# Gregori Ujaque

List of Publications by Year
in descending order



| 133 | 6,751 | 50276 | 69250 |
|---|---|---|---|
| papers | citations | 46 h-index | 77 g-index |

| 146 | 146 | 146 | 5690 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Beyond Continuum Solvent Models in Computational Homogeneous Catalysis. Topics in Catalysis, 2022, 65, 118-140. | 2.8 | 24 |
| 2 | Computational Analysis on the Pd-Catalyzed Câ€“N Coupling of Ammonia with Aryl Bromides Using a Chelate Phosphine Ligand. Journal of Organic Chemistry, 2021, 86, 4007-4017. | 3.2 | 10 |
| 3 | Origin of the Rate Acceleration in the Câ^'C Reductive Elimination from Pt(IV)â€complex in a [Ga<sub>4</sub>L<sub>6</sub>]<sup>12â^'</sup> Supramolecular Metallocage. Chemistry - A European Journal, 2021, 27, 15973-15980. | 3.3 | 9 |
| 4 | Modeling Kinetics and Thermodynamics of Guest Encapsulation into the [M4L6]12â€“ Supramolecular Organometallic Cage. Journal of Chemical Information and Modeling, 2021, 61, 4370-4381. | 5.4 | 10 |
| 5 | What Makes a Good (Computed) Energy Profile?. Topics in Organometallic Chemistry, 2020, , 1-38. | 0.7 | 15 |
| 6 | Comparative Mechanistic Study on the [Au(NHC)]<sup>+</sup>-Catalyzed Hydration of Alkynes, Alkenes, and Allenes. Organometallics, 2020, 39, 3469-3479. | 2.3 | 14 |
| 7 | Catalytic Regioselective Isomerization of 2,2â€Disubstituted Oxetanes to Homoallylic Alcohols. Angewandte Chemie, 2020, 132, 7591-7597. | 2.0 | 1 |
| 8 | Reaction Rate Inside the Cavity of [Ga<sub>4</sub>L<sub>6</sub>]<sup>12â^'</sup> Supramolecular Metallocage is Regulated by the Encapsulated Solvent. Chemistry - A European Journal, 2020, 26, 6988-6992. | 3.3 | 18 |
| 9 | Catalytic Regioselective Isomerization of 2,2â€Disubstituted Oxetanes to Homoallylic Alcohols. Angewandte Chemie - International Edition, 2020, 59, 7521-7527. | 13.8 | 16 |
| 10 | Skeletal diversity in Pt- and Au-catalyzed annulations of allenedienes: dissecting unconventional mechanistic pathways. Chemical Science, 2020, 11, 4209-4220. | 7.4 | 1 |
| 11 | A resorcinarene-based tetrabenzoimidazolylidene complex of rhodium. Dalton Transactions, 2020, 49, 3181-3186. | 3.3 | 2 |
| 12 | Microsolvation and Encapsulation Effects on Supramolecular Catalysis: Câ€“C Reductive Elimination inside [Ga<sub>4</sub>L<sub>6</sub>]<sup>12â€“</sup> Metallocage. Journal of the American Chemical Society, 2019, 141, 13114-13123. | 13.7 | 40 |
| 13 | A Reversible Phase Transition of 2D Coordination Layers by Bâ€“Hâ^™â^™â^™Cu(II) Interactions in a Coordination Polymer. Molecules, 2019, 24, 3204. | 3.8 | 7 |
| 14 | Mild Iridiumâ€Catalysed Isomerization of Epoxides. Computational Insights and Application to the Synthesis of Î²â€Alkyl Amines. Advanced Synthesis and Catalysis, 2019, 361, 3624-3631. | 4.3 | 12 |
| 15 | Origin of the Anti-Markovnikov Hydroamination of Alkenes Catalyzed by Lâ€“Au(I) Complexes: Coordination Mode Determines Regioselectivity. ACS Catalysis, 2019, 9, 848-858. | 11.2 | 45 |
| 16 | GARLEEK: Adding an extra flavor to ONIOM. Journal of Computational Chemistry, 2019, 40, 381-386. | 3.3 | 6 |
| 17 | Well-Defined Î²-Diketiminatocobalt(II) Complexes for Alkene Cyclohydroamination of Primary Amines. ACS Catalysis, 2018, 8, 4446-4451. | 11.2 | 16 |
| 18 | Calculation of Reaction Free Energies in Solution: A Comparison of Current Approaches. Journal of Physical Chemistry A, 2018, 122, 1392-1399. | 2.5 | 101 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Direct Asymmetric Hydrogenation of N-Methyl and N-Alkyl Imines with an Ir(III)H Catalyst. Journal of the American Chemical Society, 2018, 140, 16967-16970. | 13.7 | 47 |
| 20 | Iridium-Catalyzed Isomerization of N-Sulfonyl Aziridines to Allyl Amines. Organic Letters, 2018, 20, 5747-5751. | 4.6 | 25 |
| 21 | Mechanistic Insights on the Hydration of Terminal and Internal Allenes Catalyzed by [(NHC)Au]<sup>+</sup>. Organometallics, 2018, 37, 3543-3551. | 2.3 | 10 |
| 22 | Tripodal halogen bonding iodo-azolium receptors for anion recognition. RSC Advances, 2017, 7, 11253-11258. | 3.6 | 23 |
| 23 | The Origin of Antiâ€Markovnikov Regioselectivity in Alkene Hydroamination Reactions Catalyzed by [Rh(DPEphos)]<sup>+</sup>. Chemistry - A European Journal, 2016, 22, 9311-9320. | 3.3 | 28 |
| 24 | Acid Activation in Phenyliodine Dicarboxylates: Direct Observation, Structures, and Implications. Journal of the American Chemical Society, 2016, 138, 12747-12750. | 13.7 | 127 |
| 25 | Rim, Side Arms, and Cavity: Three Sites for the Recognition of Anions by Tetraazolium Resorcinarene Cavitands. Chemistry - A European Journal, 2016, 22, 15800-15806. | 3.3 | 8 |
| 26 | Mechanistic implications of the enantioselective addition of alkylzinc reagents to aldehydes catalyzed by nickel complexes with Î±-amino amide ligands. Organic and Biomolecular Chemistry, 2016, 14, 11125-11136. | 2.8 | 7 |
| 27 | First-Principles Molecular Dynamics Studies of Organometallic Complexes and Homogeneous Catalytic Processes. Accounts of Chemical Research, 2016, 49, 1271-1278. | 15.6 | 64 |
| 28 | Realistic Simulation of Organometallic Reactivity in Solution by Means of First-Principles Molecular Dynamics. Structure and Bonding, 2015, , 81-106. | 1.0 | 7 |
| 29 | A Tetraferrocenylâ€Resorcinarene Cavitand as a Redoxâ€Switchable Host of Ammonium Salts. Chemistry - A European Journal, 2015, 21, 10558-10565. | 3.3 | 19 |
| 30 | Hydroamination of Câ€“C Multiple Bonds with Hydrazine Catalyzed by N-Heterocyclic Carbeneâ€“Gold(I) Complexes: Substrate and Ligand Effects. ACS Catalysis, 2015, 5, 815-829. | 11.2 | 49 |
| 31 | Ketone Hydrogenation with Iridium Complexes with â€œnon Nâ€“Hâ€•Ligands: The Key Role of the Strong Base. ACS Catalysis, 2015, 5, 4368-4376. | 11.2 | 29 |
| 32 | Experimental and Theoretical Approaches to the Influence of the Addition of Pyrene to a Series of Pd and Ni NHCâ€Based Complexes: Catalytic Consequences. Chemistry - A European Journal, 2015, 21, 1578-1588. | 3.3 | 44 |
| 33 | Palladium monophosphine Pd(PPh<sub>3</sub>): is it really accessible in solution?. Chemical Communications, 2014, 50, 661-663. | 4.1 | 34 |
| 34 | Challenges in modelling homogeneous catalysis: new answers from ab initio molecular dynamics to the controversy over the Wacker process. Chemical Society Reviews, 2014, 43, 4940-4952. | 38.1 | 65 |
| 35 | Counteranion-Dependent Reaction Pathways in the Protonation of Cationic Rutheniumâ€“Vinylidene Complexes. Organometallics, 2014, 33, 2549-2560. | 2.3 | 8 |
| 36 | The Transmetalation Process in Suzukiâ€“Miyaura Reactions: Calculations Indicate Lower Barrier via Boronate Intermediate. ChemCatChem, 2014, 6, 3132-3138. | 3.7 | 68 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Computational Perspective on Pd-Catalyzed Câ€“C Cross-Coupling Reaction Mechanisms. Accounts of Chemical Research, 2013, 46, 2626-2634. | 15.6 | 306 |
| 38 | Mechanistic Studies on the Pd-Catalyzed Vinylation of Aryl Halides with Vinylalkoxysilanes in Water: The Effect of the Solvent and NaOH Promoter. Journal of the American Chemical Society, 2013, 135, 13749-13763. | 13.7 | 46 |
| 39 | Counteranion and Solvent Assistance in Ruthenium-Mediated Alkyne to Vinylidene Isomerizations. Inorganic Chemistry, 2013, 52, 8919-8932. | 4.0 | 36 |
| 40 | Solution dynamics of agostic interactions in T-shaped Pt(ii) complexes from ab initio molecular dynamics simulations. Dalton Transactions, 2013, 42, 12165. | 3.3 | 25 |
| 41 | Unraveling the Pathway of Gold(I)-Catalyzed Olefin Hydrogenation: An Ionic Mechanism. Journal of the American Chemical Society, 2013, 135, 1295-1305. | 13.7 | 53 |
| 42 | Mechanistic Intricacies of Goldâ€Catalyzed Intermolecular Cycloadditions between Allenamides and Dienes. Chemistry - A European Journal, 2013, 19, 15248-15260. | 3.3 | 57 |
| 43 | Mechanistic Exploration of the Pd-Catalyzed Copper-Free Sonogashira Reaction. ACS Catalysis, 2012, 2, 135-144. | 11.2 | 103 |
| 44 | PtII as a proton shuttle during Câ€“H bond activation in the Shilov process. Chemical Communications, 2012, 48, 1979. | 4.1 | 26 |
| 45 | Rearrangement of Tridentate [OSO]-Type Ligands and Migratory Insertion Reaction Mechanisms in Cyclopentadienyl Tantalum Complexes. Organometallics, 2012, 31, 7052-7062. | 2.3 | 8 |
| 46 | Experimental and Theoretical Studies of the Hydrogenation of Î±,Î²-Unsaturated Acids by an 18e Hydride Carbonylniobocene Complex. Organometallics, 2012, 31, 5177-5184. | 2.3 | 8 |
| 47 | Homogeneous Computational Catalysis: The Mechanism for Cross-Coupling and Other C-C Bond Formation Processes. NATO Science for Peace and Security Series B: Physics and Biophysics, 2012, , 185-206. | 0.3 | 1 |
| 48 | The Nature of [PdCl<sub>2</sub>(C<sub>2</sub>H<sub>4</sub>)(H<sub>2</sub>O)] as an Active Species in the Wacker Process: New Insights from Ab Initio Molecular Dynamics Simulations. Chemistry - A European Journal, 2012, 18, 5612-5619. | 3.3 | 31 |
| 49 | Highly Efficient Redox Isomerisation of Allylic Alcohols Catalysed by Pyrazoleâ€Based Ruthenium(IV) Complexes in Water: Mechanisms of Bifunctional Catalysis in Water. Chemistry - A European Journal, 2012, 18, 7749-7765. | 3.3 | 68 |
| 50 | A Versatile Ru Catalyst for the Asymmetric Transfer Hydrogenation of Both Aromatic and Aliphatic Sulfinylimines. Chemistry - A European Journal, 2012, 18, 1969-1983. | 3.3 | 53 |
| 51 | Theoretical study on intramolecular allene-diene cycloadditions catalyzed by PtCl2 and Au(i) complexes. Dalton Transactions, 2011, 40, 11095. | 3.3 | 19 |
| 52 | Internal Alkyne Isomerization to Vinylidene versus Stable Ï€-Alkyne: Theoretical and Experimental Study on the Divergence of Analogous Cp*Ru and TpRu Systems. Organometallics, 2011, 30, 4014-4031. | 2.3 | 36 |
| 53 | Gold-Catalyzed Cycloadditions Involving Allenes: Mechanistic Insights from Theoretical Studies. Topics in Current Chemistry, 2011, 302, 225-248. | 4.0 | 33 |
| 54 | Cationic Intermediates in the Pd-Catalyzed Negishi Coupling. Kinetic and Density Functional Theory Study of Alternative Transmetalation Pathways in the Meâ€“Me Coupling of ZnMe<sub>2</sub>andtrans-[PdMeCl(PMePh<sub>2</sub>)<sub>2</sub>]. Journal of the American Chemical Society, 2011, 133, 13519-13526. | 13.7 | 69 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | Theoretical Evaluation of Phosphine Effects in Cross-Coupling Reactions. Catalysis By Metal Complexes, 2011, , 57-84. | 0.6 | 12 |
| 56 | The importance of conformational search: a test case on the catalytic cycle of the Suzukiâ€“Miyaura cross-coupling. Theoretical Chemistry Accounts, 2011, 128, 639-646. | 1.4 | 67 |
| 57 | Gold versus Silverâ€Catalyzed Intermolecular Hydroaminations of Alkenes and Dienes. Advanced Synthesis and Catalysis, 2011, 353, 3451-3466. | 4.3 | 44 |
| 58 | Do Metalâ‹…â‹…â‹…Water Hydrogen Bonds Hold in Solution? Insight from Ab Initio Molecular Dynamics Simulations. ChemPhysChem, 2011, 12, 1666-1668. | 2.1 | 22 |
| 59 | Hydroamination of Alkynes with Ammonia: Unforeseen Role of the Gold(I) Catalyst. Angewandte Chemie - International Edition, 2011, 50, 11147-11151. | 13.8 | 67 |
| 60 | The Wacker Process: Innerâ€•or Outerâ€Sphere Nucleophilic Addition? New Insights from Ab Initio Molecular Dynamics. Chemistry - A European Journal, 2010, 16, 8738-8747. | 3.3 | 55 |
| 61 | Palladium Round Trip in the Negishi Coupling of transâ€[PdMeCl(PMePh<sub>2</sub>)<sub>2</sub>] with ZnMeCl: An Experimental and DFT Study of the Transmetalation Step. Chemistry - A European Journal, 2010, 16, 8596-8599. | 3.3 | 76 |
| 62 | Inner- and Outer-Sphere Hydrogenation Mechanisms: A Computational Perspective. Advances in Inorganic Chemistry, 2010, 62, 231-260. | 1.0 | 34 |
| 63 | Mechanistic Comparison of Acid- and Gold(I)-Catalyzed Nucleophilic Addition Reactions to Olefins. Organometallics, 2010, 29, 5919-5926. | 2.3 | 46 |
| 64 | Proton-Transfer Reactions to Half-Sandwich Ruthenium Trihydride Complexes Bearing Hemilabile P,N Ligands: Experimental and Density Functional Theory Studiesâ€Dedicated to Prof. Serafin Bernal in recognition of his contribution to inorganic chemistry, on the occasion of his retirement.. Inorganic Chemistry, 2010, 49, 6035-6057. | 4.0 | 28 |
| 65 | Reaction Mechanism of the Gold(I)-Catalyzed Addition of Phenols to Olefins: A Concerted Process Accelerated by Phenol and Water. Organometallics, 2010, 29, 3252-3260. | 2.3 | 67 |
| 66 | Goldâ€Catalyzed [4C+3C] Intramolecular Cycloaddition of Allenedienes: Synthetic Potential and Mechanistic Implications. Chemistry - A European Journal, 2009, 15, 3336-3339. | 3.3 | 138 |
| 67 | Experimental and Computational Studies on the Iridium Activation of Aliphatic and Aromatic Cï£¿H Bonds of Alkyl Aryl Ethers and Related Molecules. Chemistry - A European Journal, 2009, 15, 9034-9045. | 3.3 | 26 |
| 68 | Synthetic, Mechanistic, and Theoretical Studies on the Generation of Iridium Hydride Alkylidene and Iridium Hydride Alkene Isomers. Chemistry - A European Journal, 2009, 15, 9046-9057. | 3.3 | 25 |
| 69 | The role of amide ligands in the stabilization of Pd(II) tricoordinated complexes: is the Pdâ€“NR2 bond order single or higher?. Theoretical Chemistry Accounts, 2009, 123, 75-84. | 1.4 | 10 |
| 70 | Mechanistic evaluation of metal-catalyzed hydrogen-transfer processes: The Shvo catalyst as an example of computational unravelling. Computational and Theoretical Chemistry, 2009, 903, 123-132. | 1.5 | 41 |
| 71 | Why Is the Suzukiâ^'Miyaura Cross-Coupling of sp<sup>3</sup>Carbons in Î±-Bromo Sulfoxide Systems Fast and Stereoselective? A DFT Study on the Mechanism. Journal of Organic Chemistry, 2009, 74, 4049-4054. | 3.2 | 54 |
| 72 | Gold(I)-Catalyzed Intermolecular Oxyarylation of Alkynes: Unexpected Regiochemistry in the Alkylation of Arenes. Organic Letters, 2009, 11, 4906-4909. | 4.6 | 148 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Gold-Catalyzed [4C+2C] Cycloadditions of Allenedienes, including an Enantioselective Version with New Phosphoramidite-Based Catalysts: Mechanistic Aspects of the Divergence between [4C+3C] and [4C+2C] Pathways. Journal of the American Chemical Society, 2009, 131, 13020-13030. | 13.7 | 258 |
| 74 | Aromatic Câ€“F activation by complexes containing the {Pt2S2} core via nucleophilic substitution: a combined experimental and theoretical study. Dalton Transactions, 2009, , 5980. | 3.3 | 24 |
| 75 | Câˆ’C Reductive Elimination in Palladium Complexes, and the Role of Coupling Additives. A DFT Study Supported by Experiment. Journal of the American Chemical Society, 2009, 131, 3650-3657. | 13.7 | 178 |
| 76 | Mechanism of the Rhodiumâ€Catalyzed Asymmetric Isomerization of Allylamines to Enamines. Chemistry - A European Journal, 2008, 14, 3323-3329. | 3.3 | 17 |
| 77 | When Are Tricoordinated Pd<sup>II</sup>Species Accessible? Stability Trends and Mechanistic Consequences. Chemistry - A European Journal, 2008, 14, 8986-8994. | 3.3 | 50 |
| 78 | New chiral tetraaza ligands for the efficient enantioselective addition of dialkylzinc to aromatic aldehydes. Tetrahedron, 2008, 64, 9717-9724. | 1.9 | 34 |
| 79 | Mechanistic analogies and differences between gold- and palladium-supported Schiff base complexes as hydrogenation catalysts: A combined kinetic and DFT study. Journal of Catalysis, 2008, 254, 226-237. | 6.2 | 29 |
| 80 | The Reaction Mechanism of the Hydroamination of Alkenes Catalyzed by Gold(I)âˆ’Phosphine:â€‰ The Role of the Counterion and the N-Nucleophile Substituents in the Proton-Transfer Step. Journal of the American Chemical Society, 2008, 130, 853-864. | 13.7 | 197 |
| 81 | Csp3â€“F bond activation by nucleophilic attack of the {Pt2S2} core assisted by non-covalent interactions. Chemical Communications, 2008, , 3130. | 4.1 | 26 |
| 82 | Theoretical Analysis of the Hydrogen-Transfer Reaction to Câ•N, Câ•C, and Câ‰¡C Bonds Catalyzed by Shvoâ€™s Ruthenium Complex. Organometallics, 2008, 27, 4854-4863. | 2.3 | 44 |
| 83 | Effect of thetert-butiloxycarbonyl protecting group on the adsorption of protected amino-cyclopentene on the Si(100) surface. Physical Review B, 2007, 75, . | 3.2 | 2 |
| 84 | Hydrogen Transfer to Ketones Catalyzed by Shvo's Ruthenium Hydride Complex:â€‰ A Mechanistic Insight. Organometallics, 2007, 26, 4135-4144. | 2.3 | 130 |
| 85 | Mechanism of Formation of Silver N-Heterocyclic Carbenes Using Silver Oxide:â€‰ A Theoretical Study. Organometallics, 2007, 26, 6170-6183. | 2.3 | 58 |
| 86 | Nature of Cp*MoO2+in Water and Intramolecular Proton-Transfer Mechanism by Stopped-Flow Kinetics and Density Functional Theory Calculations. Inorganic Chemistry, 2007, 46, 4103-4113. | 4.0 | 39 |
| 87 | How does the Achiral Base Decide the Stereochemical Outcome in the Dynamic Kinetic Resolution of Sulfinyl Chlorides? A Computational Study. Advanced Synthesis and Catalysis, 2007, 349, 2103-2110. | 4.3 | 18 |
| 88 | The Role of Water in the Stereoselective Hydrogenation of 1,2-Diphenylacetylene Catalyzed by the Water-Soluble [{RuCl2(mtppms)2}2]. European Journal of Inorganic Chemistry, 2007, 2007, 2879-2889. | 2.0 | 14 |
| 89 | Proton-Transfer and H2-Elimination Reactions of Main-Group Hydrides EH4-(E = B, Al, Ga) with Alcohols. Inorganic Chemistry, 2006, 45, 3086-3096. | 4.0 | 49 |
| 90 | Formation of a Vinyliminium Palladium Complex by Câˆ’C Coupling in Vinylcarbene Palladium Aryl Complexes. Organometallics, 2006, 25, 1293-1297. | 2.3 | 42 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | A DFT Study of the Full Catalytic Cycle of the Suzukiâˆ'Miyaura Cross-Coupling on a Model System. Organometallics, 2006, 25, 3647-3658. | 2.3 | 348 |
| 92 | A Critical Analysis of the Cyclic and Open Alternatives of the Transmetalation Step in the Stille Cross-Coupling Reaction. Journal of the American Chemical Society, 2006, 128, 14571-14578. | 13.7 | 100 |
| 93 | Single-Site Homogeneous and Heterogeneized Gold(III) Hydrogenation Catalysts:Â Mechanistic Implications. Journal of the American Chemical Society, 2006, 128, 4756-4765. | 13.7 | 161 |
| 94 | The Active Role of the Water Solvent in the Regioselective CO Hydrogenation of Unsaturated Aldehydes by [RuH2(mtppms)x] in Basic Media. Organometallics, 2006, 25, 5010-5023. | 2.3 | 52 |
| 95 | Mechanism of the Base-Assisted Displacement of Chloride by Alcohol in Sulfinyl Derivatives. Journal of Organic Chemistry, 2006, 71, 6388-6396. | 3.2 | 39 |
| 96 | Câˆ'H Oxidative Addition of Bisimidazolium Salts to Iridium and Rhodium Complexes, and N-Heterocyclic Carbene Generation. A Combined Experimental and Theoretical Study. Organometallics, 2006, 25, 1120-1134. | 2.3 | 96 |
| 97 | Theoretical Investigation of the Selective CC Hydrogenation of Unsaturated Aldehydes Catalyzed by [{RuCl2(mtppms)2}2] in Acidic Media. Organometallics, 2006, 25, 862-872. | 2.3 | 27 |
| 98 | Aliphatic Câ€"X (X=halogen) bond activation by transition metal complexes containing the {Pt2S2} core: A theoretical study of the reaction mechanism. Inorganica Chimica Acta, 2006, 359, 3736-3744. | 2.4 | 12 |
| 99 | Computational study of the transmetalation process in the Suzukiâ€"Miyaura cross-coupling of aryls. Journal of Organometallic Chemistry, 2006, 691, 4459-4466. | 1.8 | 140 |
| 100 | Chemical and Constitutional Influences in the Self-Assembly of Functional Supramolecular Hydrogen-Bonded Nanoscopic Fibres. Chemistry - A European Journal, 2006, 12, 9161-9175. | 3.3 | 46 |
| 101 | QM/QM study of the coverage effects on the adsorption of amino-cyclopentene at the Si(100) surface. Journal of Computational Chemistry, 2006, 27, 1892-1897. | 3.3 | 4 |
| 102 | A QM/MM Study of the Asymmetric Dihydroxylation of Terminal Aliphaticn-Alkenes with OsO4â‹…(DHQD)2PYDZ: Enantioselectivity as a Function of Chain Length. Chemistry - A European Journal, 2005, 11, 1017-1029. | 3.3 | 24 |
| 103 | Computational Characterization of the Role of the Base in the Suzukiâˆ'Miyaura Cross-Coupling Reaction. Journal of the American Chemical Society, 2005, 127, 9298-9307. | 13.7 | 317 |
| 104 | Computational Rationalization of the Dependence of the Enantioselectivity on the Nature of the Catalyst in the Vanadium-Catalyzed Oxidation of Sulfides by Hydrogen Peroxide. Journal of the American Chemical Society, 2005, 127, 3624-3634. | 13.7 | 73 |
| 105 | Self-Assembly of Mercaptaneâˆ'Metallacarborane Complexes by an Unconventional Cooperative Effect:Â A Câˆ'HÂ·Â·Â·Sâˆ'HÂ·Â·Â·Hâˆ'B Hydrogen/Dihydrogen Bond Interaction. Journal of the American Chemical Society, 2005, 127, 15976-15982. | 13.7 | 105 |
| 106 | Applications of Hybrid DFT/Molecular Mechanics to Homogeneous Catalysis. Structure and Bonding, 2004, , 117-150. | 1.0 | 41 |
| 107 | A Measureable Equilibrium between Iridium Hydride Alkylidene and Iridium Hydride Alkene Isomers. Angewandte Chemie - International Edition, 2004, 43, 3708-3711. | 13.8 | 44 |
| 108 | A computational study on the acceleration of the Prins reaction by indium trichloride. Comptes Rendus Chimie, 2004, 7, 885-893. | 0.5 | 1 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | Unusual Câ^'H Allylic Activation in the {PtII(cod)} Fragment Bonded to a {Pt2(Î¼-S)2} Core. Organometallics, 2004, 23, 2522-2532. | 2.3 | 16 |
| 110 | Catalysis on the coastline: Theozyme, molecular dynamics, and free energy perturbation analysis of antibody 21D8 catalysis of the decarboxylation of 5-nitro-3-carboxybenzisoxazole. Journal of Computational Chemistry, 2003, 24, 98-110. | 3.3 | 22 |
| 111 | Diradical versus Concerted Mechanisms for the Dihydroxylation of Protoanemonin by OsO4 and OsO4â^'NH3 â^' The Effect of the Base in the Reaction. European Journal of Organic Chemistry, 2003, 2003, 833-839. | 2.4 | 8 |
| 112 | Some critical issues in the application of quantum mechanics/molecular mechanics methods to the study of transition metal complexes. Faraday Discussions, 2003, 124, 429-441. | 3.2 | 26 |
| 113 | Ortho-CH Activation of Aromatic Ketones, Partially Fluorinated Aromatic Ketones, and Aromatic Imines by a Trihydride-Stannyl-Osmium(IV) Complex. Organometallics, 2003, 22, 3753-3765. | 2.3 | 52 |
| 114 | Electrostatic Interactions between Substituents as Regioselectivity Control Elements in Dielsâ^'Alder Cycloadditions. A DFT Study of Cycloadditions of 1-Methoxy-4-trimethylsiloxy Dienes with Acrylonitrile. Journal of Organic Chemistry, 2002, 67, 7179-7184. | 3.2 | 16 |
| 115 | The Origin of endo Stereoselectivity in the Hetero-Dielsâ€"Alder Reactions of Aldehydes with ortho-Xylylenes: CHâ€"Ï€, Ï€â€"Ï€, and Steric Effects on Stereoselectivity. Chemistry - A European Journal, 2002, 8, 3423. | 3.3 | 50 |
| 116 | A comparative study of DFT and traditional ab initio methodologies on the OsO4 molecule. International Journal of Quantum Chemistry, 2000, 77, 544-551. | 2.0 | 9 |
| 117 | Edge-Sharing Binuclear d8 Complexes with XR Bridges: Theoretical and Structural Database Study of their Molecular Conformation. Chemistry - A European Journal, 1999, 5, 1391-1410. | 3.3 | 65 |
| 118 | Theoretical Study on the Origin of Enantioselectivity in the Bis(dihydroquinidine)-3,6-pyridazineÂ·Osmium Tetroxide-Catalyzed Dihydroxylation of Styrene. Journal of the American Chemical Society, 1999, 121, 1317-1323. | 13.7 | 94 |
| 119 | Theoretical and Synthetic Studies on Dihaptoacyl and Î²-Agostic Acyl Complexes of Molybdenum. Organometallics, 1999, 18, 3294-3305. | 2.3 | 24 |
| 120 | Edge-Sharing Binuclear d8 Complexes with XR Bridges: Theoretical and Structural Database Study of their Molecular Conformation. Chemistry - A European Journal, 1999, 5, 1391-1410. | 3.3 | 1 |
| 121 | Palladium(II) complexes with Pd2S2 rings. Synthesis and theoretical characterization of [Pd2(dppe)2(Î¼-S)2] and X-ray characterization of [Pd3(dppe)3(Î¼3-S)2]Cl2. Inorganic Chemistry Communication, 1998, 1, 466-468. | 3.9 | 18 |
| 122 | The first stable copper(II) complex containing four sulfide ligands: synthesis and structural characterization of [Pt2(dppe)2(Î¼-S)2] and [Cu{Pt2(dppe)2(Î¼3-S)2}2]2+. Chemical Communications, 1998, , 597-598. | 4.1 | 30 |
| 123 | Breaking an electronically preferred symmetry by steric effects in a series of [Ir(biph)X(QR3)2] compounds (X=Cl or I, Q=P or As). New Journal of Chemistry, 1998, 22, 1493-1498. | 2.8 | 22 |
| 124 | Computational Evidence of the Importance of Substituent Bulk on Agostic Interactions in Ir(H)2(PtBu2Ph)2+. Journal of the American Chemical Society, 1998, 120, 361-365. | 13.7 | 121 |
| 125 | To Bend or Not To Bend:Â Dilemma of the Edge-Sharing Binuclear Square Planar Complexes of d8Transition Metal Ions. Inorganic Chemistry, 1998, 37, 804-813. | 4.0 | 126 |
| 126 | Theoretical Characterization of an Intermediate for the [3 + 2] Cycloaddition Mechanism in the Bis(dihydroxy- quinidine)â^'3,6-PyridazineÂ·Osmium Tetroxide-Catalyzed Dihydroxylation of Styrene. Journal of Organic Chemistry, 1997, 62, 7892-7894. | 3.2 | 27 |

| # | Article | IF | Citations |
|---|---|---|---|
| 127 | Theoretical, structural and NMR studies of fluxionality in thiolato-bridged platinum(II)-platinum(IV) dinuclear complexes. Inorganica Chimica Acta, 1997, 265, 89-102. | 2.4 | 20 |
| 128 | Different van der Waals radii for organic and inorganic halogen atoms: a significant improvement in IMOMM performance. Theoretical Chemistry Accounts, 1997, 96, 146-150. | 1.4 | 34 |
| 129 | Theory Does Not Support an Osmaoxetane Intermediate in the Osmium-Catalyzed Dihydroxylation of Olefins. Journal of the American Chemical Society, 1996, 118, 11660-11661. | 13.7 | 121 |
| 130 | A theoretical evaluation of steric and electronic effects on the structure of [OSO4 (NR3)] (NR3 =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 | 0.8 | 1 |
| 131 | Basis set influence on the ab initio description of the dihydrogen complex [Os(PH3)2Cl(CO)H(H2)]1. Computational and Theoretical Chemistry, 1996, 371, 59-68. | 1.5 | 3 |
| 132 | A theoretical evaluation of steric and electronic effects on the structure of [OsO. Theoretica Chimica Acta, 1996, 94, 67. | 0.8 | 11 |
| 133 | Mechanism of Palladium-Catalyzed Cross-Coupling Reactions. , 0, , 109-130. | | 4 |