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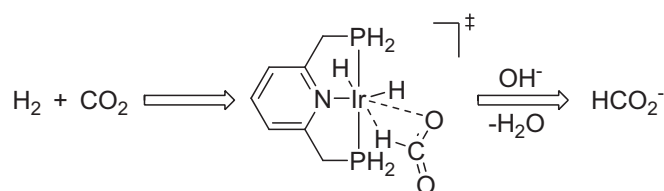
Articles

Mårten S.G. Ahlquist

Journal of Molecular Catalysis A: Chemical 324 (2010) 3

Iridium catalyzed hydrogenation of CO₂ under basic conditions—Mechanistic insight from theory

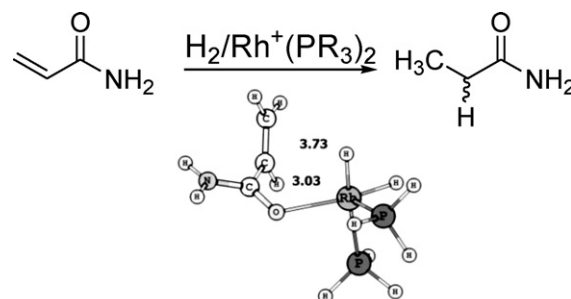
A density functional theory study of the mechanism of the iridium catalyzed hydrogenation of carbon dioxide is presented. The rate-limiting step is found to be the regeneration of the iridium(III) trihydride.



Vincenzo Verdolino, Aaron Forbes, Paul Helquist, Per-Ola Norrby, Olaf Wiest

Journal of Molecular Catalysis A: Chemical 324 (2010) 9

On the mechanism of the rhodium catalyzed acrylamide hydrogenation

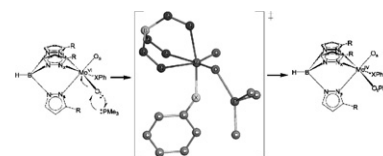


Jason M. Keith, Zoran D. Tomić, Snežana D. Zarić, Michael B. Hall

Journal of Molecular Catalysis A: Chemical 324 (2010) 15

Oxygen atom transfer catalysis: Ligand effects on the key reaction barrier in molybdenum (VI) dioxo systems

The mechanistic details of oxygen atom transfer from Tp^RMoO₂(XPh) to PMe₃ were investigated for R = 3-*i*Pr and 3-Me and X = O and S by density functional theory (DFT) calculations. The transition state exhibits a hypervalent structure at P and is both lower in energy and later, in contrast to the Hammond postulate.

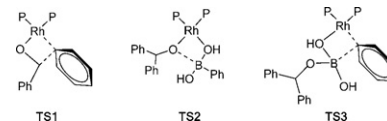


Alma Itzel Olivos Suarez, Joost N.H. Reek, Bas de Bruin

Journal of Molecular Catalysis A: Chemical 324 (2010) 24

Rhodium(I) mediated arylation of aldehydes with arylboronic acids under base and water free conditions: A computational study

DFT calculations suggest that rhodium mediated arylation of aldehydes with arylboronic acids under base and water free conditions proceeds via an internal base mechanism whereby the initially formed alcoholate (obtained by rate limiting aryl migration to the aldehyde) attacks the electrophilic boron atom of the coordinated arylboronic acid substrate to facilitate aryl transfer to the metal.

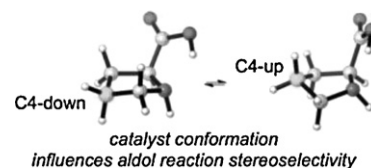


Christophe Allemann, Joann M. Um, K.N. Houk

Journal of Molecular Catalysis A: Chemical 324 (2010) 31

Computational investigations of the stereoselectivities of proline-related catalysts for aldol reactions

The aldol reaction of benzaldehyde with acetone catalyzed by proline and proline-related catalysts was studied using density functional theory. Subtle differences in the structures and conformations of these catalysts influence reaction stereoselectivities.

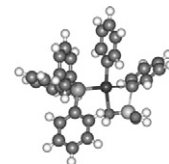


Jesús Jover, Natalie Fey, Mark Purdie, Guy C. Lloyd-Jones, Jeremy N. Harvey

Journal of Molecular Catalysis A: Chemical 324 (2010) 39

A computational study of phosphine ligand effects in Suzuki–Miyaura coupling

DFT calculations and linear regression model building show, e.g. that transmetalation is favoured by electron-withdrawing ligands.

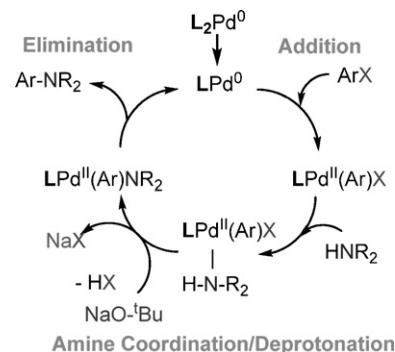


Claire L. McMullin, Bastian Rühle, Maria Besora, A. Guy Orpen, Jeremy N. Harvey, Natalie Fey

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Computational study of P^tBu_3 as ligand in the palladium-catalysed amination of phenylbromide with morpholine

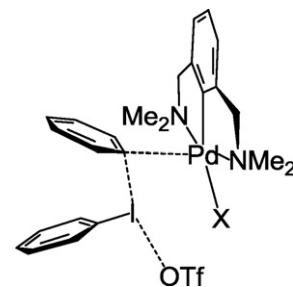
Computational study of the full catalytic cycle for the coupling of phenylbromide with morpholine (amination), catalysed by $Pd(P^tBu_3)_2$ complex, related to ligand design criteria.



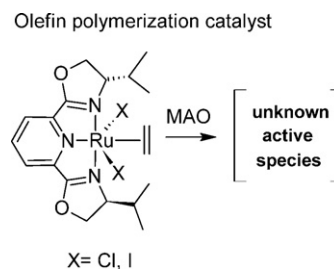
Kálmán J. Szabó*Journal of Molecular Catalysis A: Chemical* 324 (2010) 56

Mechanism of the oxidative addition of hypervalent iodonium salts to palladium(II) pincer-complexes

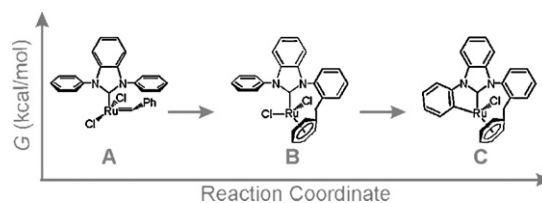
DFT modeling studies were performed for oxidative addition of hypervalent iodonium salts to Pd(II) pincer-complexes. The focus was directed to steric and electronic effects, which are important in the key-step of the Pd(II)/Pd(IV) redox cycle based catalytic reactions.

**Wouter Heyndrickx, Giovanni Occhipinti, Yury Minenkov, Vidar R. Jensen***Journal of Molecular Catalysis A: Chemical* 324 (2010) 64

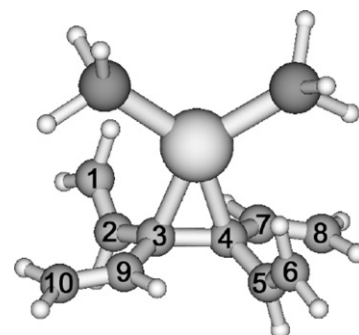
On the nature of the active site in ruthenium olefin coordination–insertion polymerization catalysts

Various candidate active centers and mechanisms of ruthenium-based olefin polymerization have been investigated by means of DFT. The calculations strongly suggest that the olefin polymerization activity observed for the (bis(oxazoline)pyridine)RuCl₂(ethylene)/MAO system is not due to a mononuclear ruthenium center bearing an intact bis(oxazoline)pyridine ligand.**Albert Poater, Luigi Cavallo***Journal of Molecular Catalysis A: Chemical* 324 (2010) 75

Mechanistic insights into the double C–H (de)activation route of a Ru-based olefin metathesis catalyst

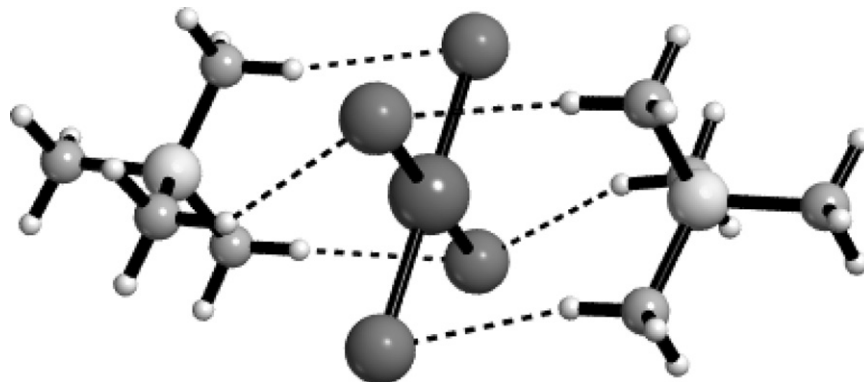
Ru-complexes relevant to olefin catalysis suffer from deactivation reactions whose mechanism is often difficult to understand. We report here a detailed DFT study showing all the steps that convert the starting complex **A** into the product **B** first, and then to evolution of **B** into product **C**.**Boris B. Averkiev, Yan Zhao, Donald G. Truhlar***Journal of Molecular Catalysis A: Chemical* 324 (2010) 80Binding energy of d¹⁰ transition metals to alkenes by wave function theory and density functional theory

It is shown that new density functionals provide accurate binding energies for conjugated alkenes in Pd and Pt complexes.



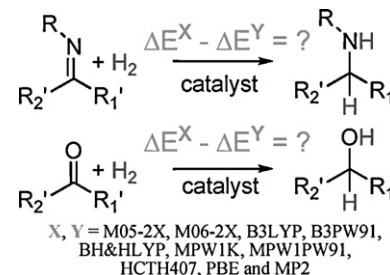
Pavel A. Dub, Rinaldo Poli*Journal of Molecular Catalysis A: Chemical* 324 (2010) 89

A computational study of solution equilibria of platinum-based ethylene hydroamination catalytic species including solvation and counterion effects: Proper treatment of the free energy of solvation

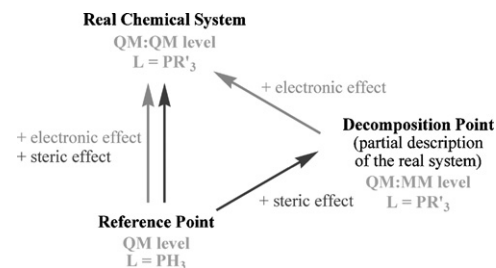
**Jonas Nyhlén, Timofei Privalov***Journal of Molecular Catalysis A: Chemical* 324 (2010) 97

Hydrogenation of carbon-heteroatom unsaturated bonds: An assessment of consistency of density functional methods

The relation between the form of density functionals, namely M05-2X, M06-2X, B3LYP, B3PW91, BH&HLYP, MPW1K, MPW1PW91, HCTH407 and PBE, and the calculated energy change in hydrogenation of unsaturated carbon-heteroatom bonds was assessed for a series of 12 imines (selected according to Stephan's H₂-addition reactions) as well as a series of 11 ketones/aldehydes.

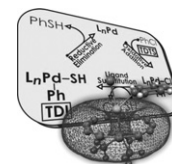
**Valentine P. Ananikov, Djamaladdin G. Musaev, Keiji Morokuma***Journal of Molecular Catalysis A: Chemical* 324 (2010) 104

Real size of ligands, reactants and catalysts: Studies of structure, reactivity and selectivity by ONIOM and other hybrid computational approaches

**Sebastian Kozuch, Sason Shaik***Journal of Molecular Catalysis A: Chemical* 324 (2010) 120

Defining the optimal inductive and steric requirements for a cross-coupling catalyst using the energetic span model

The energetic span model for kinetic assessment of catalytic cycles identifies the best phosphine ligand for a theoretically computed cross-coupling reaction.

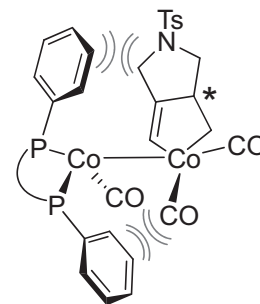


Torstein Fjermestad, Miquel A. Pericàs, FelIU Maseras

Journal of Molecular Catalysis A: Chemical 324 (2010) 127

Origin of enantioselectivity in asymmetric Pauson–Khand reactions catalyzed by [(BINAP)Co₂(CO)₆]

The selectivity in the Pauson–Khand intramolecular cyclization of prochiral enynes catalyzed by [(BINAP)Co₂(CO)₆] is controlled by enyne–phenyl and carbonyl–phenyl steric repulsions.

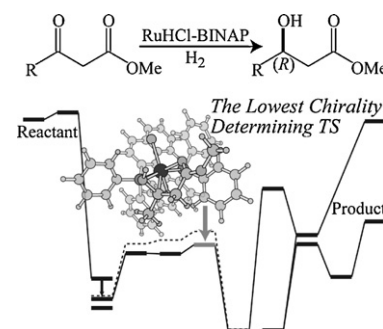


Koichi Ohno, Satoshi Maeda

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A systematic study on the RuHCl–BINAP-catalyzed asymmetric hydrogenation mechanism by the global reaction route mapping method

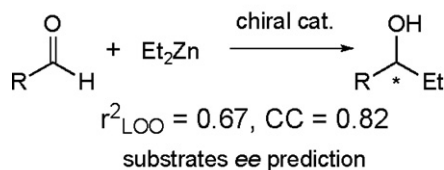
The full mechanism of a RuHCl–BINAP-catalyzed asymmetric hydrogenation reaction was systematically explored by the global reaction route mapping (GRRM) method.



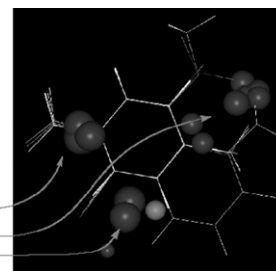
Marisa C. Kozlowski, James C. Ianni

Journal of Molecular Catalysis A: Chemical 324 (2010) 141

Quantum molecular interaction field models of substrate enantioselection in asymmetric processes



areas of substrates correlated to ee



Christopher R. Corbeil, Nicolas Moitessier

Journal of Molecular Catalysis A: Chemical 324 (2010) 146

Theory and application of medium to high throughput prediction method techniques for asymmetric catalyst design

With the use of computational methods in the field of drug design becoming ever more prevalent, there is pressure to port these technologies to other fields. One of the fields ripe for application of computational drug design techniques; specifically virtual screening and computer-aided molecular design, is the design and synthesis of asymmetric catalysts. Such methods could either guide the selection of the optimal catalyst(s) for a given reaction and a given substrate or provide an enriched selection of highly efficient asymmetric catalysts which enable the synthetic chemists to focus on the most promising candidates. This would in turn provide savings in time and reduce the costs associated with the synthesis and evaluation of large libraries of molecules. However, to be applicable to the evaluation of a large number of potential catalysts, speed is of utmost importance. This impetus has led to the development of medium to high throughput virtual screening (HTVS) methods for asymmetric catalyst development or assessment, although a very few applications have been reported. These methods typically fall into four classes: methods combining quantum mechanics and molecular mechanics (QM/MM), pure molecular mechanics-based methods – a class which can be subdivided into static and dynamic transition state modeling – and lastly quantitative structure selectivity relationship methods (QSSR). This review will cover specific methods within these classes and their application to selected reactions.

