Gregori Ujaque

List of Publications by Year
in descending order

133	6,751	50170	69108
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.	1.3	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.	1.7	10
3	Origin of the Rate Acceleration in the Câˆ’C Reductive Elimination from Pt(IV)â€complex in a [Ga₄L₆]^{12âˆ’} Supramolecular Metallocage. Chemistry - A European Journal, 2021, 27, 15973-15980.	1.7	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.	2.5	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)]⁺-Catalyzed Hydration of Alkynes, Alkenes, and Allenes. Organometallics, 2020, 39, 3469-3479.	1.1	14
7	Catalytic Regioselective Isomerization of 2,2â€Disubstituted Oxetanes to Homoallylic Alcohols. Angewandte Chemie, 2020, 132, 7591-7597.	1.6	1
8	Reaction Rate Inside the Cavity of [Ga₄L₆]^{12âˆ’} Supramolecular Metallocage is Regulated by the Encapsulated Solvent. Chemistry - A European Journal, 2020, 26, 6988-6992.	1.7	18
9	Catalytic Regioselective Isomerization of 2,2â€Disubstituted Oxetanes to Homoallylic Alcohols. Angewandte Chemie - International Edition, 2020, 59, 7521-7527.	7.2	16
10	Skeletal diversity in Pt- and Au-catalyzed annulations of allenedienes: dissecting unconventional mechanistic pathways. Chemical Science, 2020, 11, 4209-4220.	3.7	1
11	A resorcinarene-based tetrabenzoimidazolylidene complex of rhodium. Dalton Transactions, 2020, 49, 3181-3186.	1.6	2
12	Microsolvation and Encapsulation Effects on Supramolecular Catalysis: Câ€“C Reductive Elimination inside [Ga₄L₆]^{12â€“} Metallocage. Journal of the American Chemical Society, 2019, 141, 13114-13123.	6.6	40
13	A Reversible Phase Transition of 2D Coordination Layers by Bâ€“Hâˆ™âˆ™âˆ™Cu(II) Interactions in a Coordination Polymer. Molecules, 2019, 24, 3204.	1.7	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.	2.1	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.	5.5	45
16	GARLEEK: Adding an extra flavor to ONIOM. Journal of Computational Chemistry, 2019, 40, 381-386.	1.5	6
17	Well-Defined Î²-Diketiminatocobalt(II) Complexes for Alkene Cyclohydroamination of Primary Amines. ACS Catalysis, 2018, 8, 4446-4451.	5.5	16
18	Calculation of Reaction Free Energies in Solution: A Comparison of Current Approaches. Journal of Physical Chemistry A, 2018, 122, 1392-1399.	1.1	101

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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.	6.6	47
20	Iridium-Catalyzed Isomerization of N-Sulfonyl Aziridines to Allyl Amines. Organic Letters, 2018, 20, 5747-5751.	2.4	25
21	Mechanistic Insights on the Hydration of Terminal and Internal Allenes Catalyzed by [(NHC)Au]⁺. Organometallics, 2018, 37, 3543-3551.	1.1	10
22	Tripodal halogen bonding iodo-azolium receptors for anion recognition. RSC Advances, 2017, 7, 11253-11258.	1.7	23
23	The Origin of Antiâ€Markovnikov Regioselectivity in Alkene Hydroamination Reactions Catalyzed by [Rh(DPEphos)]⁺. Chemistry - A European Journal, 2016, 22, 9311-9320.	1.7	28
24	Acid Activation in Phenyliodine Dicarboxylates: Direct Observation, Structures, and Implications. Journal of the American Chemical Society, 2016, 138, 12747-12750.	6.6	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.	1.7	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.	1.5	7
27	First-Principles Molecular Dynamics Studies of Organometallic Complexes and Homogeneous Catalytic Processes. Accounts of Chemical Research, 2016, 49, 1271-1278.	7.6	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.	1.7	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.	5.5	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.	5.5	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.	1.7	44
33	Palladium monophosphine Pd(PPh₃): is it really accessible in solution?. Chemical Communications, 2014, 50, 661-663.	2.2	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.	18.7	65
35	Counteranion-Dependent Reaction Pathways in the Protonation of Cationic Rutheniumâ€“Vinylidene Complexes. Organometallics, 2014, 33, 2549-2560.	1.1	8
36	The Transmetalation Process in Suzukiâ€“Miyaura Reactions: Calculations Indicate Lower Barrier via Boronate Intermediate. ChemCatChem, 2014, 6, 3132-3138.	1.8	68

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37	Computational Perspective on Pd-Catalyzed Câ€“C Cross-Coupling Reaction Mechanisms. Accounts of Chemical Research, 2013, 46, 2626-2634.	7.6	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.	6.6	46
39	Counteranion and Solvent Assistance in Ruthenium-Mediated Alkyne to Vinylidene Isomerizations. Inorganic Chemistry, 2013, 52, 8919-8932.	1.9	36
40	Solution dynamics of agostic interactions in T-shaped Pt(ii) complexes from ab initio molecular dynamics simulations. Dalton Transactions, 2013, 42, 12165.	1.6	25
41	Unraveling the Pathway of Gold(I)-Catalyzed Olefin Hydrogenation: An Ionic Mechanism. Journal of the American Chemical Society, 2013, 135, 1295-1305.	6.6	53
42	Mechanistic Intricacies of Goldâ€Catalyzed Intermolecular Cycloadditions between Allenamides and Dienes. Chemistry - A European Journal, 2013, 19, 15248-15260.	1.7	57
43	Mechanistic Exploration of the Pd-Catalyzed Copper-Free Sonogashira Reaction. ACS Catalysis, 2012, 2, 135-144.	5.5	103
44	PtII as a proton shuttle during Câ€“H bond activation in the Shilov process. Chemical Communications, 2012, 48, 1979.	2.2	26
45	Rearrangement of Tridentate [OSO]-Type Ligands and Migratory Insertion Reaction Mechanisms in Cyclopentadienyl Tantalum Complexes. Organometallics, 2012, 31, 7052-7062.	1.1	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.	1.1	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.	0.2	1
48	The Nature of [PdCl₂(C₂H₄)(H₂O)] 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
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.	1.7	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.	1.7	53
51	Theoretical study on intramolecular allene-diene cycloadditions catalyzed by PtCl2 and Au(i) complexes. Dalton Transactions, 2011, 40, 11095.	1.6	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.	1.1	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 ZnMe₂andtrans-[PdMeCl(PMePh₂)₂]. Journal of the American Chemical Society, 2011, 133, 13519-13526.	6.6	69

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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.	0.5	67
57	Gold versus Silverâ€Catalyzed Intermolecular Hydroaminations of Alkenes and Dienes. Advanced Synthesis and Catalysis, 2011, 353, 3451-3466.	2.1	44
58	Do Metalâ‹…â‹…â‹…Water Hydrogen Bonds Hold in Solution? Insight from Ab Initio Molecular Dynamics Simulations. ChemPhysChem, 2011, 12, 1666-1668.	1.0	22
59	Hydroamination of Alkynes with Ammonia: Unforeseen Role of the Gold(I) Catalyst. Angewandte Chemie - International Edition, 2011, 50, 11147-11151.	7.2	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.	1.7	55
61	Palladium Round Trip in the Negishi Coupling of transâ€[PdMeCl(PMePh₂)₂] with ZnMeCl: An Experimental and DFT Study of the Transmetalation Step. Chemistry - A European Journal, 2010, 16, 8596-8599.	1.7	76
62	Inner- and Outer-Sphere Hydrogenation Mechanisms: A Computational Perspective. Advances in Inorganic Chemistry, 2010, 62, 231-260.	0.4	34
63	Mechanistic Comparison of Acid- and Gold(I)-Catalyzed Nucleophilic Addition Reactions to Olefins. Organometallics, 2010, 29, 5919-5926.	1.1	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.	1.9	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.	1.1	67
66	Goldâ€Catalyzed [4C+3C] Intramolecular Cycloaddition of Allenedienes: Synthetic Potential and Mechanistic Implications. Chemistry - A European Journal, 2009, 15, 3336-3339.	1.7	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.	1.7	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.	1.7	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.	0.5	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 sp³Carbons in Î±-Bromo Sulfoxide Systems Fast and Stereoselective? A DFT Study on the Mechanism. Journal of Organic Chemistry, 2009, 74, 4049-4054.	1.7	54
72	Gold(I)-Catalyzed Intermolecular Oxyarylation of Alkynes: Unexpected Regiochemistry in the Alkylation of Arenes. Organic Letters, 2009, 11, 4906-4909.	2.4	148

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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.	6.6	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.	1.6	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.	6.6	178
76	Mechanism of the Rhodiumâ€Catalyzed Asymmetric Isomerization of Allylamines to Enamines. Chemistry - A European Journal, 2008, 14, 3323-3329.	1.7	17
77	When Are Tricoordinated Pd^{II}Species Accessible? Stability Trends and Mechanistic Consequences. Chemistry - A European Journal, 2008, 14, 8986-8994.	1.7	50
78	New chiral tetraaza ligands for the efficient enantioselective addition of dialkylzinc to aromatic aldehydes. Tetrahedron, 2008, 64, 9717-9724.	1.0	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.	3.1	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.	6.6	197
81	Csp3â€“F bond activation by nucleophilic attack of the {Pt2S2} core assisted by non-covalent interactions. Chemical Communications, 2008, , 3130.	2.2	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.	1.1	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, .	1.1	2
84	Hydrogen Transfer to Ketones Catalyzed by Shvo's Ruthenium Hydride Complex:â€‰ A Mechanistic Insight. Organometallics, 2007, 26, 4135-4144.	1.1	130
85	Mechanism of Formation of Silver N-Heterocyclic Carbenes Using Silver Oxide:â€‰ A Theoretical Study. Organometallics, 2007, 26, 6170-6183.	1.1	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.	1.9	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.	2.1	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.	1.0	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.	1.9	49
90	Formation of a Vinyliminium Palladium Complex by Câˆ’C Coupling in Vinylcarbene Palladium Aryl Complexes. Organometallics, 2006, 25, 1293-1297.	1.1	42

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91	A DFT Study of the Full Catalytic Cycle of the Suzukiâˆ'Miyaura Cross-Coupling on a Model System. Organometallics, 2006, 25, 3647-3658.	1.1	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.	6.6	100
93	Single-Site Homogeneous and Heterogeneized Gold(III) Hydrogenation Catalysts:Â Mechanistic Implications. Journal of the American Chemical Society, 2006, 128, 4756-4765.	6.6	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.	1.1	52
95	Mechanism of the Base-Assisted Displacement of Chloride by Alcohol in Sulfinyl Derivatives. Journal of Organic Chemistry, 2006, 71, 6388-6396.	1.7	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.	1.1	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.	1.1	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.	1.2	12
99	Computational study of the transmetalation process in the Suzukiâ€"Miyaura cross-coupling of aryls. Journal of Organometallic Chemistry, 2006, 691, 4459-4466.	0.8	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.	1.7	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.	1.5	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.	1.7	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.	6.6	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.	6.6	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.	6.6	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.	7.2	44
108	A computational study on the acceleration of the Prins reaction by indium trichloride. Comptes Rendus Chimie, 2004, 7, 885-893.	0.2	1

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109	Unusual Câˆ’H Allylic Activation in the {PtII(cod)} Fragment Bonded to a {Pt2(Î¼-S)2} Core. Organometallics, 2004, 23, 2522-2532.	1.1	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.	1.5	22
111	Diradical versus Concerted Mechanisms for the Dihydroxylation of Protoanemonin by OsO4 and OsO4âˆ’NH3 âˆ’ The Effect of the Base in the Reaction. European Journal of Organic Chemistry, 2003, 2003, 833-839.	1.2	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.	1.6	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.	1.1	52
114	Electrostatic Interactions between Substituents as Regioselectivity Control Elements in Dielsâˆ’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
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.	1.7	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.	1.0	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.	1.7	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.	6.6	94
119	Theoretical and Synthetic Studies on Dihaptoacyl and Î²-Agostic Acyl Complexes of Molybdenum. Organometallics, 1999, 18, 3294-3305.	1.1	24
120	Edge-Sharing Binuclear d8 Complexes with XR Bridges: Theoretical and Structural Database Study of their Molecular Conformation. , 1999, 5, 1391.		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.	1.8	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.	2.2	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.	1.4	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.	6.6	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.	1.9	126
126	Theoretical Characterization of an Intermediate for the [3 + 2] Cycloaddition Mechanism in the Bis(dihydroxy- quinidine)âˆ’3,6-PyridazineÂ·Osmium Tetroxide-Catalyzed Dihydroxylation of Styrene. Journal of Organic Chemistry, 1997, 62, 7892-7894.	1.7	27

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127	Theoretical, structural and NMR studies of fluxionality in thiolato-bridged platinum(II)-platinum(IV) dinuclear complexes. Inorganica Chimica Acta, 1997, 265, 89-102.	1.2	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.	0.5	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.	6.6	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	0.9	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.	0.9	11
133	Mechanism of Palladium-Catalyzed Cross-Coupling Reactions. , 0, , 109-130.		4