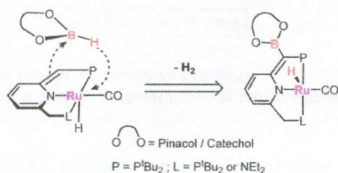
**Ruthenium(II)–Arene RAPTA Type Complexes Containing Curcumin and Bisdemethoxycurcumin Display Potent and Selective Anticancer Activity**

Riccardo Pettinari,\* Fabio Marchetti, Francesca Condello, Claudio Pettinari, Giulio Lupidi, Rosario Scopelliti, Suman Mukhopadhyay, Tina Riedel, and Paul J. Dyson\*



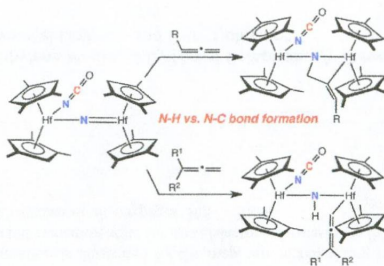
**B–H Bond Cleavage via Metal–Ligand Cooperation by Dearomatized Ruthenium Pincer Complexes**

Aviel Anby, Burkhard Butschke, Yehoshua Ben-David, Linda J. W. Shimom, Gregory Leitus, Moran Feller,\* and David Milstein\*



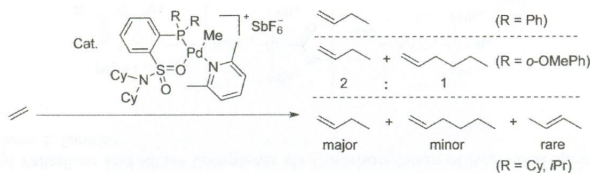
**N–H and N–C Bond Formation with an N<sub>2</sub>-Derived Dihafnium  $\mu$ -Nitrido Complex**

Scott P. Semproni and Paul J. Chirik\*

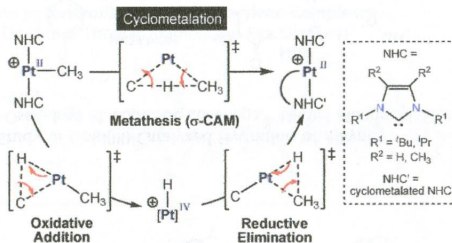


**Cationic Palladium(II) Complexes of Phosphine–Sulfonamide Ligands: Synthesis, Characterization, and Catalytic Ethylene Oligomerization**

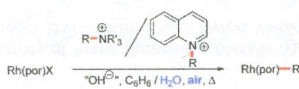
Yanlu Zhang, Yanchun Cao, Xuebing Leng, Changle Chen,\* and Zheng Huang\*


**Coordinationally Unsaturated T-Shaped Platinum(II) Complexes Stabilized by Small N-Heterocyclic Carbene Ligands. Synthesis and Cyclometalation**

Marta Roselló-Merino, Orestes Rivada-Wheleghan, Manuel A. Ortuño, Pietro Vidossich, Josefina Díez, Agustí Lledós,\* and Salvador Conejero\*


**Alkylation of Rhodium Porphyrins Using Ammonium and Quinolinium Salts**

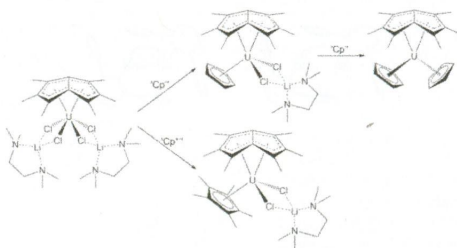
Samuel J. Thompson and Guangbin Dong\*



- Broad: various R groups can be transferred
- Robust: air and moisture are tolerated
- Convenient: ammonium salts as mild alkylating reagents

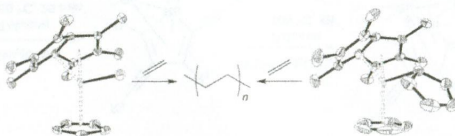
## Half- and Mixed-Sandwich Uranium Permethylpentalene Compounds

F. Mark Chadwick and Dermot M. O'Hare\*

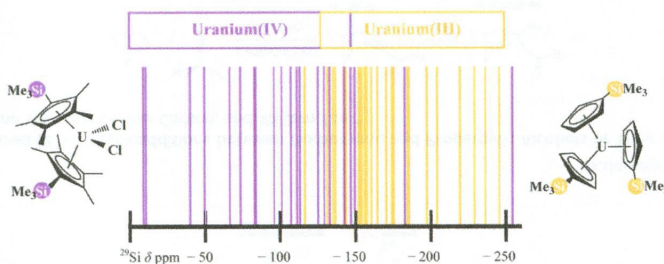


## Early Transition Metal Permethylpentalene Complexes for the Polymerization of Ethylene

F. Mark Chadwick, Robert T. Cooper, Andrew E. Ashley, Jean-Charles Buffet, and Dermot M. O'Hare\*

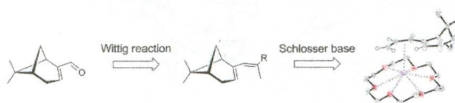
 $^{29}\text{Si}$  NMR Spectra of Silicon-Containing Uranium Complexes

Cory J. Windorff and William J. Evans\*



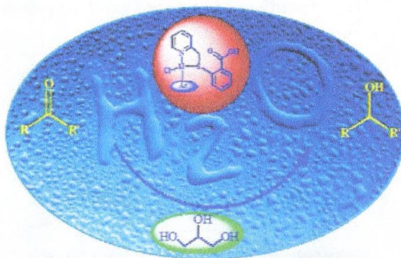
## Synthesis and Coordination Chemistry of Pentadienyl Ligands Derived from (1R)-(-)-Myrtenal

Ann Christin Fecker, Bogdan-Florin Crăciun, Matthias Freytag, Peter G. Jones, and Marc D. Walter\*



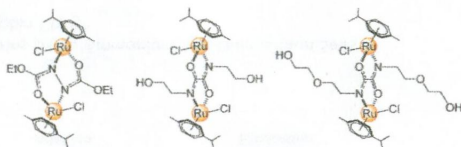
**Transfer Hydrogenation (pH Independent) of Ketones and Aldehydes in Water with Glycerol: Ru, Rh, and Ir Catalysts with a COOH Group near the Metal on a (Phenylthio)methyl-2-pyridine Scaffold**

Om Prakash, Hemant Joshi, Kamal Nayan Sharma, Pancham Lal Gupta, and Ajai K. Singh\*



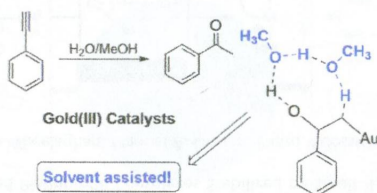
**Strategy to Optimize the Biological Activity of Arene Ruthenium Metalla-Assemblies**

Amine Garci, Anatoly A. Dobrov, Tina Riedel, Ersin Orhan, Paul J. Dyson, Vladimir B. Arion,\* and Bruno Therrien\*



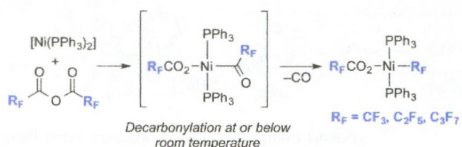
**Experimental and Theoretical Study of Gold(III)-Catalyzed Hydration of Alkynes**

Jesús Cordon, Gonzalo Jiménez-Osés, José M. López-de-Luzuriaga,\* Miguel Monge, M. Elena Olmos, and David Pascual



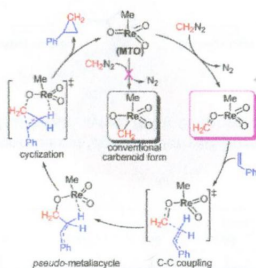
**Synthesis of Fluoroalkyl Palladium and Nickel Complexes via Decarbonylation of Acylmetal Species**

Ansis Maleckis and Melanie S. Sanford\*

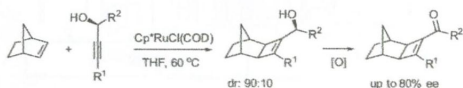


**Theoretical Mechanistic Studies on Methyltrioxorhenium-Catalyzed Olefin Cyclopropanation: Stepwise Transfer of a Terminal Methylene Group**

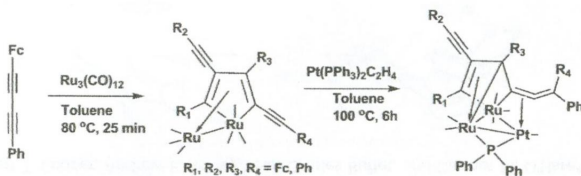
Gen Luo, Yi Luo,\* Satoshi Maeda, Jingping Qu, Zhaomin Hou, and Koichi Ohno\*


**Ruthenium-Catalyzed [2 + 2] Cycloadditions between Norbornene and Propargylic Alcohols or Their Derivatives**

Gavin C. Tsui, Karine Villeneuve, Emily Carlson, and William Tam\*


**Synthesis of Novel Allene-Coordinated, Phosphido-Bridged Ru<sub>2</sub>Pt Clusters Involving Enyne to Allene Transformation**

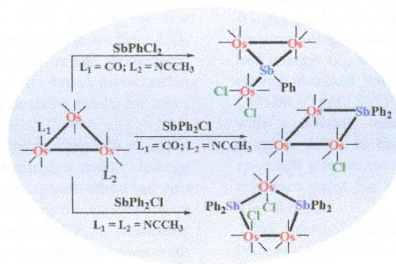
Pradeep Mathur,\* Dharendra K. Rai, Raj K. Joshi, Badrinath Jha, and Shaikh M. Mobin





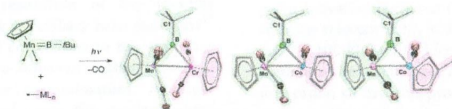
### Binuclear Oxidative Addition of Sb–Cl Bonds: A Facile Synthetic Route to Main Group–Transition Element Clusters and Rings

Ying-Zhou Li, Rakesh Ganguly, and Weng Kee Leong\*



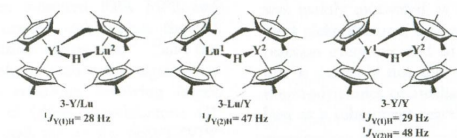
### A Simple Decarbonylative Route to Heterodinuclear Alkylborylene Complexes

Holger Braunschweig,\* Rian D. Dewhurst, Thomas Kramer, and Eva Siedler



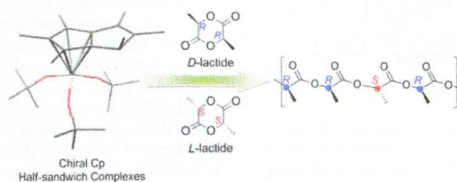
### Differentiating Chemically Similar Lewis Acid Sites in Heterobimetallic Complexes: The Rare-Earth Bridged Hydride $(C_5Me_5)_2Ln(\mu-H)_2Ln'(C_5Me_5)_2$ and Tuckover Hydride $(C_5Me_5)_2Ln(\mu-H)(\mu-\eta^5-C_5H_2Me_3)Ln'(C_5Me_5)_2$ Systems

Megan E. Fieser, Thomas J. Mueller, Jefferson E. Bates, Joseph W. Ziller, Filipp Furche,\* and William J. Evans\*



### Chiral Group 4 Cyclopentadienyl Complexes and Their Use in Polymerization of Lactide Monomers

Zoë R. Turner, Jean-Charles Buffet, and Dermot O'Hare\*



**Structural and Spectroscopic Characterization of Tin–Tin Double Bonds in Cyclic Distannenes**

Jens Henning, Klaus Eichele, Reinhold F. Fink, and Lars Wesemann\*

