

Gregori Ujaque

List of Publications by Year in descending order

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133
papers

6,751
citations

50170

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146
docs citations

146
times ranked

5690
citing authors

#	ARTICLE	IF	CITATIONS
1	A DFT Study of the Full Catalytic Cycle of the Suzuki–Miyaura Cross-Coupling on a Model System. <i>Organometallics</i> , 2006, 25, 3647-3658.	1.1	348
2	Computational Characterization of the Role of the Base in the Suzuki–Miyaura Cross-Coupling Reaction. <i>Journal of the American Chemical Society</i> , 2005, 127, 9298-9307.	6.6	317
3	Computational Perspective on Pd-Catalyzed C–C Cross-Coupling Reaction Mechanisms. <i>Accounts of Chemical Research</i> , 2013, 46, 2626-2634.	7.6	306
4	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. <i>Journal of the American Chemical Society</i> , 2009, 131, 13020-13030.	6.6	258
5	The Reaction Mechanism of the Hydroamination of Alkenes Catalyzed by Gold(I)–Phosphine: The Role of the Counterion and the N-Nucleophile Substituents in the Proton-Transfer Step. <i>Journal of the American Chemical Society</i> , 2008, 130, 853-864.	6.6	197
6	C–C Reductive Elimination in Palladium Complexes, and the Role of Coupling Additives. A DFT Study Supported by Experiment. <i>Journal of the American Chemical Society</i> , 2009, 131, 3650-3657.	6.6	178
7	Single-Site Homogeneous and Heterogenized Gold(III) Hydrogenation Catalysts: Mechanistic Implications. <i>Journal of the American Chemical Society</i> , 2006, 128, 4756-4765.	6.6	161
8	Gold(I)-Catalyzed Intermolecular Oxyarylation of Alkynes: Unexpected Regiochemistry in the Alkylation of Arenes. <i>Organic Letters</i> , 2009, 11, 4906-4909.	2.4	148
9	Computational study of the transmetalation process in the Suzuki–Miyaura cross-coupling of aryls. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 4459-4466.	0.8	140
10	Gold-Catalyzed [4C+3C] Intramolecular Cycloaddition of Allenedienes: Synthetic Potential and Mechanistic Implications. <i>Chemistry - A European Journal</i> , 2009, 15, 3336-3339.	1.7	138
11	Hydrogen Transfer to Ketones Catalyzed by Shvo's Ruthenium Hydride Complex: A Mechanistic Insight. <i>Organometallics</i> , 2007, 26, 4135-4144.	1.1	130
12	Acid Activation in Phenyliodine Dicarboxylates: Direct Observation, Structures, and Implications. <i>Journal of the American Chemical Society</i> , 2016, 138, 12747-12750.	6.6	127
13	To Bend or Not To Bend: A Dilemma of the Edge-Sharing Binuclear Square Planar Complexes of d8 Transition Metal Ions. <i>Inorganic Chemistry</i> , 1998, 37, 804-813.	1.9	126
14	Theory Does Not Support an Osmaoxetane Intermediate in the Osmium-Catalyzed Dihydroxylation of Olefins. <i>Journal of the American Chemical Society</i> , 1996, 118, 11660-11661.	6.6	121
15	Computational Evidence of the Importance of Substituent Bulk on Agostic Interactions in Ir(H) ₂ (PtBu ₂ Ph) ₂ ⁺ . <i>Journal of the American Chemical Society</i> , 1998, 120, 361-365.	6.6	121
16	Self-Assembly of Mercaptane–Metallacarborane Complexes by an Unconventional Cooperative Effect: A C–H...H–A...S–H...H–A...H–B Hydrogen/Dihydrogen Bond Interaction. <i>Journal of the American Chemical Society</i> , 2005, 127, 15976-15982.	6.6	105
17	Mechanistic Exploration of the Pd-Catalyzed Copper-Free Sonogashira Reaction. <i>ACS Catalysis</i> , 2012, 2, 135-144.	5.5	103
18	Calculation of Reaction Free Energies in Solution: A Comparison of Current Approaches. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1392-1399.	1.1	101

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19	A Critical Analysis of the Cyclic and Open Alternatives of the Transmetalation Step in the Stille Cross-Coupling Reaction. <i>Journal of the American Chemical Society</i> , 2006, 128, 14571-14578.	6.6	100
20	C ^α -H Oxidative Addition of Bisimidazolium Salts to Iridium and Rhodium Complexes, and N-Heterocyclic Carbene Generation. A Combined Experimental and Theoretical Study. <i>Organometallics</i> , 2006, 25, 1120-1134.	1.1	96
21	Theoretical Study on the Origin of Enantioselectivity in the Bis(dihydroquinidine)-3,6-pyridazine- <i>O</i> -Osmium Tetroxide-Catalyzed Dihydroxylation of Styrene. <i>Journal of the American Chemical Society</i> , 1999, 121, 1317-1323.	6.6	94
22	Palladium Round Trip in the Negishi Coupling of <i>trans</i> -[PdMeCl(PMePh) ₂] with ZnMeCl: An Experimental and DFT Study of the Transmetalation Step. <i>Chemistry - A European Journal</i> , 2010, 16, 8596-8599.	1.7	76
23	Computational Rationalization of the Dependence of the Enantioselectivity on the Nature of the Catalyst in the Vanadium-Catalyzed Oxidation of Sulfides by Hydrogen Peroxide. <i>Journal of the American Chemical Society</i> , 2005, 127, 3624-3634.	6.6	73
24	Cationic Intermediates in the Pd-Catalyzed Negishi Coupling. Kinetic and Density Functional Theory Study of Alternative Transmetalation Pathways in the Me ^α -Me Coupling of ZnMe ₂ and <i>trans</i> -[PdMeCl(PMePh) ₂]. <i>Journal of the American Chemical Society</i> , 2011, 133, 13519-13526.	6.6	69
25	Highly Efficient Redox Isomerisation of Allylic Alcohols Catalysed by Pyrazole-Based Ruthenium(IV) Complexes in Water: Mechanisms of Bifunctional Catalysis in Water. <i>Chemistry - A European Journal</i> , 2012, 18, 7749-7765.	1.7	68
26	The Transmetalation Process in Suzuki-Miyaura Reactions: Calculations Indicate Lower Barrier via Boronate Intermediate. <i>ChemCatChem</i> , 2014, 6, 3132-3138.	1.8	68
27	Reaction Mechanism of the Gold(I)-Catalyzed Addition of Phenols to Olefins: A Concerted Process Accelerated by Phenol and Water. <i>Organometallics</i> , 2010, 29, 3252-3260.	1.1	67
28	The importance of conformational search: a test case on the catalytic cycle of the Suzuki-Miyaura cross-coupling. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 639-646.	0.5	67
29	Hydroamination of Alkynes with Ammonia: Unforeseen Role of the Gold(I) Catalyst. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 11147-11151.	7.2	67
30	Edge-Sharing Binuclear d8 Complexes with XR Bridges: Theoretical and Structural Database Study of their Molecular Conformation. <i>Chemistry - A European Journal</i> , 1999, 5, 1391-1410.	1.7	65
31	Challenges in modelling homogeneous catalysis: new answers from ab initio molecular dynamics to the controversy over the Wacker process. <i>Chemical Society Reviews</i> , 2014, 43, 4940-4952.	18.7	65
32	First-Principles Molecular Dynamics Studies of Organometallic Complexes and Homogeneous Catalytic Processes. <i>Accounts of Chemical Research</i> , 2016, 49, 1271-1278.	7.6	64
33	Mechanism of Formation of Silver <i>N</i> -Heterocyclic Carbenes Using Silver Oxide: A Theoretical Study. <i>Organometallics</i> , 2007, 26, 6170-6183.	1.1	58
34	Mechanistic Intricacies of Gold-Catalyzed Intermolecular Cycloadditions between Allenamides and Dienes. <i>Chemistry - A European Journal</i> , 2013, 19, 15248-15260.	1.7	57
35	The Wacker Process: Inner- or Outer-Sphere Nucleophilic Addition? New Insights from Ab Initio Molecular Dynamics. <i>Chemistry - A European Journal</i> , 2010, 16, 8738-8747.	1.7	55
36	Why Is the Suzuki-Miyaura Cross-Coupling of sp ³ Carbons in <i>±</i> -Bromo Sulfoxide Systems Fast and Stereoselective? A DFT Study on the Mechanism. <i>Journal of Organic Chemistry</i> , 2009, 74, 4049-4054.	1.7	54

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37	A Versatile Ru Catalyst for the Asymmetric Transfer Hydrogenation of Both Aromatic and Aliphatic Sulfinylimines. <i>Chemistry - A European Journal</i> , 2012, 18, 1969-1983.	1.7	53
38	Unraveling the Pathway of Gold(I)-Catalyzed Olefin Hydrogenation: An Ionic Mechanism. <i>Journal of the American Chemical Society</i> , 2013, 135, 1295-1305.	6.6	53
39	Ortho-CH Activation of Aromatic Ketones, Partially Fluorinated Aromatic Ketones, and Aromatic Imines by a Trihydride-Stannyl-Osmium(IV) Complex. <i>Organometallics</i> , 2003, 22, 3753-3765.	1.1	52
40	The Active Role of the Water Solvent in the Regioselective CO Hydrogenation of Unsaturated Aldehydes by [RuH ₂ (mtppm)x] in Basic Media. <i>Organometallics</i> , 2006, 25, 5010-5023.	1.1	52
41	The Origin of endo Stereoselectivity in the Hetero-Diels-Alder Reactions of Aldehydes with ortho-Xylylenes: CH ₂ =C=C ₂ and Steric Effects on Stereoselectivity. <i>Chemistry - A European Journal</i> , 2002, 8, 3423.	1.7	50
42	When Are Tricoordinated Pd ^{II} Species Accessible? Stability Trends and Mechanistic Consequences. <i>Chemistry - A European Journal</i> , 2008, 14, 8986-8994.	1.7	50
43	Proton-Transfer and H ₂ -Elimination Reactions of Main-Group Hydrides EH ₄ (E = B, Al, Ga) with Alcohols. <i>Inorganic Chemistry</i> , 2006, 45, 3086-3096.	1.9	49
44	Hydroamination of C=C Multiple Bonds with Hydrazine Catalyzed by N-Heterocyclic Carbene-Gold(I) Complexes: Substrate and Ligand Effects. <i>ACS Catalysis</i> , 2015, 5, 815-829.	5.5	49
45	Direct Asymmetric Hydrogenation of <i>N</i> -Methyl and <i>N</i> -Alkyl Imines with an Ir(III)H Catalyst. <i>Journal of the American Chemical Society</i> , 2018, 140, 16967-16970.	6.6	47
46	Chemical and Constitutional Influences in the Self-Assembly of Functional Supramolecular Hydrogen-Bonded Nanoscopic Fibres. <i>Chemistry - A European Journal</i> , 2006, 12, 9161-9175.	1.7	46
47	Mechanistic Comparison of Acid- and Gold(I)-Catalyzed Nucleophilic Addition Reactions to Olefins. <i>Organometallics</i> , 2010, 29, 5919-5926.	1.1	46
48	Mechanistic Studies on the Pd-Catalyzed Vinylation of Aryl Halides with Vinylalkoxysilanes in Water: The Effect of the Solvent and NaOH Promoter. <i>Journal of the American Chemical Society</i> , 2013, 135, 13749-13763.	6.6	46
49	Origin of the Anti-Markovnikov Hydroamination of Alkenes Catalyzed by L ¹ -Au(I) Complexes: Coordination Mode Determines Regioselectivity. <i>ACS Catalysis</i> , 2019, 9, 848-858.	5.5	45
50	A Measureable Equilibrium between Iridium Hydride Alkylidene and Iridium Hydride Alkene Isomers. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 3708-3711.	7.2	44
51	Theoretical Analysis of the Hydrogen-Transfer Reaction to C=N, C=C, and C=C Bonds Catalyzed by Shvo's Ruthenium Complex. <i>Organometallics</i> , 2008, 27, 4854-4863.	1.1	44
52	Gold versus Silver-Catalyzed Intermolecular Hydroaminations of Alkenes and Dienes. <i>Advanced Synthesis and Catalysis</i> , 2011, 353, 3451-3466.	2.1	44
53	Experimental and Theoretical Approaches to the Influence of the Addition of Pyrene to a Series of Pd and Ni NHC-Based Complexes: Catalytic Consequences. <i>Chemistry - A European Journal</i> , 2015, 21, 1578-1588.	1.7	44
54	Formation of a Vinyliminium Palladium Complex by C=C Coupling in Vinylcarbene Palladium Aryl Complexes. <i>Organometallics</i> , 2006, 25, 1293-1297.	1.1	42

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55	Applications of Hybrid DFT/Molecular Mechanics to Homogeneous Catalysis. Structure and Bonding, 2004, , 117-150.	1.0	41
56	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
57	Microsolvation and Encapsulation Effects on Supramolecular Catalysis: C ⁺ C Reductive Elimination inside [Ga ₄ L ₆] ¹²⁺ Metallo cage. Journal of the American Chemical Society, 2019, 141, 13114-13123.	6.6	40
58	Mechanism of the Base-Assisted Displacement of Chloride by Alcohol in Sulfinyl Derivatives. Journal of Organic Chemistry, 2006, 71, 6388-6396.	1.7	39
59	Nature of Cp*MoO ₂ in Water and Intramolecular Proton-Transfer Mechanism by Stopped-Flow Kinetics and Density Functional Theory Calculations. Inorganic Chemistry, 2007, 46, 4103-4113.	1.9	39
60	Internal Alkyne Isomerization to Vinylidene versus Stable η -Alkyne: Theoretical and Experimental Study on the Divergence of Analogous Cp*Ru and TpRu Systems. Organometallics, 2011, 30, 4014-4031.	1.1	36
61	Counteranion and Solvent Assistance in Ruthenium-Mediated Alkyne to Vinylidene Isomerizations. Inorganic Chemistry, 2013, 52, 8919-8932.	1.9	36
62	Different van der Waals radii for organic and inorganic halogen atoms: a significant improvement in IMOMM performance. Theoretical Chemistry Accounts, 1997, 96, 146-150.	0.5	34
63	New chiral tetraaza ligands for the efficient enantioselective addition of dialkylzinc to aromatic aldehydes. Tetrahedron, 2008, 64, 9717-9724.	1.0	34
64	Inner- and Outer-Sphere Hydrogenation Mechanisms: A Computational Perspective. Advances in Inorganic Chemistry, 2010, 62, 231-260.	0.4	34
65	Palladium monophosphine Pd(PPh ₃): is it really accessible in solution?. Chemical Communications, 2014, 50, 661-663.	2.2	34
66	Gold-Catalyzed Cycloadditions Involving Allenes: Mechanistic Insights from Theoretical Studies. Topics in Current Chemistry, 2011, 302, 225-248.	4.0	33
67	The Nature of [PdCl ₂ (C ₂ H ₄)(H ₂ 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.	1.7	31
68	The first stable copper(II) complex containing four sulfide ligands: synthesis and structural characterization of [Pt ₂ (dppe) ₂ (μ -S) ₂] and [Cu{Pt ₂ (dppe) ₂ (μ -S) ₂ } ₂] ²⁺ . Chemical Communications, 1998, , 597-598.	2.2	30
69	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.	3.1	29
70	Ketone Hydrogenation with Iridium Complexes with α -enon N ⁺ H ⁻ Ligands: The Key Role of the Strong Base. ACS Catalysis, 2015, 5, 4368-4376.	5.5	29
71	Proton-Transfer Reactions to Half-Sandwich Ruthenium Trihydride Complexes Bearing Hemilabile P,N Ligands: Experimental and Density Functional Theory Studies ^{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.	1.9	28
72	The Origin of Anti-Markovnikov Regioselectivity in Alkene Hydroamination Reactions Catalyzed by [Rh(DPEphos)] ⁺ . Chemistry - A European Journal, 2016, 22, 9311-9320.	1.7	28

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73	Theoretical Characterization of an Intermediate for the [3 + 2] Cycloaddition Mechanism in the Bis(dihydroxy-quinidine)-3,6-Pyridazine-Osmium Tetroxide-Catalyzed Dihydroxylation of Styrene. <i>Journal of Organic Chemistry</i> , 1997, 62, 7892-7894.	1.7	27
74	Theoretical Investigation of the Selective CC Hydrogenation of Unsaturated Aldehydes Catalyzed by $[RuCl_2(mtppps)_2]$ in Acidic Media. <i>Organometallics</i> , 2006, 25, 862-872.	1.1	27
75	Some critical issues in the application of quantum mechanics/molecular mechanics methods to the study of transition metal complexes. <i>Faraday Discussions</i> , 2003, 124, 429-441.	1.6	26
76	Csp ³ -F bond activation by nucleophilic attack of the {Pt ₂ S ₂ } core assisted by non-covalent interactions. <i>Chemical Communications</i> , 2008, , 3130.	2.2	26
77	Experimental and Computational Studies on the Iridium Activation of Aliphatic and Aromatic C-H Bonds of Alkyl Aryl Ethers and Related Molecules. <i>Chemistry - A European Journal</i> , 2009, 15, 9034-9045.	1.7	26
78	PtII as a proton shuttle during C-H bond activation in the Shilov process. <i>Chemical Communications</i> , 2012, 48, 1979.	2.2	26
79	Synthetic, Mechanistic, and Theoretical Studies on the Generation of Iridium Hydride Alkylidene and Iridium Hydride Alkene Isomers. <i>Chemistry - A European Journal</i> , 2009, 15, 9046-9057.	1.7	25
80	Solution dynamics of agostic interactions in T-shaped Pt(II) complexes from ab initio molecular dynamics simulations. <i>Dalton Transactions</i> , 2013, 42, 12165.	1.6	25
81	Iridium-Catalyzed Isomerization of <i>N</i> -Sulfonyl Aziridines to Allyl Amines. <i>Organic Letters</i> , 2018, 20, 5747-5751.	2.4	25
82	Theoretical and Synthetic Studies on Dihaptoacyl and η^2 -Agostic Acyl Complexes of Molybdenum. <i>Organometallics</i> , 1999, 18, 3294-3305.	1.1	24
83	A QM/MM Study of the Asymmetric Dihydroxylation of Terminal Aliphatic Alkenes with OsO ₄ -(DHQD)2PYDZ: Enantioselectivity as a Function of Chain Length. <i>Chemistry - A European Journal</i> , 2005, 11, 1017-1029.	1.7	24
84	Aromatic C-F activation by complexes containing the {Pt ₂ S ₂ } core via nucleophilic substitution: a combined experimental and theoretical study. <i>Dalton Transactions</i> , 2009, , 5980.	1.6	24
85	Beyond Continuum Solvent Models in Computational Homogeneous Catalysis. <i>Topics in Catalysis</i> , 2022, 65, 118-140.	1.3	24
86	Tripodal halogen bonding iodo-azolium receptors for anion recognition. <i>RSC Advances</i> , 2017, 7, 11253-11258.	1.7	23
87	Breaking an electronically preferred symmetry by steric effects in a series of [Ir(biph)X(QR ₃) ₂] compounds (X=Cl or I, Q=P or As). <i>New Journal of Chemistry</i> , 1998, 22, 1493-1498.	1.4	22
88	Catalysis on the coastline: Theozyme, molecular dynamics, and free energy perturbation analysis of antibody 21D8 catalysis of the decarboxylation of 5-nitro-3-carboxybenzoxazole. <i>Journal of Computational Chemistry</i> , 2003, 24, 98-110.	1.5	22
89	Do Metal...Water Hydrogen Bonds Hold in Solution? Insight from Ab Initio Molecular Dynamics Simulations. <i>ChemPhysChem</i> , 2011, 12, 1666-1668.	1.0	22
90	Theoretical, structural and NMR studies of fluxionality in thiolato-bridged platinum(II)-platinum(IV) dinuclear complexes. <i>Inorganica Chimica Acta</i> , 1997, 265, 89-102.	1.2	20

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91	Theoretical study on intramolecular allene-diene cycloadditions catalyzed by PtCl ₂ and Au(I) complexes. Dalton Transactions, 2011, 40, 11095.	1.6	19
92	A Tetraferrocenyl-Resorcinarene Cavitand as a Redox-Switchable Host of Ammonium Salts. Chemistry - A European Journal, 2015, 21, 10558-10565.	1.7	19
93	Palladium(II) complexes with Pd ₂ S ₂ rings. Synthesis and theoretical characterization of [Pd ₂ (dppe) ₂ (η^4 -S) ₂] and X-ray characterization of [Pd ₃ (dppe) ₃ (η^4 -S) ₂]Cl ₂ . Inorganic Chemistry Communication, 1998, 1, 466-468.	1.8	18
94	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.	2.1	18
95	Reaction Rate Inside the Cavity of [Ga ₄ L ₆] ¹²⁺ Supramolecular Metallocage is Regulated by the Encapsulated Solvent. Chemistry - A European Journal, 2020, 26, 6988-6992.	1.7	18
96	Mechanism of the Rhodium-Catalyzed Asymmetric Isomerization of Allylamines to Enamines. Chemistry - A European Journal, 2008, 14, 3323-3329.	1.7	17
97	Electrostatic Interactions between Substituents as Regioselectivity Control Elements in Diels-Alder Cycloadditions. A DFT Study of Cycloadditions of 1-Methoxy-4-trimethylsiloxy Dienes with Acrylonitrile. Journal of Organic Chemistry, 2002, 67, 7179-7184.	1.7	16
98	Unusual C-H Allylic Activation in the {PtII(cod)} Fragment Bonded to a {Pt ₂ (η^4 -S) ₂ } Core. Organometallics, 2004, 23, 2522-2532.	1.1	16
99	Well-Defined η^2 -Diketiminatocobalt(II) Complexes for Alkene Cyclohydroamination of Primary Amines. ACS Catalysis, 2018, 8, 4446-4451.	5.5	16
100	Catalytic Regioselective Isomerization of 2,2-Disubstituted Oxetanes to Homoallylic Alcohols. Angewandte Chemie - International Edition, 2020, 59, 7521-7527.	7.2	16
101	What Makes a Good (Computed) Energy Profile?. Topics in Organometallic Chemistry, 2020, , 1-38.	0.7	15
102	The Role of Water in the Stereoselective Hydrogenation of 1,2-Diphenylacetylene Catalyzed by the Water-Soluble [RuCl ₂ (mtppps) ₂]. European Journal of Inorganic Chemistry, 2007, 2007, 2879-2889.	1.0	14
103	Comparative Mechanistic Study on the [Au(NHC)] ⁺ -Catalyzed Hydration of Alkynes, Alkenes, and Allenes. Organometallics, 2020, 39, 3469-3479.	1.1	14
104	Aliphatic C-X (X=halogen) bond activation by transition metal complexes containing the {Pt ₂ S ₂ } core: A theoretical study of the reaction mechanism. Inorganica Chimica Acta, 2006, 359, 3736-3744.	1.2	12
105	Theoretical Evaluation of Phosphine Effects in Cross-Coupling Reactions. Catalysis By Metal Complexes, 2011, , 57-84.	0.6	12
106	Mild Iridium-Catalysed Isomerization of Epoxides. Computational Insights and Application to the Synthesis of η^2 -Alkyl Amines. Advanced Synthesis and Catalysis, 2019, 361, 3624-3631.	2.1	12
107	A theoretical evaluation of steric and electronic effects on the structure of [OsO]. Theoretica Chimica Acta, 1996, 94, 67.	0.9	11
108	The role of amide ligands in the stabilization of Pd(II) tricoordinated complexes: is the Pd-NR ₂ bond order single or higher?. Theoretical Chemistry Accounts, 2009, 123, 75-84.	0.5	10

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109	Mechanistic Insights on the Hydration of Terminal and Internal Allenes Catalyzed by [(NHC)Au] ⁺ . <i>Organometallics</i> , 2018, 37, 3543-3551.	1.1	10
110	Computational Analysis on the Pd-Catalyzed C ^α -N Coupling of Ammonia with Aryl Bromides Using a Chelate Phosphine Ligand. <i>Journal of Organic Chemistry</i> , 2021, 86, 4007-4017.	1.7	10
111	Modeling Kinetics and Thermodynamics of Guest Encapsulation into the [M ₄ L ₆] ¹²⁺ Supramolecular Organometallic Cage. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4370-4381.	2.5	10
112	A comparative study of DFT and traditional ab initio methodologies on the OsO ₄ molecule. <i>International Journal of Quantum Chemistry</i> , 2000, 77, 544-551.	1.0	9
113	Origin of the Rate Acceleration in the C ^α -C Reductive Elimination from Pt(IV) η^6 -complex in a [Ga ₄ L ₆] ¹²⁺ Supramolecular Metallocage. <i>Chemistry - A European Journal</i> , 2021, 27, 15973-15980.	1.7	9
114	Diradical versus Concerted Mechanisms for the Dihydroxylation of Protoanemonin by OsO ₄ and OsO ₄ \cdot NH ₃ \cdot . The Effect of the Base in the Reaction. <i>European Journal of Organic Chemistry</i> , 2003, 2003, 833-839.	1.2	8
115	Rearrangement of Tridentate [OSO]-Type Ligands and Migratory Insertion Reaction Mechanisms in Cyclopentadienyl Tantalum Complexes. <i>Organometallics</i> , 2012, 31, 7052-7062.	1.1	8
116	Experimental and Theoretical Studies of the Hydrogenation of $\hat{1},\hat{2}$ -Unsaturated Acids by an 18 <i>e</i> Hydride Carbonylniobocene Complex. <i>Organometallics</i> , 2012, 31, 5177-5184.	1.1	8
117	Counteranion-Dependent Reaction Pathways in the Protonation of Cationic Ruthenium η^6 -Vinylidene Complexes. <i>Organometallics</i> , 2014, 33, 2549-2560.	1.1	8
118	Rim, Side Arms, and Cavity: Three Sites for the Recognition of Anions by Tetraazolium Resorcinarene Cavitands. <i>Chemistry - A European Journal</i> , 2016, 22, 15800-15806.	1.7	8
119	Realistic Simulation of Organometallic Reactivity in Solution by Means of First-Principles Molecular Dynamics. <i>Structure and Bonding</i> , 2015, , 81-106.	1.0	7
120	Mechanistic implications of the enantioselective addition of alkylzinc reagents to aldehydes catalyzed by nickel complexes with $\hat{1},\hat{2}$ -amino amide ligands. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 11125-11136.	1.5	7
121	A Reversible Phase Transition of 2D Coordination Layers by η^6 -H TM $\hat{1},\hat{2}$ -Cu(II) Interactions in a Coordination Polymer. <i>Molecules</i> , 2019, 24, 3204.	1.7	7
122	GARLEEK: Adding an extra flavor to ONIOM. <i>Journal of Computational Chemistry</i> , 2019, 40, 381-386.	1.5	6
123	QM/QM study of the coverage effects on the adsorption of amino-cyclopentene at the Si(100) surface. <i>Journal of Computational Chemistry</i> , 2006, 27, 1892-1897.	1.5	4
124	Mechanism of Palladium-Catalyzed Cross-Coupling Reactions. , 0, , 109-130.		4
125	Basis set influence on the ab initio description of the dihydrogen complex [Os(PH ₃) ₂ Cl(CO)H(H ₂)] ₁ . <i>Computational and Theoretical Chemistry</i> , 1996, 371, 59-68.	1.5	3
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