Agusti Lledos

List of Publications by Year
in descending order

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374	13,379	26610 56	54882 84
papers	citations	h-index	g-index

405	405	405	8822
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Transition Metal Polyhydrides:â€‰ From Qualitative Ideas to Reliable Computational Studies. Chemical Reviews, 2000, 100, 601-636.	23.0	341
2	Computational Perspective on Pd-Catalyzed Câ€“C Cross-Coupling Reaction Mechanisms. Accounts of Chemical Research, 2013, 46, 2626-2634.	7.6	306
3	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
4	The Reaction Mechanism of the Hydroamination of Alkenes Catalyzed by Gold(I)â^'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
5	Elongated dihydrogen complexes: what remains of the Hâ€“H Bond?. Chemical Society Reviews, 2004, 33, 175-182.	18.7	178
6	Gold(I)-Catalyzed Intermolecular Oxyarylation of Alkynes: Unexpected Regiochemistry in the Alkylation of Arenes. Organic Letters, 2009, 11, 4906-4909.	2.4	148
7	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
8	Goldâ€Catalyzed [4C+3C] Intramolecular Cycloaddition of Allenedienes: Synthetic Potential and Mechanistic Implications. Chemistry - A European Journal, 2009, 15, 3336-3339.	1.7	138
9	Hydrogen Transfer to Ketones Catalyzed by Shvo's Ruthenium Hydride Complex:â€‰ A Mechanistic Insight. Organometallics, 2007, 26, 4135-4144.	1.1	130
10	Acid Activation in Phenyliodine Dicarboxylates: Direct Observation, Structures, and Implications. Journal of the American Chemical Society, 2016, 138, 12747-12750.	6.6	127
11	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
12	Analysis of solvent effects on the Menshutkin reaction. Journal of the American Chemical Society, 1991, 113, 2873-2879.	6.6	123
13	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
14	Ligand Macrocycle Structural Effects on Copperâ^'Dioxygen Reactivity. Inorganic Chemistry, 2000, 39, 4059-4072.	1.9	116
15	Breaking Câ€“F Bonds via Nucleophilic Attack of Coordinated Ligands: Transformations from Câ€“F to Câ€“X Bonds (X= H, N, O, S). Organometallics, 2012, 31, 1245-1256.	1.1	110
16	Self-Assembly of Mercaptaneâ^'Metallacarborane Complexes by an Unconventional Cooperative Effect:Â A Câ^'HÂ·Â·Â·Sâ^'HÂ·Â·Â·Hâ^'B Hydrogen/Dihydrogen Bond Interaction. Journal of the American Chemical Society, 2005, 127, 15976-15982.	6.6	105
17	Mechanistic Exploration of the Pd-Catalyzed Copper-Free Sonogashira Reaction. ACS Catalysis, 2012, 2, 135-144.	5.5	103
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	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
20	Protonation of transition-metal hydrides: a not so simple process. Chemical Society Reviews, 2009, 38, 957.	18.7	99
21	An Artificial Heme Enzyme for Cyclopropanation Reactions. Angewandte Chemie - International Edition, 2018, 57, 7785-7789.	7.2	98
22	Câ^'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
23	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
24	Highly Enantioselective Electrophilic Amination and Michael Addition of Cyclic Î²-Ketoesters Induced by Lanthanides and (S,S)-ip-pybox:Â The MechanismâŠ¥. Journal of Organic Chemistry, 2007, 72, 2077-2087.	1.7	94
25	First X-ray Characterization and Theoretical Study of Ï€-Alkyne, Alkynyl-Hydride, and Vinylidene Isomers for the Same Transition Metal Fragment [Cp*Ru(PEt3)2]+. Journal of the American Chemical Society, 2003, 125, 3311-3321.	6.6	90
26	Introducing Copper as Catalyst for Oxidative Alkane Dehydrogenation. Journal of the American Chemical Society, 2013, 135, 3887-3896.	6.6	89
27	Reactions of a Hexahydrideâ^'Osmium Complex with Aromatic Ketones:Â Câ^'H Activation versus Câ^'F ActivationÂ§. Organometallics, 2001, 20, 442-452.	1.1	88
28	Bond-stretch isomerism in transition-metal complexes. Journal of the American Chemical Society, 1988, 110, 4506-4516.	6.6	85
29	A Computational Study of the Olefin Epoxidation Mechanism Catalyzed by Cyclopentadienyloxidomolybdenum(VI) Complexes. Chemistry - A European Journal, 2010, 16, 2147-2158.	1.7	84
30	Synthesis and Characterization of OsX{NHC(Ph)C6H4}H2(PiPr3)2(X = H, Cl, Br, I):Â Nature of the H2Unit and Its Behavior in Solution. Organometallics, 1998, 17, 4065-4076.	1.1	81
31	Synthesis and Properties of Compressed Dihydride Complexes of Iridium:Â Theoretical and Spectroscopic Investigations. Journal of the American Chemical Society, 2004, 126, 8813-8822.	6.6	79
32	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
33	Structural, Kinetic, and Docking Studies of Artificial Imine Reductases Based on Biotinâ€“Streptavidin Technology: An Induced Lock-and-Key Hypothesis. Journal of the American Chemical Society, 2014, 136, 15676-15683.	6.6	75
34	A Density Functional Study on the Effect of the Trans Axial Ligand of Cobalamin on the Homolytic Cleavage of the Coâ^'C Bond. Journal of Physical Chemistry B, 2001, 105, 7564-7571.	1.2	74
35	Influence of Media and Homoconjugate Pairing on Transition Metal Hydride Protonation. An IR and DFT Study on Proton Transfer to CpRuH(CO)(PCy3). Journal of the American Chemical Society, 2003, 125, 7715-7725.	6.6	74
36	Incorporation of Manganese Complexes into Xylanase: New Artificial Metalloenzymes for Enantioselective Epoxidation. ChemBioChem, 2012, 13, 240-251.	1.3	72

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37	Ab initio study of the hydration of carbon dioxide by carbonic anhydrase. A comparison between the Lipscomb and Lindskog mechanisms. Journal of the American Chemical Society, 1992, 114, 869-877.	6.6	70
38	A Quantum Mechanics/Molecular Mechanics Study of the Highly Enantioselective Addition of Diethylzinc to Benzaldehyde Promoted by (R)-2-Piperidino-1,1,2-triphenylethanol. Journal of Organic Chemistry, 2000, 65, 7303-7309.	1.7	70
39	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
40	Design of an enantioselective artificial metallo-hydratase enzyme containing an unnatural metal-binding amino acid. Chemical Science, 2017, 8, 7228-7235.	3.7	69
41	Experimental and Theoretical Studies of Bonding and Oxidative Addition of Germanes and Silanes, EH4-nPhn(E = Si, Ge;n= 0â^'3), to Mo(CO)(diphosphine)2. The First Structurally Characterized Germane Ïƒ Complex. Organometallics, 2003, 22, 5307-5323.	1.1	68
42	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
43	The Transmetalation Process in Suzukiâ€“Miyaura Reactions: Calculations Indicate Lower Barrier via Boronate Intermediate. ChemCatChem, 2014, 6, 3132-3138.	1.8	68
44	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
45	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
46	Hydroamination of Alkynes with Ammonia: Unforeseen Role of the Gold(I) Catalyst. Angewandte Chemie - International Edition, 2011, 50, 11147-11151.	7.2	67
47	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
48	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
49	Elongated Dihydrogen Complexes:Â A Combined Electronic DFT + Nuclear Dynamics Study of the [Ru(HÂ·Â·Â·H)(C5H5)(H2PCH2PH2)]+Complex. Journal of the American Chemical Society, 1997, 119, 9840-9847.	6.6	64
50	First-Principles Molecular Dynamics Studies of Organometallic Complexes and Homogeneous Catalytic Processes. Accounts of Chemical Research, 2016, 49, 1271-1278.	7.6	64
51	Theoretical Study of the Hydrogen Exchange Coupling in the Metallocene Trihydride Complexes [(C5H5)2MH3]n+(M = Mo, W,n= 1; M = Nb, Ta,n= 0). Journal of the American Chemical Society, 1996, 118, 4617-4621.	6.6	60
52	Experimental and Computational Studies of Hydrogen Bonding and Proton Transfer to [Cp*Fe(dppe)H]. Chemistry - A European Journal, 2005, 11, 873-888.	1.7	58
53	Mechanism of Formation of Silver N-Heterocyclic Carbenes Using Silver Oxide:â€‰ A Theoretical Study. Organometallics, 2007, 26, 6170-6183.	1.1	58
54	Hydride Exchange Processes in the Coordination Sphere of Transition Metal Complexes:â€‰ The OsH3(BH4)(PR3)2 System. Journal of the American Chemical Society, 1996, 118, 8388-8394.	6.6	57

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55	Synthesis and Spectroscopic Properties of Dihydrogen Isocyanide Niobocene [Nb(Î·5-C5H4SiMe3)2(Î·2-H2)(CNR)]+Complexes. Experimental and Theoretical Study of the Blocked Rotation of a Coordinated Dihydrogen. Journal of the American Chemical Society, 1997, 119, 6107-6114.	6.6	57
56	Density Functional Study on the Mechanism of the Vanadium-Catalyzed Oxidation of Sulfides by Hydrogen Peroxide. Journal of Organic Chemistry, 2003, 68, 4265-4274.	1.7	57
57	Water-Assisted Hâ‹¯H Bond Splitting Mediated by [CpRu(PTA)2Cl] (PTA=1,3,5-triaza-7-phosphaadamantane). A DFT Analysis. Organometallics, 2007, 26, 3289-3296.	1.1	57
58	Mechanistic Intricacies of Goldâ€Catalyzed Intermolecular Cycloadditions between Allenamides and Dienes. Chemistry - A European Journal, 2013, 19, 15248-15260.	1.7	57
59	Synthesis, Structure, and Catalytic Applications for ortho- and meta-Carboranyl Based NBN Pincer-Pd Complexes. Inorganic Chemistry, 2014, 53, 9284-9295.	1.9	57
60	Theoretical study of reaction mechanisms for the ketonization of vinyl alcohol in gas phase and aqueous solution. Theoretica Chimica Acta, 1987, 72, 175-195.	0.9	56
61	Dynamic Behavior in Solution of the Transâ€Hydridodihydrogen Complex [OsHCl(n²â€H₂)(CO)(PiPr₃)₂]: Ab Initio and NMR Studies. Chemistry - A European Journal, 1996, 2, 815-825.	1.7	56
62	Lactam/lactim tautomeric interconversion mechanism of 2-pyridone in aqueous solution. Tetrahedron Letters, 1981, 22, 775-778.	0.7	55
63	Bonding in Elongated Dihydrogen Complexes. Theoretical Analysis of the Electron Density in [MLn(HÂ·Â·Â·H)] Species. Organometallics, 1996, 15, 2947-2953.	1.1	55
64	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
65	Imidazole Based Ruthenium(IV) Complexes as Highly Efficient Bifunctional Catalysts for the Redox Isomerization of Allylic Alcohols in Aqueous Medium: Water as Cooperating Ligand. ACS Catalysis, 2012, 2, 2087-2099.	5.5	55
66	True and masked three-coordinate T-shaped platinum(II) intermediates. Beilstein Journal of Organic Chemistry, 2013, 9, 1352-1382.	1.3	55
67	Two- and Four-Electron Alkyne Ligands in Osmiumâ‹¯Cyclopentadienyl Chemistry:Â Consequences of the Ï€âŠ¥â†’M Interaction. Organometallics, 2002, 21, 305-314.	1.1	54
68	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
69	Prediction of the interaction of metallic moieties with proteins: An update for proteinâ€ligand docking techniques. Journal of Computational Chemistry, 2018, 39, 42-51.	1.5	54
70	Concerted and Stepwise Mechanisms in Metalâ€Free and Metalâ€Assisted [4+3] Cycloadditions Involving Allyl Cations. Chemistry - A European Journal, 2010, 16, 12147-12157.	1.7	53
71	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
72	Oxidative Addition of Group 14 Element Hydrido Compounds to OsH2(Î·2-CH2CHEt)(CO)(PiPr3)2:Â Synthesis and Characterization of the First Trihydridoâ‹¯Silyl, Trihydridoâ‹¯Germyl, and Trihydridoâ‹¯Stannyl Derivatives of Osmium(IV). Inorganic Chemistry, 1996, 35, 1250-1256.	1.9	52

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73	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
74	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
75	Molecular hydrogen complexes with a hydride ligand. An ab initio study on the iron hydride, [Fe(PR3)4H(H2)]+, system. Journal of the American Chemical Society, 1991, 113, 2879-2884.	6.6	51
76	Crucial Role of Anions on the Deprotonation of the Cationic Dihydrogen Complex trans-[FeH(Î·2-H2)(dppe)2]+. Journal of the American Chemical Society, 2007, 129, 6608-6618.	6.6	51
77	Coordination and Rupture of Methyl C(sp³)â^'H Bonds in Osmiumâ^'Polyhydride Complexes with Î´ Agostic Interaction. Organometallics, 2007, 26, 5140-5152.	1.1	51
78	Toward the Computational Design of Artificial Metalloenzymes: From Proteinâ€“Ligand Docking to Multiscale Approaches. ACS Catalysis, 2015, 5, 2469-2480.	5.5	51
79	Diverse Evolution of [{Ph2P(CH2)nPPh2}Pt(Î¼-S)2Pt{Ph2P(CH2)nPPh2}] (n = 2, 3) Metalloligands in CH2Cl2. Inorganic Chemistry, 2002, 41, 3218-3229.	1.9	50
80	First Investigation of Non-Classical Dihydrogen Bonding between an Early Transition-Metal Hydride and Alcohols: IR, NMR, and DFT Approach. Chemistry - A European Journal, 2004, 10, 661-671.	1.7	50
81	When Are Tricoordinated Pd^{II}Species Accessible? Stability Trends and Mechanistic Consequences. Chemistry - A European Journal, 2008, 14, 8986-8994.	1.7	50
82	Acidâ€“Base Interaction between Transitionâ€Metal Hydrides: Dihydrogen Bonding and Dihydrogen Evolution. Angewandte Chemie - International Edition, 2011, 50, 1367-1370.	7.2	50
83	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
84	Palladium Complexes of a Phosphorus Ylide with Two Stabilizing Groups:Â Synthesis, Structure, and DFT Study of the Bonding Modesâ€. Inorganic Chemistry, 2006, 45, 6803-6815.	1.9	49
85	Cobalt-Catalyzed Vinylation of Aromatic Halides Using Î²-Halostyrene: Experimental and DFT Studies. Journal of Organic Chemistry, 2012, 77, 5056-5062.	1.7	49
86	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
87	Structure and Dynamics of LRhâ€œH4â€•(L = Cp, Tp) Systems. A Theoretical Study. Organometallics, 1997, 16, 3805-3814.	1.1	48
88	Density Functional Study on the Effect of the trans Axial Ligand ofB12Cofactors on the Heterolytic Cleavage of the Coâ^'C Bond. Journal of Physical Chemistry B, 2003, 107, 306-315.	1.2	48
89	Influence of the Cis Ligand on the Hâ^'H Separation and the Rotation Barrier of the Dihydrogen in Osmium-Elongated Dihydrogen Complexes Containing an Ortho-Metalated Ketoneâ€. Organometallics, 2004, 23, 3008-3015.	1.1	48
90	Tuning Nâ€Heterocyclic Carbenes in Tâ€Shaped Pt^{II} Complexes for Intermolecular Cï£¿H Bond Activation of Arenes. Angewandte Chemie - International Edition, 2012, 51, 3936-3939.	7.2	48

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91	NHâ€Heterocyclic Aryliodonium Salts and their Selective Conversion into N1â€Arylâ€5â€iodoimidazoles. Angewandte Chemie - International Edition, 2016, 55, 7152-7156.	7.2	48
92	Intramolecular atom exchange between molecular hydrogen and hydride ligands in cis-[Fe(PR3)4H(H2)]+ complexes. An ab initio theoretical study. Journal of the American Chemical Society, 1992, 114, 2922-2928.	6.6	47
93	Hinge Distortion in Platinum(II) Dimers with a Pt2S2Ring. Anab InitioMolecular Orbital Study. Inorganic Chemistry, 1996, 35, 490-497.	1.9	47
94	Linear Mâ‰¡Eâ€”Me Versus Bent Mâ€”Eâ€”Me: Bonding Analysis in Heavier Metal-ylidyne Complexes [(Cp)(CO)₂Mâ‰¡EMe] and Metallo-ylidenes [(Cp)(CO)₃Mâ•EMe] (M = Cr, Mo, W; E =) TjETQq0 0 0 rgBT /O	47	
95	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
96	Quantum Mechanical Hydrogen Exchange Coupling in [(C5H5)Ir(L)H3]+ Complexes (L = PH3, CO). A Combined ab Initio/Tunneling Dynamics Study. Journal of the American Chemical Society, 1995, 117, 1069-1075.	6.6	46
97	Preparation and Characterization of Osmiumâ•Stannyl Polyhydrides:Â d4â•d2Oxidative Addition of Neutral Molecules in a Late Transition Metal. Organometallics, 2003, 22, 2087-2096.	1.1	46
98	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
99	Mechanistic Comparison of Acid- and Gold(I)-Catalyzed Nucleophilic Addition Reactions to Olefins. Organometallics, 2010, 29, 5919-5926.	1.1	46
100	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
101	Preparation and Spectroscopic and Theoretical Characterization of the Tetrahydroborate Complex OsH3(.eta.2-H2BH2)(P-i-Pr3)2. Inorganic Chemistry, 1994, 33, 3609-3611.	1.9	45
102	Effect of the Spinning Motion of the Dihydrogen Ligand on the Properties of an Elongated Dihydrogen Complex. A Theoretical Study of the trans-[Os(HÂ·Â·Â·H)Cl(H2PCH2CH2PH2)2]+ Complex. Journal of the American Chemical Society, 1998, 120, 8168-8176.	6.6	45
103	Extending The Reaction Landscape of the {Pt(Î¼â€S) 2 Pt} Core: From Metal Centers to Nonâ€Metallic Electrophiles. European Journal of Inorganic Chemistry, 2004, 2004, 3585-3599.	1.0	45
104	Basic ancillary ligands promote Oâ€“O bond formation in iridium-catalyzed water oxidation: A DFT study. Dalton Transactions, 2011, 40, 11241.	1.6	45
105	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
106	A Measureable Equilibrium between Iridium Hydride Alkylidene and Iridium Hydride Alkene Isomers. Angewandte Chemie - International Edition, 2004, 43, 3708-3711.	7.2	44
107	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
108	Selective Bâ€“H versus Nâ€“H Bond Activation in Ammonia Borane by [Ir(dppm)₂]OTf. European Journal of Inorganic Chemistry, 2009, 2009, 3055-3059.	1.0	44

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109	Gold versus Silverâ€Catalyzed Intermolecular Hydroaminations of Alkenes and Dienes. Advanced Synthesis and Catalysis, 2011, 353, 3451-3466.	2.1	44
110	Selective Catalytic Deuterium Labeling of Alcohols during a Transfer Hydrogenation Process of Ketones Using D2O as the Only Deuterium Source. Theoretical and Experimental Demonstration of a Ruâ€“H/D+Exchange as the Key Step. ACS Catalysis, 2014, 4, 1040-1053.	5.5	44
111	Synthesis and Spectroscopic and Theoretical Characterization of the Elongated Dihydrogen Complex OsCl2(Î·2-H2)(NHCPh2)(PiPr3)2. Inorganic Chemistry, 1998, 37, 5033-5035.	1.9	43
112	Coordination Modes and Hydride Exchange Dynamics in Transition Metal Tetrahydroborate Complexes. , 2007, , 149-202.		43
113	Theoretical study of the addition of hydrogen halides to olefins: reaction of dimeric hydrogen fluoride with ethylene. Journal of the American Chemical Society, 1986, 108, 923-928.	6.6	42
114	AM1 study of hydrogen bonded complexes of water. Computational and Theoretical Chemistry, 1989, 187, 55-68.	1.5	42
115	Analysis of the gas-phase addition of water to formaldehyde: A semiempirical andab initiostudy of bifunctional catalysis by H2O. Journal of Computational Chemistry, 1992, 13, 1037-1046.	1.5	42
116	The use of localised orbitals for the bonding and mechanistic analysis of organometallic compounds. Dalton Transactions, 2014, 43, 11145.	1.6	42
117	Selective Cyclopalladation of R3PNCH2Aryl Iminophosphoranes. Experimental and Computational Study. Inorganic Chemistry, 2007, 46, 10133-10142.	1.9	41
118	Regioselective Ortho Palladation of Stabilized Iminophosphoranes in Exo Positions: Scope, Limitations, and Mechanistic Insights. Organometallics, 2008, 27, 2929-2936.	1.1	41
119	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
120	Elucidation of Binding Site and Chiral Specificity of Oxidovanadium Drugs with Lysozyme through Theoretical Calculations. Inorganic Chemistry, 2017, 56, 12938-12951.	1.9	40
121	Theoretical modeling of the heme group with a hybrid QM/MM method. Journal of Computational Chemistry, 2000, 21, 282-294.	1.5	39
122	The Effect of the â€œInertâ€•Counteranions in the Deprotonation of the Dihydrogen Complextrans-[FeH(Î·2-H2)(dppe)2]+:Â Kinetic and Theoretical Studies. Journal of the American Chemical Society, 2004, 126, 2320-2321.	6.6	39
123	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
124	The Kubas Complex Revisited. A Theoretical Study of Dihydrogen Addition and Structure of the Dihydride Form. Organometallics, 1998, 17, 190-195.	1.1	38
125	Thermally Activated Site Exchange and Quantum Exchange Coupling Processes in Unsymmetrical Trihydride Osmium Compounds. Inorganic Chemistry, 1999, 38, 1814-1824.	1.9	38
126	The Evolution of[{Ph2P(CH2)nPPh2}Pt(Î¼-S)2Pt{Ph2P(CH2)nPPh2}] (n=2, 3) Metalloligands in Protic Acids: A Cascade of Sequential Reactions. Chemistry - A European Journal, 2003, 9, 5023-5035.	1.7	38

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127	Ruthenium‚€Catalyzed Oxidative Coupling of Primary Amines with Internal Alkynes through Cï£¿H Bond Activation: Scope and Mechanistic Studies. Chemistry - A European Journal, 2015, 21, 8626-8636.	1.7	38
128	Electric fields acting as catalysts in chemical reactions. An ab initio study of the walden inversion reaction. Chemical Physics Letters, 1988, 153, 82-86.	1.2	37
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