# Odile Eisenstein

List of Publications by Year
in descending order

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|---|---|---|---|
| 330<br>papers | 21,933<br>citations | 6250<br>80<br>h-index | 13758<br>129<br>g-index |
| 385<br>all docs | 385<br>docs citations | 385<br>times ranked | 11524<br>citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Computational Catalysis: A Land of Opportunities. Topics in Catalysis, 2022, 65, 1-5. | 1.3 | 3 |
| 2 | From the Felkinâ€Anh Rule to the Grignard Reaction: an Almost Circular 50â€…Year Adventure in the World of Molecular Structures and Reaction Mechanisms with Computational Chemistry**. Israel Journal of Chemistry, 2022, 62, . | 1.0 | 2 |
| 3 | What Makes a Good (Computed) Energy Profile?. Topics in Organometallic Chemistry, 2020, , 1-38. | 0.7 | 15 |
| 4 | <sup>31</sup>P Chemical Shifts in Ru(II) Phosphine Complexes. A Computational Study of the Influence of the Coordination Sphere. Inorganic Chemistry, 2020, 59, 17038-17048. | 1.9 | 12 |
| 5 | The Grignard Reaction â€“ Unraveling a Chemical Puzzle. Journal of the American Chemical Society, 2020, 142, 2984-2994. | 6.6 | 84 |
| 6 | Efficient alkene hydrosilation with bis(8-quinolyl)phosphine (NPN) nickel catalysts. The dominant role of silyl-over hydrido-nickel catalytic intermediates. Chemical Science, 2020, 11, 5043-5051. | 3.7 | 7 |
| 7 | Carbon-13 NMR Chemical Shift: A Descriptor for Electronic Structure and Reactivity of Organometallic Compounds. Accounts of Chemical Research, 2019, 52, 2278-2289. | 7.6 | 80 |
| 8 | Understanding unusual element-element bond formation and activation: general discussion. Faraday Discussions, 2019, 220, 376-385. | 1.6 | 0 |
| 9 | Physical methods for mechanistic understanding: general discussion. Faraday Discussions, 2019, 220, 144-178. | 1.6 | 0 |
| 10 | Mechanistic insight into organic and industrial transformations: general discussion. Faraday Discussions, 2019, 220, 282-316. | 1.6 | 8 |
| 11 | Computational and theoretical approaches for mechanistic understanding: general discussion. Faraday Discussions, 2019, 220, 464-488. | 1.6 | 3 |
| 12 | Concluding remarks for â€œMechanistic Processes in Organometallic Chemistryâ€: the importance of a multidisciplinary approach. Faraday Discussions, 2019, 220, 489-495. | 1.6 | 4 |
| 13 | Ï€-Bond Character in Metalâ€“Alkyl Compounds for Câ€“H Activation: How, When, and Why?. Journal of the American Chemical Society, 2019, 141, 648-656. | 6.6 | 46 |
| 14 | Modelling the surface of amorphous dehydroxylated silica: the influence of the potential on the nature and density of defects. New Journal of Chemistry, 2018, 42, 1356-1367. | 1.4 | 11 |
| 15 | Metal alkyls programmed to generate metal alkylidenes by Î±-H abstraction: prognosis from NMR chemical shift. Chemical Science, 2018, 9, 1912-1918. | 3.7 | 47 |
| 16 | Zirconocene-Mediated Selective Câ€“C Bond Cleavage of Strained Carbocycles: Scope and Mechanism. Journal of Organic Chemistry, 2018, 83, 3497-3515. | 1.7 | 27 |
| 17 | Catalytic Olefin Hydrosilations Mediated by Ruthenium Î·3-H2Si Ïƒ Complexes of Primary and Secondary Silanes. ACS Catalysis, 2018, 8, 11513-11523. | 5.5 | 12 |
| 18 | The Key Role of the Hemiaminal Intermediate in the Iron-Catalyzed Deaminative Hydrogenation of Amides. ACS Catalysis, 2018, 8, 8751-8762. | 5.5 | 53 |

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| 19 | NMR chemical shift analysis decodes olefin oligo- and polymerization activity of d <sup>0</sup> group 4 metal complexes. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E5867-E5876. | 3.3 | 40 |
| 20 | Orbital Analysis of Carbonâ€13 Chemical Shift Tensors Reveals Patterns to Distinguish Fischer and Schrock Carbenes. Angewandte Chemie - International Edition, 2017, 56, 10127-10131. | 7.2 | 57 |
| 21 | Orbital Analysis of Carbonâ€13 Chemical Shift Tensors Reveals Patterns to Distinguish Fischer and Schrock Carbenes. Angewandte Chemie, 2017, 129, 10261-10265. | 1.6 | 13 |
| 22 | Metathesis Activity Encoded in the Metallacyclobutane Carbon-13 NMR Chemical Shift Tensors. ACS Central Science, 2017, 3, 759-768. | 5.3 | 84 |
| 23 | How Solvent Dynamics Controls the Schlenk Equilibrium of Grignard Reagents: A Computational Study of CH<sub>3</sub>MgCl in Tetrahydrofuran. Journal of Physical Chemistry B, 2017, 121, 4226-4237. | 1.2 | 63 |
| 24 | Aromatic Câ€“H Ïƒ-Bond Activation by Ni<sup>0</sup>, Pd<sup>0</sup>, and Pt<sup>0</sup> Alkene Complexes: Concerted Oxidative Addition to Metal vs Ligand-to-Ligand H Transfer Mechanism. Organometallics, 2017, 36, 2761-2771. | 1.1 | 84 |
| 25 | Molecular and Silica-Supported Molybdenum Alkyne Metathesis Catalysts: Influence of Electronics and Dynamics on Activity Revealed by Kinetics, Solid-State NMR, and Chemical Shift Analysis. Journal of the American Chemical Society, 2017, 139, 17597-17607. | 6.6 | 80 |
| 26 | Selectivity of Câ€“H Activation and Competition between Câ€“H and Câ€“F Bond Activation at Fluorocarbons. Chemical Reviews, 2017, 117, 8710-8753. | 23.0 | 265 |
| 27 | Experimental and DFT Computational Study of Î²-Me and Î²-H Elimination Coupled with Proton Transfer: From Amides to Enamides in Cp*<sub>2</sub>MX (M = La, Ce). Organometallics, 2017, 36, 97-108. | 1.1 | 11 |
| 28 | Deciphering Selectivity in Organic Reactions: A Multifaceted Problem. Accounts of Chemical Research, 2016, 49, 1070-1078. | 7.6 | 31 |
| 29 | Elucidating the Link between NMR Chemical Shifts and Electronic Structure in d<sup>0</sup> Olefin Metathesis Catalysts. Journal of the American Chemical Society, 2016, 138, 2261-2272. | 6.6 | 99 |
| 30 | Coordination and insertion of alkenes and alkynes in Au<sup>III</sup>complexes: nature of the intermediates from a computational perspective. Dalton Transactions, 2016, 45, 5504-5513. | 1.6 | 20 |
| 31 | FemExâ€”female excellence in theoretical and computational chemistry. International Journal of Quantum Chemistry, 2015, 115, 1195-1196. | 1.0 | 3 |
| 32 | Hydrazine Nâ€“N Bond Cleavage over Silica-Supported Tantalum-Hydrides. Inorganic Chemistry, 2015, 54, 11648-11659. | 1.9 | 8 |
| 33 | Remote functionalization of hydrocarbons with reversibility enhanced stereocontrol. Chemical Science, 2015, 6, 2770-2776. | 3.7 | 65 |
| 34 | Metallacyclobutanes from Schrock-Type d<sup>0</sup> Metal Alkylidene Catalysts: Structural Preferences and Consequences in Alkene Metathesis. Organometallics, 2015, 34, 1668-1680. | 1.1 | 55 |
| 35 | Donor-Promoted 1,2-Hydrogen Migration from Silicon to a Saturated Ruthenium Center and Access to Silaoxiranyl and Silaiminyl Complexes. Journal of the American Chemical Society, 2015, 137, 9186-9194. | 6.6 | 14 |
| 36 | Modelling and Rationalizing Organometallic Chemistry with Computation: Where Are We?. Structure and Bonding, 2015, , 1-37. | 1.0 | 13 |

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| 37 | An Unusual Example of Hypervalent Silicon: A Fiveâ€Coordinate Silyl Group Bridging Two Palladium or Nickel Centers through a Nonsymmetrical Fourâ€Center Twoâ€Electron Bond. Angewandte Chemie - International Edition, 2014, 53, 1103-1108. | 7.2 | 37 |
| 38 | Stereoselectivity through a network of non-classical CH weak interactions: a prospective study of a bicyclic organocatalytic scaffold. New Journal of Chemistry, 2014, 38, 5975-5982. | 1.4 | 5 |
| 39 | Conformational complexity of morphine and morphinum in the gas phase and in water. A DFT and MP2 study. RSC Advances, 2014, 4, 24729-24735. | 1.7 | 2 |
| 40 | Linear-Selective Hydroarylation of Unactivated Terminal and Internal Olefins with Trifluoromethyl-Substituted Arenes. Journal of the American Chemical Society, 2014, 136, 13098-13101. | 6.6 | 263 |
| 41 | Cyclometalated N-Heterocyclic Carbene Complexes of Ruthenium for Access to Electron-Rich Silylene Complexes That Bind the Lewis Acids CuOTf and AgOTf. Journal of the American Chemical Society, 2014, 136, 11473-11482. | 6.6 | 29 |
| 42 | Nonclassical CHâ‹¯Ï€ Supramolecular Interactions in Artemisinic Acid Favor a Single Conformation, Yielding High Diastereoselectivity in the Reduction with Diazene. Journal of Organic Chemistry, 2014, 79, 5939-5947. | 1.7 | 13 |
| 43 | 1,2-Hydrogen Migration to a Saturated Ruthenium Complex via Reversal of Electronic Properties for Tin in a Stannylene-to-Metallostannylene Conversion. Journal of the American Chemical Society, 2014, 136, 13991-13994. | 6.6 | 35 |
| 44 | Computational Studies Explain the Importance of Two Different Substituents on the Chelating Bis(amido) Ligand for Transfer Hydrogenation by Bifunctional Cp*Rh(III) Catalysts. Organometallics, 2014, 33, 3433-3442. | 1.1 | 39 |
| 45 | Two [1,2,4-(Me<sub>3</sub>C)<sub>3</sub>C<sub>5</sub>H<sub>2</sub>]<sub>2</sub>CeH Molecules are Involved in Hydrogenation of Pyridine to Piperidine as Shown by Experiments and Computations. Inorganic Chemistry, 2014, 53, 6361-6373. | 1.9 | 19 |
| 46 | Mechanistic Insights on the Stereoselective Nucleophilic 1,2-Addition to Sulfinyl Imines. Journal of Organic Chemistry, 2014, 79, 2514-2521. | 1.7 | 18 |
| 47 | Theoretical Studies on the Reaction Mechanism of Metal-Assisted CH Activation. , 2013, , 695-726. | | 8 |
| 48 | Decamethylscandocinium-hydrido-(perfluorophenyl)borate: fixation and tandem tris(perfluorophenyl)borane catalysed deoxygenative hydrosilation of carbon dioxide. Chemical Science, 2013, 4, 2152. | 3.7 | 132 |
| 49 | Outer sphere hydrogenation catalysis. New Journal of Chemistry, 2013, 37, 21-27. | 1.4 | 161 |
| 50 | Cleaving bonds in CH<sub>3</sub>OSO<sub>2</sub>CF<sub>3</sub>with [1,2,4-(Me<sub>3</sub>C)<sub>3</sub>C<sub>5</sub>H<sub>2</sub>]<sub>2</sub>CeH; an experimental and computational study. New Journal of Chemistry, 2013, 37, 132-142. | 1.4 | 14 |
| 51 | Generation and Structural Characterization of a Gold(III) Alkene Complex. Angewandte Chemie - International Edition, 2013, 52, 1660-1663. | 7.2 | 58 |
| 52 | Successive Heterolytic Cleavages of H<sub>2</sub> Achieve N<sub>2</sub> Splitting on Silica-Supported Tantalum Hydrides: A DFT Proposed Mechanism. Inorganic Chemistry, 2012, 51, 7237-7249. | 1.9 | 35 |
| 53 | Selectivity in the Câ€“H Activation Reaction of CH<sub>3</sub>OSO<sub>2</sub>CH<sub>3</sub> with [1,2,4-(Me<sub>3</sub>C)<sub>3</sub>C<sub>5</sub>H<sub>2</sub>]<sub>2</sub>CeH or [1,2,4-(Me<sub>3</sub>C)<sub>3</sub>C<sub>5</sub>H<sub>2</sub>][1,2-(Me<sub>3</sub>C)<sub>2</sub>-4-(Me<sub>2</sub> To Choose or Not To Choose. Organometallics, 2012, 31, 870-881. | 1.1 | 14 |
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| 55 | Cp* Iridium Precatalysts for Selective Câ€“H Oxidation via Direct Oxygen Insertion: A Joint Experimental/Computational Study. ACS Catalysis, 2012, 2, 208-218. | 5.5 | 82 |
| 56 | Hydrofluoroarylation of Alkynes with Ni Catalysts. Câ€“H Activation via Ligand-to-Ligand Hydrogen Transfer, an Alternative to Oxidative Addition. Organometallics, 2012, 31, 1300-1314. | 1.1 | 161 |
| 57 | Structures of d4MH3X: a Computational Study of the Influence of the Metal and the Ligands. Inorganic Chemistry, 2012, 51, 5705-5715. | 1.9 | 0 |
| 58 | Oxo vs Imido Alkylidene d<sup>0</sup>-Metal Species: How and Why Do They Differ in Structure, Activity, and Efficiency in Alkene Metathesis?. Organometallics, 2012, 31, 6812-6822. | 1.1 | 81 |
| 59 | Carbon Monoxide Activation via O-Bound CO Using Decamethylscandociniumâ€“Hydridoborate Ion Pairs. Journal of the American Chemical Society, 2012, 134, 10843-10851. | 6.6 | 90 |
| 60 | DFT calculations of 29Si-NMR chemical shifts in Ru(ii) silyl complexes: Searching for trends and accurate values. Dalton Transactions, 2011, 40, 11321. | 1.6 | 12 |
| 61 | Heterolytic cleavage of ammonia Nâ€“H bond by bifunctional activation in silica-grafted single site Ta(V) imido amido surface complex. Importance of the outer sphere NH3 assistance. New Journal of Chemistry, 2011, 35, 1011. | 1.4 | 11 |
| 62 | Câˆ’F and Câˆ’H Bond Activation of Fluorobenzenes and Fluoropyridines at Transition Metal Centers: How Fluorine Tips the Scales. Accounts of Chemical Research, 2011, 44, 333-348. | 7.6 | 430 |
| 63 | Iridium-Catalyzed Hydrogenation of N-Heterocyclic Compounds under Mild Conditions by an Outer-Sphere Pathway. Journal of the American Chemical Society, 2011, 133, 7547-7562. | 6.6 | 296 |
| 64 | Facile Interconversion of [Cp<sub>2</sub>(Cl)Hf(SnH<sub>3</sub>)] and [Cp<sub>2</sub>(Cl)Hf(Ï¼â€Ħ)SnH<sub>2</sub>]: DFT Investigations of Hafnocene Stannyl Complexes as Masked Stannylenes. Angewandte Chemie - International Edition, 2010, 49, 1816-1819. | 7.2 | 14 |
| 65 | Mechanistic investigation of vinylic carbonâ€“fluorine bond activation of perfluorinated cycloalkenes using Cp*2ZrH2 and Cp*2ZrHF. Journal of Fluorine Chemistry, 2010, 131, 1122-1132. | 0.9 | 42 |
| 66 | Half-Sandwich Iridium Complexes for Homogeneous Water-Oxidation Catalysis. Journal of the American Chemical Society, 2010, 132, 16017-16029. | 6.6 | 507 |
| 67 | An Experimentalâˆ’Theoretical Study of the Factors That Affect the Switch between Ruthenium-Catalyzed Dehydrogenative Amide Formation versus Amine Alkylation. Organometallics, 2010, 29, 6548-6558. | 1.1 | 103 |
| 68 | Shutting Down Secondary Reaction Pathways: The Essential Role of the Pyrrolyl Ligand in Improving Silica Supported d<sup>0</sup>-ML<sub>4</sub> Alkene Metathesis Catalysts from DFT Calculations. Journal of the American Chemical Society, 2010, 132, 7750-7757. | 6.6 | 121 |
| 69 | Bridging Silyl Groups in Ïƒ-Bond Metathesis and [1,2]-Shifts. Experimental and Computational Study of the Reaction between Cerium Metallocenes and MeOSiMe<sub>3</sub>. Organometallics, 2010, 29, 5103-5110. | 1.1 | 24 |
| 70 | Intermediate-Valence Tautomerism in Decamethylytterbocene Complexes of Methyl-Substituted Bipyridines. Journal of the American Chemical Society, 2010, 132, 17537-17549. | 6.6 | 92 |
| 71 | Câ€”H Bond Activation in Transition Metal Species from a Computational Perspective. Chemical Reviews, 2010, 110, 749-823. | 23.0 | 959 |
| 72 | Manganese Catalysts for Câˆ’H Activation: An Experimental/Theoretical Study Identifies the Stereoelectronic Factor That Controls the Switch between Hydroxylation and Desaturation Pathways. Journal of the American Chemical Society, 2010, 132, 7605-7616. | 6.6 | 100 |

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| 73 | Importance of palladiumâ€“carbon bond energies in direct arylation of polyfluorinated benzenes. Dalton Transactions, 2010, 39, 10510. | 1.6 | 54 |
| 74 | Catalytic hydrosilylation of olefins with organolanthanides: a DFT study. Part I: Hydrosilylation of propene by SiH4. Dalton Transactions, 2010, 39, 10749. | 1.6 | 15 |
| 75 | The reaction of bis(1,2,4-tri-t-butylcyclopentadienyl)ceriumbenzyl, Cpâ€²2CeCH2Ph, with methylhalides: a metathesis reaction that does not proceed by a metathesis transition state. Dalton Transactions, 2010, 39, 6648. | 1.6 | 34 |
| 76 | Splitting a Câ€“O bond in dialkylethers with bis(1,2,4-tri-tert-butylcyclopentadienyl)cerium hydride does not occur by a Ïƒ-bond metathesis pathway: a combined experimental and DFT computational study. New Journal of Chemistry, 2010, 34, 2189. | 1.4 | 11 |
| 77 | Catalytic hydrosilylation of olefins with organolanthanide complexes: A DFT study. Part II: Influence of the substitution on olefin and silane. Dalton Transactions, 2010, 39, 10757. | 1.6 | 11 |
| 78 | Synthesis, structure, and reductive elimination in the series Tpâ€²Rh(PR3)(ArF)H; Determination of rhodiumâ€“carbon bond energies of fluoroaryl substituents. Dalton Transactions, 2010, 39, 10495. | 1.6 | 35 |
| 79 | H/D Exchange on Silica-Grafted Tantalum(V) Imido Amido [(â‰¡SiO)2Ta(V)(NH)(NH2)] Synthesized from Either Ammonia or Dinitrogen: IR and DFT Evidence for Heterolytic Splitting of D2. Topics in Catalysis, 2009, 52, 1482-1491. | 1.3 | 14 |
| 80 | Bond Activations of PhSiH<sub>3</sub> by Cp<sub>2</sub>SmH: A Mechanistic Investigation by the DFT Method. Organometallics, 2009, 28, 3767-3775. | 1.1 | 32 |
| 81 | The Bond between CO and Cpâ€²<sub>3</sub>U in Cpâ€²<sub>3</sub>U(CO) Involves Back-bonding from the Cpâ€²<sub>3</sub>U Ligand-Based Orbitals of Ï€-Symmetry, where Cpâ€² Represents a Substituted Cyclopentadienyl Ligand. Organometallics, 2009, 28, 3629-3635. | 1.1 | 59 |
| 82 | Hydrogen for X-Group Exchange in CH<sub>3</sub>X (X = Cl, Br, I, OMe, and NMe<sub>2</sub>) by Monomeric [1,2,4-(Me<sub>3</sub>C)<sub>3</sub>C<sub>5</sub>H<sub>2</sub>]<sub>2</sub>CeH: Experimental and Computational Support for a Carbenoid Mechanism. Organometallics, 2009, 28, 3173-3185. | 1.1 | 43 |
| 83 | Energetics of Câ^'H Bond Activation of Fluorinated Aromatic Hydrocarbons Using a [Tpâ€²Rh(CNneopentyl)] Complex. Journal of the American Chemical Society, 2009, 131, 13464-13473. | 6.6 | 117 |
| 84 | Highly Active and Robust Cp* Iridium Complexes for Catalytic Water Oxidation. Journal of the American Chemical Society, 2009, 131, 8730-8731. | 6.6 | 561 |
| 85 | Exceptional Sensitivity of Metalâ^'Aryl Bond Energies to ortho-Fluorine Substituents: Influence of the Metal, the Coordination Sphere, and the Spectator Ligands on Mâ^'C/Hâ^'C Bond Energy Correlations. Journal of the American Chemical Society, 2009, 131, 7817-7827. | 6.6 | 172 |
| 86 | Synthesis and structure of â€œ16-electronâ€•rhodium(iii) catalysts for transfer hydrogenation of a cyclic imine: mechanistic implications. Chemical Communications, 2009, , 6801. | 2.2 | 35 |
| 87 | Decamethylytterbocene Complexes of Bipyridines and Diazabutadienes: Multiconfigurational Ground States and Open-Shell Singlet Formation. Journal of the American Chemical Society, 2009, 131, 6480-6491. | 6.6 | 112 |
| 88 | Molecular recognition in Mn-catalyzed Câ€“H oxidation. Reaction mechanism and origin of selectivity from a DFT perspective. Dalton Transactions, 2009, , 5989. | 1.6 | 27 |
| 89 | Metal fragment isomerisation upon grafting a d2 ML4 perhydrocarbyl Os complex on a silica surface: origin and consequence. Dalton Transactions, 2009, , 5879. | 1.6 | 16 |
| 90 | The mechanism of N-vinylindole formation via tandem imine formation and cycloisomerisation of o-ethynylanilines. Dalton Transactions, 2009, , 10296. | 1.6 | 10 |

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| 92 | A NMR, X-ray, and DFT combined study on the regio-chemistry of nucleophilic addition to platinum(II) coordinated terminal olefins. Journal of Organometallic Chemistry, 2008, 693, 2819-2827. | 0.8 | 17 |
| 93 | Mechanism of Homogeneous Iridium-Catalyzed Alkylation of Amines with Alcohols from a DFT Study. Organometallics, 2008, 27, 2529-2535. | 1.1 | 149 |
| 94 | The rebound mechanism in catalytic Câ€“H oxidation by MnO(tpp)Cl from DFT studies: electronic nature of the active species. Chemical Communications, 2008, , 744-746. | 2.2 | 68 |
| 95 | Stereochemical Nonrigidity of a Chiral Rhodium Boryl Hydride Complex:Â A Ïƒ-Borane Complex as Transition State for Isomerization. Journal of the American Chemical Society, 2008, 130, 4375-4385. | 6.6 | 20 |
| 96 | Î²-H Transfer from the Metallacyclobutane: A Key Step in the Deactivation and Byproduct Formation for the Well-Defined Silica-Supported Rhenium Alkylidene Alkene Metathesis Catalyst. Journal of the American Chemical Society, 2008, 130, 6288-6297. | 6.6 | 88 |
| 97 | Cationic Methyl Complexes of the Rare-Earth Metals: An Experimental and Computational Study on Synthesis, Structure, and Reactivity. Inorganic Chemistry, 2008, 47, 9265-9278. | 1.9 | 49 |
| 98 | A Rational Basis for the Axial Ligand Effect in Câˆ’H Oxidation by [MnO(porphyrin)(X)]+ (X = H2O, OHâˆ’,) Tj ETQq0 0 0 rgBT /Overlock 1 | 1.9 | 87 |
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| 101 | Structural and dynamic properties of propane coordinated to TpRh(CNR) from a confrontation between theory and experiment. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 6939-6944. | 3.3 | 33 |
| 102 | Understanding d0-Olefin Metathesis Catalysts:Â Which Metal, Which Ligands?. Journal of the American Chemical Society, 2007, 129, 8207-8216. | 6.6 | 210 |
| 103 | Dinitrogen Dissociation on an Isolated Surface Tantalum Atom. Science, 2007, 317, 1056-1060. | 6.0 | 163 |
| 104 | Chemoselectivity in Ïƒ bond activation by lanthanocene complexes from a DFT perspective: reactions of Cp2LnR (R = CH3, H, SiH3) with SiH4and CH3â€“SiH3. New Journal of Chemistry, 2007, 31, 549-555. | 1.4 | 37 |
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| 106 | Reflections on 30 years in the life of a journal. New Journal of Chemistry, 2007, 31, 1995. | 1.4 | 0 |
| 107 | Computational structureâ€“activity relationships in H2storage: how placement of N atoms affects release temperatures in organic liquid storage materials. Chemical Communications, 2007, , 2231-2233. | 2.2 | 163 |
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| 110 | Imidazolium Carboxylates as Versatile and Selective N-Heterocyclic Carbene Transfer Agents:â€‰ Synthesis, Mechanism, and Applications. Journal of the American Chemical Society, 2007, 129, 12834-12846. | 6.6 | 213 |
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| 112 | DFT studies of the methyl exchange reaction between Cp2Mâ€“CH3or Cp*2Mâ€“CH3(Cp = C5H5, Cp* = C5Me5,) Tj ETQq0 0 0 rgBT /O 3052-3057. | 1.6 | 47 |
| 113 | Validation of the Mâˆ’C/Hâˆ’C Bond Enthalpy Relationship through Application of Density Functional Theory. Journal of the American Chemical Society, 2006, 128, 8350-8357. | 6.6 | 73 |
| 114 | DFT calculations of d0M(NR)(CHtBu)(X)(Y) (M = Mo, W; R = CPh3, 2,6-iPrâ€“C6H3; X and Y = CH2tBu, OtBu,) Tj ETQq0 0 0 rgBT /Overlo Transactions, 2006, , 3077-3087. | 1.6 | 58 |
| 115 | A Well-Defined, Silica-Supported Tungsten Imido Alkylidene Olefin Metathesis Catalyst. Organometallics, 2006, 25, 3554-3557. | 1.1 | 152 |
| 116 | Silyl, Hydrido Silylene or Alternative Bonding Modes:Â The Many Possible Structures of [(C5H5)(PH3)IrX]+(X = SiHR2and SiR3; R = H, CH3, SiH3, and Cl). Organometallics, 2006, 25, 4748-4755. | 1.1 | 11 |
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| 121 | Hydrogen for Fluorine Exchange in C6F6and C6F5H by Monomeric [1,3,4-(Me3C)3C5H2]2CeH:Â Experimental and Computational Studies. Journal of the American Chemical Society, 2005, 127, 279-292. | 6.6 | 190 |
| 122 | An Anion-Dependent Switch in Selectivity Results from a Change of Câˆ’H Activation Mechanism in the Reaction of an Imidazolium Salt with IrH5(PPh3)2. Journal of the American Chemical Society, 2005, 127, 16299-16311. | 6.6 | 172 |
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