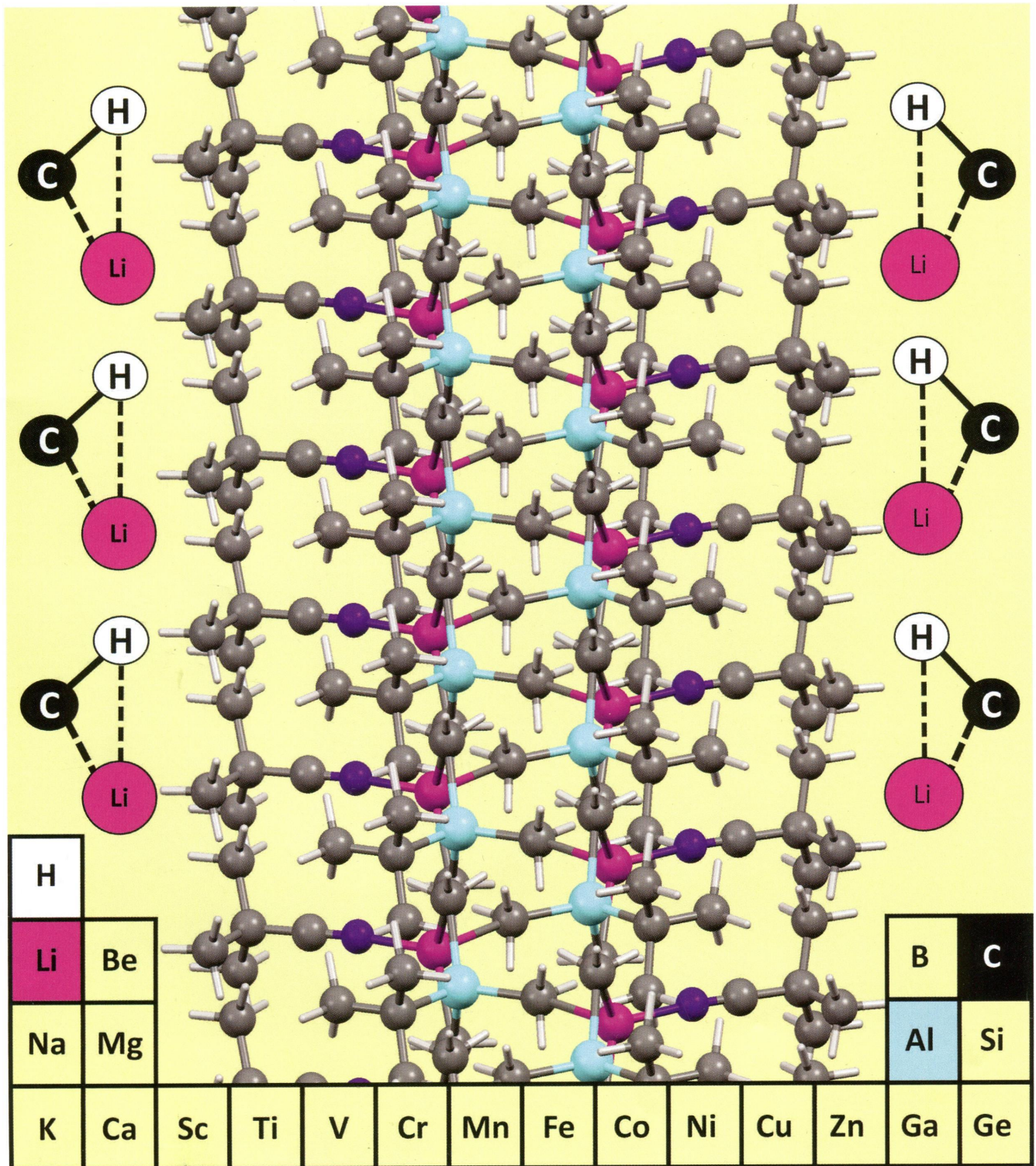


ORGANOMETALLICS



ON THE COVER: Organoaluminum complexes are of interest for catalysis and synergic base chemistry. The exact nature of ligand bridging between the two metals requires elucidation since this has an impact on their chemical reactivity. The cover article provides such clarity via the neutron structure of an organoaluminum polymer which evidences C–H...Li agostic interactions, three-center-two-electron interactions; these are revealed in the bridging methyl groups and serve to stabilize the alkali metal. The bridging methyl groups run down the center of the structure shown in the cover graphic, with cartoons of the agostic interactions alongside. This study is the first to use neutrons to evidence C–H...Li agostic interactions in a lithium aluminate species. Neutron diffraction is ideally suited to determine these types of interactions, given the significant neutron scattering cross section of hydrogen. The study is nonetheless challenging owing to the substantial neutron absorption cross section of lithium. The project was led by Cambridge University, where Cole undertook the neutron diffraction work and data interpretation, while Wheatley headed up the synthetic aspects of the project. Contributions spanned scientists from three central facilities: Argonne National Laboratory, USA; the Australian Nuclear Science and Technology Organisation, Australia; and the Institut Laue Langevin, Grenoble, France (the data source). Further details may be found in the article by Cole et al. on pages 3919–3923. View the article.

Articles

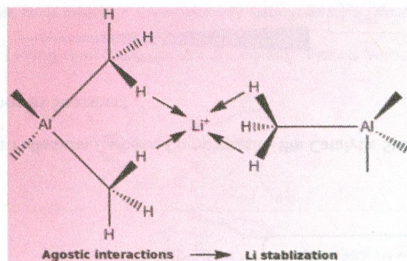
Cover Paper

3919


[dx.doi.org/10.1021/om500271p](https://doi.org/10.1021/om500271p)

Neutron Diffraction Characterization of C–H...Li Interactions in a Lithium Aluminate Polymer

Jacqueline M. Cole,* Paul G. Waddell, Andrew E. H. Wheatley, Garry J. McIntyre, Andrew J. Peel, Christopher W. Tate, and David J. Linton

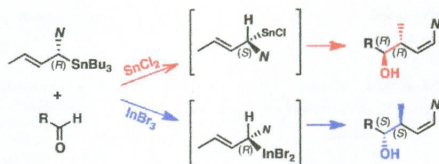


3924 **S**

dx.doi.org/10.1021/om500768e

Chiral Transfer in the Reaction of Aminoallylic Stannanes with Carbonyls in Two Different Modes using Tin(II) and Indium(III) Halides for the Synthesis of Each Enantiomer

Makoto Yasuda,* Yoshitaka Nagano, Hiroshi Yunoki, Kensuke Tsuruwa, and Akio Baba*



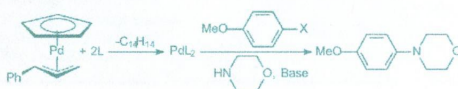
Articles

3928

dx.doi.org/10.1021/om500617p

$\text{Pd}(\eta^3\text{-1-PhC}_3\text{H}_4)(\eta^5\text{-C}_5\text{H}_5)$ as a Catalyst Precursor for Buchwald–Hartwig Amination Reactions

Sogol Borjian, David M. E. Tom, and Michael C. Baird*

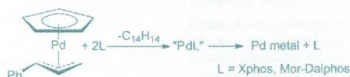


3936

dx.doi.org/10.1021/om500618e

NMR Studies of the Species Present in Cross-Coupling Catalysis Systems Involving $\text{Pd}(\eta^3\text{-1-Ph-C}_3\text{H}_4)(\eta^5\text{-C}_5\text{H}_5)$ and $\text{Pd}(\eta^3\text{-1-Ph-C}_3\text{H}_4)\text{Cl}_2$ Activated by PBu_3 , XPhos, and Mor-Dalpos: Nonexistence of $\text{Pd}(\text{XPhos})_n$ and $\text{Pd}(\text{Mor-Dalpos})_n$ ($n = 1, 2$) at Moderate Temperatures

Sogol Borjian and Michael C. Baird*

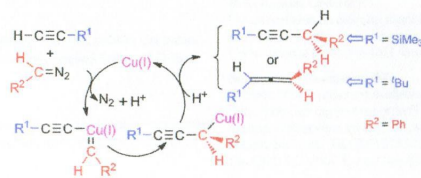


3941 **S**

dx.doi.org/10.1021/om4010803

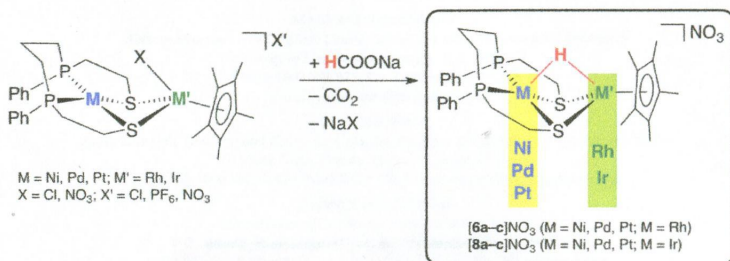
DFT Studies on Cu-Catalyzed Cross-Coupling of Diazo Compounds with Trimethylsilylethyne and *tert*-Butylethyne: Formation of Alkynes for Trimethylsilylethyne while Allenes for *tert*-Butylethyne

Ting Wang, Meiyang Wang,* Sheng Fang, and Jing-yao Liu*



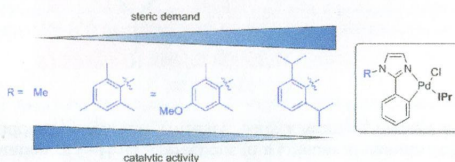
Systematic Heterodinuclear Complexes with MM' (μ -meppp) Centers That Tune the Properties of a Nesting Hydride (M = Ni, Pd, Pt; M' = Rh, Ir; H_2 meppp = *meso*-1,3-Bis[(mercaptoethyl)phenylphosphino]propane)

Bunsho Kure,* Mikie Sano, Takayuki Nakajima, and Tomoaki Tanase*



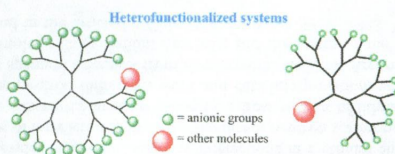
Cyclometalated 2-Phenylimidazole Palladium Carbene Complexes in the Catalytic Suzuki–Miyaura Cross-Coupling Reaction

Maik Micksch, Mario Tenne, and Thomas Strassner*



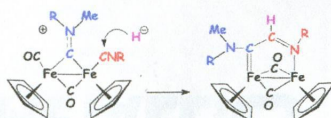
Heterofunctionalized Carbosilane Dendritic Systems: Bifunctionalized Dendrons as Building Blocks versus Statistically Decorated Dendrimers

Marta Galán, Elena Fuentes-Paniagua, F. Javier de la Mata,* and Rafael Gómez*



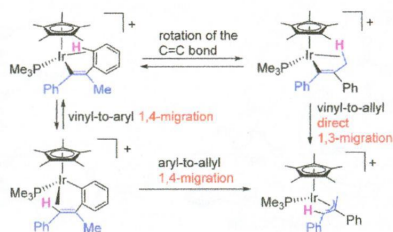
Coupling of Isocyanide and μ -Aminocarbene Ligands in Diiron Complexes Promoted by Hydride Addition

Fabio Marchetti, Stefano Zacchini, and Valerio Zanotti*



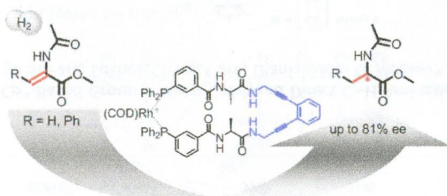
1,4- and 1,3-Metal Migration in a Cp*Ir^{III} Complex: Experimental Evidence of Direct 1,3-Metal Migration

Yousuke Ikeda, Koichi Takano, Shintaro Kodama, and Youichi Ishii*



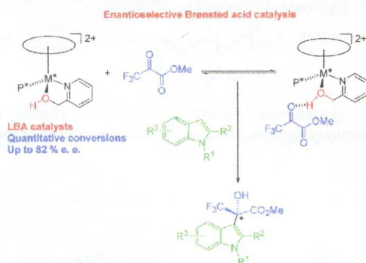
"Backdoor Induction" of Chirality: Asymmetric Hydrogenation with Rhodium(I) Complexes of Triphenylphosphane-Substituted β -Turn Mimetics

Zoran Kokan, Zoran Glasovac, Maja Majerić Elenkov, Matija Gredičak, Ivanka Jerić, and Srećko I. Kirin*



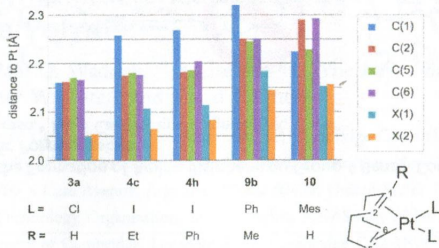
Chiral Brønsted Acid Catalysts. Activation of Methyl 3,3-Trifluoropropylate by Hydroxymethylpyridine-Containing Half-Sandwich Complexes

Daniel Carmona,* Pilar Lamata,* Antonio Sánchez, Pilar Pardo, Ricardo Rodríguez, Paola Ramírez, Fernando J. Lahoz, Pilar García-Orduña, and Luis A. Oro



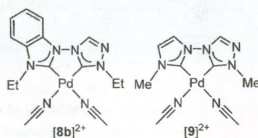
Cytotoxicity and NMR Studies of Platinum Complexes with Cyclooctadiene Ligands

Mirja Enders, Benjamin Görling, Alexander B. Braun, Judith E. Seltenreich, Linus F. Reichenbach, Kari Rissanen, Martin Nieger, Burkhard Luy, Ute Schepers, and Stefan Bräse*



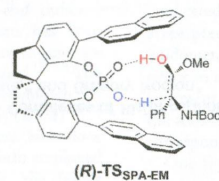
Coordination Chemistry of Bidentate Bis(NHC) Ligands with Two Different NHC Donors

Sabrina Schick, Tania Pape, and F. Ekkehardt Hahn*



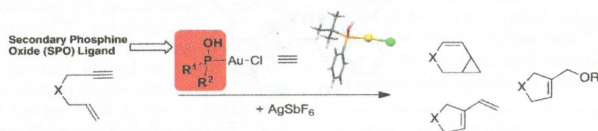
Mechanistic Insight into Asymmetric N–H Insertion Cooperatively Catalyzed by a Dirhodium Compound and a Spiro Chiral Phosphoric Acid

Xu-Chao Wang, Xian-Shuang Song, Li-Ping Guo, Deyu Qu, Zhi-Zhong Xie,* Francis Verpoort,* and Jun Cao*

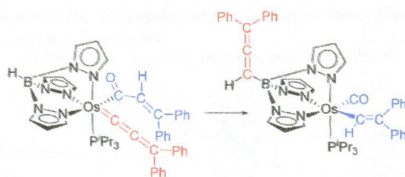


Secondary Phosphine Oxide–Gold(I) Complexes and Their First Application in Catalysis

Felix Schröder, Coralie Tugny, Elise Salanoue, Hervé Clavier, Laurent Giordano, Delphine Moraleda, Yves Gimbert, Virginie Mouriès-Mansuy, Jean-Philippe Goddard, and Louis Fensterbank*

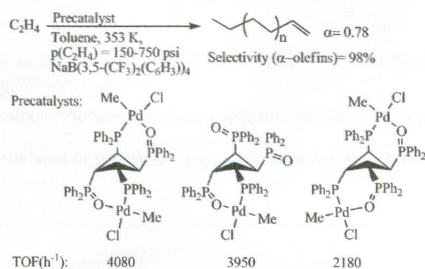


Osmium-Acyl Decarbonylation Promoted by Tp-Mediated Allenylidene Abstraction: A New Role of the Tp Ligand
 Sonia Bajo, Miguel A. Esteruelas,* Ana M. López, and Enrique Oñate



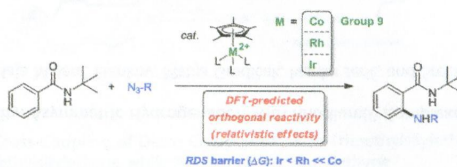
Linear α -Olefins Obtained with Palladium(II) Complexes Bearing a Partially Oxidized Tetraphosphane

Werner Oberhauser,* Gabriele Manca, Andrea Ienco, Christof Strabler, Johannes Prock, Alexander Weninger, Rene Gutmann, and Peter Brüggeleer*



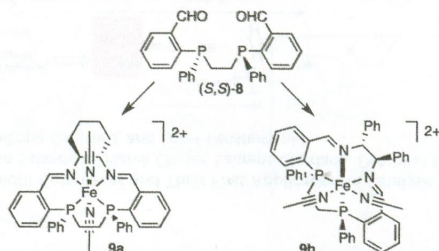
Comparative Investigations of Cp*-Based Group 9 Metal-Catalyzed Direct C–H Amination of Benzamides

Travis M. Figg, Sehoon Park, Juhyeon Park, Sukbok Chang,* and Djameladdin G. Musaev*



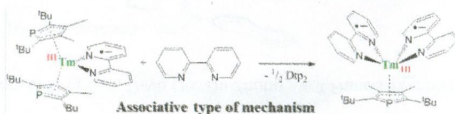
Chiral Macrocyclic N₂P₂ Ligands and Iron(II): A Marriage of Interest

Raphael Bigler, Elisabeth Otth, and Antonio Mezzetti*



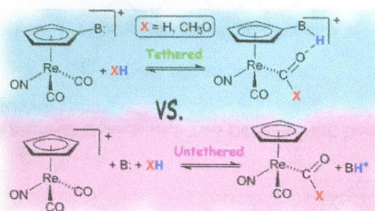
Multiple One-Electron Transfers in Bipyridine Complexes of Bis(phospholy) Thulium

Léa Jacquot, Mathieu Xémard, Carine Clavaguéra,* and Grégory Nocton*



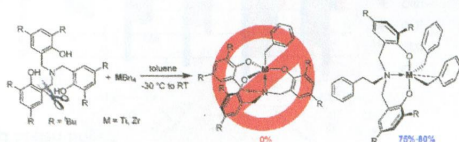
Guanidine-Functionalized Rhenium Cyclopentadienyl Carbonyl Complexes: Synthesis and Cooperative Activation of H–H and O–H Bonds

Thomas S. Teets, Jay A. Labinger,* and John E. Bercaw*



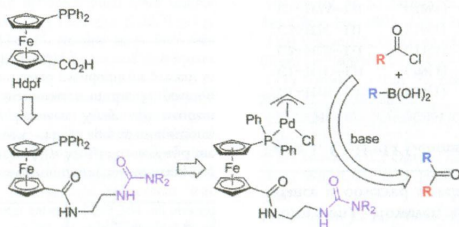
Unusual C–C Bond Cleavage in the Formation of Amine-Bis(phenoxy) Group 4 Benzyl Complexes: Mechanism of Formation and Application to Stereospecific Polymerization

Ravikumar R. Gowda, Lucia Caporaso,* Luigi Cavallo, and Eugene Y.-X. Chen*

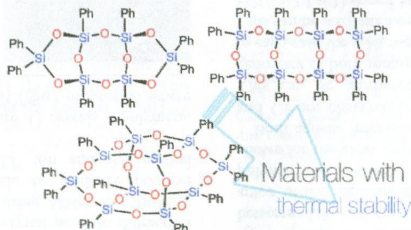


Synthesis, Structural Characterization, and Catalytic Evaluation of Phosphinoferrrocene Ligands Bearing Extended Urea-Amide Substituents

Hana Solařová, Ivana Cisařová, and Petr Štěpnička*

**Notes****Synthesis and Properties of Phenylsilsesquioxanes with Ladder and Double-Decker Structures**

Hisayuki Endo, Nobuhiro Takeda, and Masafumi Unno*

**Hydrogenation of Esters Catalyzed by Ruthenium PN^3 -Pincer Complexes Containing an Aminophosphine Arm**

Tao Chen, Huaifeng Li, Shuanglin Qu, Bin Zheng, Lipeng He, Zhiping Lai, Zhi-Xiang Wang,* and Kuo-Wei Huang*

