

# Agusti Lledos

## List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Transition Metal Polyhydrides: From Qualitative Ideas to Reliable Computational Studies. <i>Chemical Reviews</i> , 2000, 100, 601-636.	23.0	341
2	Computational Perspective on Pd-Catalyzed C-C Cross-Coupling Reaction Mechanisms. <i>Accounts of Chemical Research</i> , 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. <i>Journal of the American Chemical Society</i> , 2009, 131, 13020-13030.	6.6	258
4	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
5	Elongated dihydrogen complexes: what remains of the H-H Bond?. <i>Chemical Society Reviews</i> , 2004, 33, 175-182.	18.7	178
6	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
7	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
8	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
9	Hydrogen Transfer to Ketones Catalyzed by Shvo's Ruthenium Hydride Complex: A Mechanistic Insight. <i>Organometallics</i> , 2007, 26, 4135-4144.	1.1	130
10	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
11	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
12	Analysis of solvent effects on the Menshutkin reaction. <i>Journal of the American Chemical Society</i> , 1991, 113, 2873-2879.	6.6	123
13	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
14	Ligand Macrocyclic Structural Effects on Copper-Dioxygen Reactivity. <i>Inorganic Chemistry</i> , 2000, 39, 4059-4072.	1.9	116
15	Breaking C-F Bonds via Nucleophilic Attack of Coordinated Ligands: Transformations from C-F to C-X Bonds (X= H, N, O, S). <i>Organometallics</i> , 2012, 31, 1245-1256.	1.1	110
16	Self-Assembly of Mercaptane-Metallacarborane Complexes by an Unconventional Cooperative Effect: A C-H...H-S...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	Protonation of transition-metal hydrides: a not so simple process. <i>Chemical Society Reviews</i> , 2009, 38, 957.	18.7	99
21	An Artificial Heme Enzyme for Cyclopropanation Reactions. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 7785-7789.	7.2	98
22	C <sup>α</sup> -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
23	Theoretical Study on the Origin of Enantioselectivity in the Bis(dihydroquinidine)-3,6-pyridazine- <i>Os</i> -Osmium Tetroxide-Catalyzed Dihydroxylation of Styrene. <i>Journal of the American Chemical Society</i> , 1999, 121, 1317-1323.	6.6	94
24	Highly Enantioselective Electrophilic Amination and Michael Addition of Cyclic $\alpha$ -Ketoesters Induced by Lanthanides and (S,S)-ip-pybox: A Theoretical Study. <i>Journal of Organic Chemistry</i> , 2007, 72, 2077-2087.	1.7	94
25	First X-ray Characterization and Theoretical Study of $\eta^5$ -Alkyne, Alkynyl-Hydride, and Vinylidene Isomers for the Same Transition Metal Fragment [Cp* <i>Ru</i> (PEt <sub>3</sub> ) <sub>2</sub> ] <sup>+</sup> . <i>Journal of the American Chemical Society</i> , 2003, 125, 3311-3321.	6.6	90
26	Introducing Copper as Catalyst for Oxidative Alkane Dehydrogenation. <i>Journal of the American Chemical Society</i> , 2013, 135, 3887-3896.	6.6	89
27	Reactions of a Hexahydride- <i>Os</i> Osmium Complex with Aromatic Ketones: $\alpha$ -C-H Activation versus $\alpha$ -F Activation. <i>Organometallics</i> , 2001, 20, 442-452.	1.1	88
28	Bond-stretch isomerism in transition-metal complexes. <i>Journal of the American Chemical Society</i> , 1988, 110, 4506-4516.	6.6	85
29	A Computational Study of the Olefin Epoxidation Mechanism Catalyzed by Cyclopentadienyloxidomolybdenum(VI) Complexes. <i>Chemistry - A European Journal</i> , 2010, 16, 2147-2158.	1.7	84
30	Synthesis and Characterization of OsX{NHC(Ph)C <sub>6</sub> H <sub>4</sub> }H <sub>2</sub> (PiPr <sub>3</sub> ) <sub>2</sub> (X = H, Cl, Br, I): Nature of the H <sub>2</sub> Unit and Its Behavior in Solution. <i>Organometallics</i> , 1998, 17, 4065-4076.	1.1	81
31	Synthesis and Properties of Compressed Dihydride Complexes of Iridium: A Theoretical and Spectroscopic Investigations. <i>Journal of the American Chemical Society</i> , 2004, 126, 8813-8822.	6.6	79
32	Palladium Round Trip in the Negishi Coupling of <i>trans</i> - $\eta^5$ -PdMeCl(PMePh) <sub>2</sub> with ZnMeCl: An Experimental and DFT Study of the Transmetalation Step. <i>Chemistry - A European Journal</i> , 2010, 16, 8596-8599.	1.7	76
33	Structural, Kinetic, and Docking Studies of Artificial Imine Reductases Based on Biotin-Streptavidin Technology: An Induced Lock-and-Key Hypothesis. <i>Journal of the American Chemical Society</i> , 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 Co-C Bond. <i>Journal of Physical Chemistry B</i> , 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)(PCy <sub>3</sub> ). <i>Journal of the American Chemical Society</i> , 2003, 125, 7715-7725.	6.6	74
36	Incorporation of Manganese Complexes into Xylanase: New Artificial Metalloenzymes for Enantioselective Epoxidation. <i>ChemBioChem</i> , 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. <i>Journal of the American Chemical Society</i> , 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. <i>Journal of Organic Chemistry</i> , 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 Me <sup>α</sup> Me Coupling of ZnMe <sub>2</sub> and <i>trans</i> -[PdMeCl(PMePh) <sub>2</sub> ]. <i>Journal of the American Chemical Society</i> , 2011, 133, 13519-13526.	6.6	69
40	Design of an enantioselective artificial metallo-hydratase enzyme containing an unnatural metal-binding amino acid. <i>Chemical Science</i> , 2017, 8, 7228-7235.	3.7	69
41	Experimental and Theoretical Studies of Bonding and Oxidative Addition of Germanes and Silanes, EH <sub>4</sub> -nPhn (E = Si, Ge; n = 0-3), to Mo(CO)(diphosphine) <sub>2</sub> . The First Structurally Characterized Germane $\pi$ Complex. <i>Organometallics</i> , 2003, 22, 5307-5323.	1.1	68
42	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
43	The Transmetalation Process in Suzuki-Miyaura Reactions: Calculations Indicate Lower Barrier via Boronate Intermediate. <i>ChemCatChem</i> , 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. <i>Organometallics</i> , 2010, 29, 3252-3260.	1.1	67
45	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
46	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
47	Edge-Sharing Binuclear d <sub>8</sub> 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
48	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
49	Elongated Dihydrogen Complexes: A Combined Electronic DFT + Nuclear Dynamics Study of the [Ru(H $\pi$ -H)(C <sub>5</sub> H <sub>5</sub> )(H <sub>2</sub> PCH <sub>2</sub> PH <sub>2</sub> )] <sup>+</sup> Complex. <i>Journal of the American Chemical Society</i> , 1997, 119, 9840-9847.	6.6	64
50	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
51	Theoretical Study of the Hydrogen Exchange Coupling in the Metallocene Trihydride Complexes [(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> MH <sub>3</sub> ] <sub>n</sub> (M = Mo, W, n = 1; M = Nb, Ta, n = 0). <i>Journal of the American Chemical Society</i> , 1996, 118, 4617-4621.	6.6	60
52	Experimental and Computational Studies of Hydrogen Bonding and Proton Transfer to [Cp*Fe(dppe)H]. <i>Chemistry - A European Journal</i> , 2005, 11, 873-888.	1.7	58
53	Mechanism of Formation of Silver $\pi$ -Heterocyclic Carbenes Using Silver Oxide: A Theoretical Study. <i>Organometallics</i> , 2007, 26, 6170-6183.	1.1	58
54	Hydride Exchange Processes in the Coordination Sphere of Transition Metal Complexes: The OsH <sub>3</sub> (BH <sub>4</sub> )(PR <sub>3</sub> ) <sub>2</sub> System. <i>Journal of the American Chemical Society</i> , 1996, 118, 8388-8394.	6.6	57

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55	Synthesis and Spectroscopic Properties of Dihydrogen Isocyanide Niobocene [Nb( $\eta$ -5-C <sub>5</sub> H <sub>4</sub> SiMe <sub>3</sub> ) <sub>2</sub> ( $\eta$ -2-H <sub>2</sub> )(CNR)] <sub>2</sub> +Complexes. Experimental and Theoretical Study of the Blocked Rotation of a Coordinated Dihydrogen. <i>Journal of the American Chemical Society</i> , 1997, 119, 6107-6114.	6.6	57
56	Density Functional Study on the Mechanism of the Vanadium-Catalyzed Oxidation of Sulfides by Hydrogen Peroxide. <i>Journal of Organic Chemistry</i> , 2003, 68, 4265-4274.	1.7	57
57	Water-Assisted H $\alpha$ -H Bond Splitting Mediated by [CpRu(PTA)Cl] (PTA=1,3,5-triaza-7-phosphaadamantane). A DFT Analysis. <i>Organometallics</i> , 2007, 26, 3289-3296.	1.1	57
58	Mechanistic Intricacies of Gold-Catalyzed Intermolecular Cycloadditions between Allenamides and Dienes. <i>Chemistry - A European Journal</i> , 2013, 19, 15248-15260.	1.7	57
59	Synthesis, Structure, and Catalytic Applications for <i>ortho</i> - and <i>meta</i> -Carboranyl Based NBN Pincer-Pd Complexes. <i>Inorganic Chemistry</i> , 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. <i>Theoretica Chimica Acta</i> , 1987, 72, 175-195.	0.9	56
61	Dynamic Behavior in Solution of the <i>Trans</i> -Hydridodihydrogen Complex [OsHCl( $\eta$ -n <sup>2</sup> )( $\eta$ -H <sub>2</sub> )(CO)(P <i>i</i> -Pr <sub>3</sub> ) <sub>2</sub> ): Ab Initio and NMR Studies. <i>Chemistry - A European Journal</i> , 1996, 2, 815-825.	1.7	56
62	Lactam/lactim tautomeric interconversion mechanism of 2-pyridone in aqueous solution. <i>Tetrahedron Letters</i> , 1981, 22, 775-778.	0.7	55
63	Bonding in Elongated Dihydrogen Complexes. Theoretical Analysis of the Electron Density in [MLn(H $\alpha$ -H)] Species. <i>Organometallics</i> , 1996, 15, 2947-2953.	1.1	55
64	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
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. <i>ACS Catalysis</i> , 2012, 2, 2087-2099.	5.5	55
66	True and masked three-coordinate T-shaped platinum(II) intermediates. <i>Beilstein Journal of Organic Chemistry</i> , 2013, 9, 1352-1382.	1.3	55
67	Two- and Four-Electron Alkyne Ligands in Osmium-Cyclopentadienyl Chemistry: Consequences of the $\pi$ -M Interaction. <i>Organometallics</i> , 2002, 21, 305-314.	1.1	54
68	Why Is the Suzuki-Miyaura Cross-Coupling of sp <sup>3</sup> Carbons in $\beta$ -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
69	Prediction of the interaction of metallic moieties with proteins: An update for protein-ligand docking techniques. <i>Journal of Computational Chemistry</i> , 2018, 39, 42-51.	1.5	54
70	Concerted and Stepwise Mechanisms in Metal-Free and Metal-Assisted [4+3] Cycloadditions Involving Allyl Cations. <i>Chemistry - A European Journal</i> , 2010, 16, 12147-12157.	1.7	53
71	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
72	Oxidative Addition of Group 14 Element Hydrido Compounds to OsH <sub>2</sub> ( $\eta$ -2-CH <sub>2</sub> CH <sub>2</sub> Et)(CO)(PiPr <sub>3</sub> ) <sub>2</sub> : Synthesis and Characterization of the First Trihydrido-Silyl, Trihydrido-Germyl, and Trihydrido-Stannyl Derivatives of Osmium(IV). <i>Inorganic Chemistry</i> , 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. <i>Organometallics</i> , 2003, 22, 3753-3765.	1.1	52
74	The Active Role of the Water Solvent in the Regioselective CO Hydrogenation of Unsaturated Aldehydes by [RuH <sub>2</sub> (mtppps) <sub>x</sub> ] in Basic Media. <i>Organometallics</i> , 2006, 25, 5010-5023.	1.1	52
75	Molecular hydrogen complexes with a hydride ligand. An ab initio study on the iron hydride, [Fe(PR <sub>3</sub> ) <sub>4</sub> H(H <sub>2</sub> )] <sup>+</sup> , system. <i>Journal of the American Chemical Society</i> , 1991, 113, 2879-2884.	6.6	51
76	Crucial Role of Anions on the Deprotonation of the Cationic Dihydrogen Complex trans-[FeH(̂ <sup>2</sup> -H <sub>2</sub> )(dppe) <sub>2</sub> ] <sup>+</sup> . <i>Journal of the American Chemical Society</i> , 2007, 129, 6608-6618.	6.6	51
77	Coordination and Rupture of Methyl C(sp <sup>3</sup> )-H Bonds in Osmium <sup>II</sup> Polyhydride Complexes with $\sigma$ -Agostic Interaction. <i>Organometallics</i> , 2007, 26, 5140-5152.	1.1	51
78	Toward the Computational Design of Artificial Metalloenzymes: From Protein <sup>II</sup> Ligand Docking to Multiscale Approaches. <i>ACS Catalysis</i> , 2015, 5, 2469-2480.	5.5	51
79	Diverse Evolution of [Ph <sub>2</sub> P(CH <sub>2</sub> ) <sub>n</sub> PPh <sub>2</sub> ] <sub>2</sub> Pt(̂ <sup>4</sup> -S)Pt{Ph <sub>2</sub> P(CH <sub>2</sub> ) <sub>n</sub> PPh <sub>2</sub> } (n = 2, 3) Metalloligands in CH <sub>2</sub> Cl <sub>2</sub> . <i>Inorganic Chemistry</i> , 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. <i>Chemistry - A European Journal</i> , 2004, 10, 661-671.	1.7	50
81	When Are Tricoordinated Pd <sup>II</sup> Species Accessible? Stability Trends and Mechanistic Consequences. <i>Chemistry - A European Journal</i> , 2008, 14, 8986-8994.	1.7	50
82	Acid <sup>II</sup> -Base Interaction between Transition <sup>II</sup> -Metal Hydrides: Dihydrogen Bonding and Dihydrogen Evolution. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 1367-1370.	7.2	50
83	Proton-Transfer and H <sub>2</sub> -Elimination Reactions of Main-Group Hydrides EH <sub>4</sub> (E = B, Al, Ga) with Alcohols. <i>Inorganic Chemistry</i> , 2006, 45, 3086-3096.	1.9	49
84	Palladium Complexes of a Phosphorus Ylide with Two Stabilizing Groups: $\sigma$ -Synthesis, Structure, and DFT Study of the Bonding Modes. <i>Inorganic Chemistry</i> , 2006, 45, 6803-6815.	1.9	49
85	Cobalt-Catalyzed Vinylation of Aromatic Halides Using $\sigma$ -Halostyrene: Experimental and DFT Studies. <i>Journal of Organic Chemistry</i> , 2012, 77, 5056-5062.	1.7	49
86	Hydroamination of C=C Multiple Bonds with Hydrazine Catalyzed by N-Heterocyclic Carbene <sup>II</sup> -Gold(I) Complexes: Substrate and Ligand Effects. <i>ACS Catalysis</i> , 2015, 5, 815-829.	5.5	49
87	Structure and Dynamics of LRh $\sigma$ -H <sub>4</sub> (L = Cp, Tp) Systems. A Theoretical Study. <i>Organometallics</i> , 1997, 16, 3805-3814.	1.1	48
88	Density Functional Study on the Effect of the trans Axial Ligand of B <sub>12</sub> Cofactors on the Heterolytic Cleavage of the Co <sup>II</sup> -C Bond. <i>Journal of Physical Chemistry B</i> , 2003, 107, 306-315.	1.2	48
89	Influence of the Cis Ligand on the H $\sigma$ -H Separation and the Rotation Barrier of the Dihydrogen in Osmium-Elongated Dihydrogen Complexes Containing an Ortho-Metalated Ketone. <i>Organometallics</i> , 2004, 23, 3008-3015.	1.1	48
90	Tuning N <sup>II</sup> -Heterocyclic Carbenes in T <sup>II</sup> -Shaped Pt <sup>II</sup> Complexes for Intermolecular C $\sigma$ -H Bond Activation of Arenes. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 3936-3939.	7.2	48

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91	NH <sub>2</sub> -Heterocyclic Aryliodonium Salts and their Selective Conversion into <i>N</i> -Aryl-5-iodoimidazoles. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 7152-7156.	7.2	48
92	Intramolecular atom exchange between molecular hydrogen and hydride ligands in cis-[Fe(PR <sub>3</sub> ) <sub>4</sub> H(H <sub>2</sub> )] <sup>+</sup> complexes. An ab initio theoretical study. <i>Journal of the American Chemical Society</i> , 1992, 114, 2922-2928.	6.6	47
93	Hinge Distortion in Platinum(II) Dimers with a Pt <sub>2</sub> S <sub>2</sub> Ring. An ab Initio Molecular Orbital Study. <i>Inorganic Chemistry</i> , 1996, 35, 490-497.	1.9	47
94	Linear M <sup>n</sup> -Me Versus Bent M <sup>n</sup> -Me: Bonding Analysis in Heavier Metal-ylidyne Complexes [(Cp)(CO) <sub>2</sub> M <sup>n</sup> EMe] and Metallo-ylidenes [(Cp)(CO) <sub>3</sub> M <sup>n</sup> EMe] (M = Cr, Mo, W; E = ) <i>J. Chem. Phys.</i> 1997, 107, 1000-1007.	1.1	46
95	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
96	Quantum Mechanical Hydrogen Exchange Coupling in [(C <sub>5</sub> H <sub>5</sub> )Ir(L)H <sub>3</sub> ] <sup>+</sup> Complexes (L = PH <sub>3</sub> , CO). A Combined ab Initio/Tunneling Dynamics Study. <i>Journal of the American Chemical Society</i> , 1995, 117, 1069-1075.	6.6	46
97	Preparation and Characterization of Osmium <sup>VI</sup> Stannyl Polyhydrides: A DFT Study of the Oxidative Addition of Neutral Molecules in a Late Transition Metal. <i>Organometallics</i> , 2003, 22, 2087-2096.	1.1	46
98	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
99	Mechanistic Comparison of Acid- and Gold(I)-Catalyzed Nucleophilic Addition Reactions to Olefins. <i>Organometallics</i> , 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. <i>Journal of the American Chemical Society</i> , 2013, 135, 13749-13763.	6.6	46
101	Preparation and Spectroscopic and Theoretical Characterization of the Tetrahydroborate Complex OsH <sub>3</sub> (η <sup>2</sup> -H <sub>2</sub> BH <sub>2</sub> )(P- <i>i</i> -Pr <sub>3</sub> ) <sub>2</sub> . <i>Inorganic Chemistry</i> , 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(H <sub>2</sub> ) <sub>2</sub> Cl(H <sub>2</sub> PCH <sub>2</sub> CH <sub>2</sub> PH <sub>2</sub> ) <sub>2</sub> ] <sup>+</sup> Complex. <i>Journal of the American Chemical Society</i> , 1998, 120, 8168-8176.	6.6	45
103	Extending The Reaction Landscape of the {Pt(η <sup>5</sup> -C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> Pt} Core: From Metal Centers to Non-Metallic Electrophiles. <i>European Journal of Inorganic Chemistry</i> , 2004, 2004, 3585-3599.	1.0	45
104	Basic ancillary ligands promote O-O bond formation in iridium-catalyzed water oxidation: A DFT study. <i>Dalton Transactions</i> , 2011, 40, 11241.	1.6	45
105	Origin of the Anti-Markovnikov Hydroamination of Alkenes Catalyzed by Au(I) Complexes: Coordination Mode Determines Regioselectivity. <i>ACS Catalysis</i> , 2019, 9, 848-858.	5.5	45
106	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
107	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
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