

Agusti Lledos

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#	Paper	IF	Citations
372	Transition metal polyhydrides: from qualitative ideas to reliable computational studies. <i>Chemical Reviews</i> , 2000 , 100, 601-36	68.1	304
371	Computational perspective on Pd-catalyzed C-C cross-coupling reaction mechanisms. <i>Accounts of Chemical Research</i> , 2013 , 46, 2626-34	24.3	253
370	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, 13020-30	16.4	240
369	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, 853-64	16.4	191
368	Elongated dihydrogen complexes: what remains of the H-H bond?. <i>Chemical Society Reviews</i> , 2004 , 33, 175-82	58.5	164
367	Gold(I)-catalyzed intermolecular oxyarylation of alkynes: unexpected regiochemistry in the alkylation of arenes. <i>Organic Letters</i> , 2009 , 11, 4906-9	6.2	137
366	Gold-catalyzed [4C+3C] intramolecular cycloaddition of allenedienes: synthetic potential and mechanistic implications. <i>Chemistry - A European Journal</i> , 2009 , 15, 3336-9	4.8	133
365	Hydrogen Transfer to Ketones Catalyzed by Shvo's Ruthenium Hydride Complex: A Mechanistic Insight. <i>Organometallics</i> , 2007 , 26, 4135-4144	3.8	122
364	Computational study of the transmetalation process in the SuzukiMiyaura cross-coupling of aryls. <i>Journal of Organometallic Chemistry</i> , 2006 , 691, 4459-4466	2.3	122
363	To Bend or Not To Bend: Dilemma of the Edge-Sharing Binuclear Square Planar Complexes of d8 Transition Metal Ions. <i>Inorganic Chemistry</i> , 1998 , 37, 804-813	5.1	117
362	Analysis of solvent effects on the Menshutkin reaction. <i>Journal of the American Chemical Society</i> , 1991 , 113, 2873-2879	16.4	108
361	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	16.4	104
360	Ligand macrocycle structural effects on copper-dioxygen reactivity. <i>Inorganic Chemistry</i> , 2000 , 39, 4059-72	5.1	98
359	Breaking C σ Bonds via Nucleophilic Attack of Coordinated Ligands: Transformations from C σ to C π Bonds (X= H, N, O, S). <i>Organometallics</i> , 2012 , 31, 1245-1256	3.8	96
358	Self-assembly of mercaptane-metallacarborane complexes by an unconventional cooperative effect: a C-H...S-H...H-B hydrogen/dihydrogen bond interaction. <i>Journal of the American Chemical Society</i> , 2005 , 127, 15976-82	16.4	95
357	Protonation of transition-metal hydrides: a not so simple process. <i>Chemical Society Reviews</i> , 2009 , 38, 957-66	58.5	93
356	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, 14571-8	16.4	93

355	Acid Activation in Phenyl iodine Dicarboxylates: Direct Observation, Structures, and Implications. <i>Journal of the American Chemical Society</i> , 2016 , 138, 12747-12750	16.4	93
354	Mechanistic Exploration of the Pd-Catalyzed Copper-Free Sonogashira Reaction. <i>ACS Catalysis</i> , 2012 , 2, 135-144	13.1	90
353	C ^{II} 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	3.8	90
352	Highly enantioselective electrophilic amination and Michael addition of cyclic beta-ketoesters induced by lanthanides and (S,S)-ip-pybox: the mechanism. <i>Journal of Organic Chemistry</i> , 2007 , 72, 2077-2087	4.2	87
351	First X-ray characterization and theoretical study of pi-alkyne, alkynyl-hydride, and vinylidene isomers for the same transition metal fragment [Cp*Ru(PEt3)2]+. <i>Journal of the American Chemical Society</i> , 2003 , 125, 3311-21	16.4	85
350	Reactions of a Hexahydride Osmium Complex with Aromatic Ketones: C ^{II} Activation versus C ^{III} Activation. <i>Organometallics</i> , 2001 , 20, 442-452	3.8	85
349	Calculation of Reaction Free Energies in Solution: A Comparison of Current Approaches. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 1392-1399	2.8	82
348	Theoretical Study on the Origin of Enantioselectivity in the Bis(dihydroquinidine)-3,6-pyridazine Osmium Tetroxide-Catalyzed Dihydroxylation of Styrene. <i>Journal of the American Chemical Society</i> , 1999 , 121, 1317-1323	16.4	82
347	A computational study of the olefin epoxidation mechanism catalyzed by cyclopentadienyloxidomolybdenum(VI) complexes. <i>Chemistry - A European Journal</i> , 2010 , 16, 2147-58	4.8	75
346	Synthesis and properties of compressed dihydride complexes of iridium: theoretical and spectroscopic investigations. <i>Journal of the American Chemical Society</i> , 2004 , 126, 8813-22	16.4	74
345	Synthesis and Characterization of OsX{NHC(Ph)C6H4}H2(PiPr3)2 (X = H, Cl, Br, I): Nature of the H2 Unit and Its Behavior in Solution. <i>Organometallics</i> , 1998 , 17, 4065-4076	3.8	73
344	An Artificial Heme Enzyme for Cyclopropanation Reactions. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 7785-7789	16.4	72
343	Palladium round trip in the Negishi coupling of trans-[PdMeCl(PMePh2)2] with ZnMeCl: an experimental and DFT study of the transmetalation step. <i>Chemistry - A European Journal</i> , 2010 , 16, 8596-9	4.8	70
342	Bond-stretch isomerism in transition-metal complexes. <i>Journal of the American Chemical Society</i> , 1988 , 110, 4506-4516	16.4	69
341	Influence of media and homoconjugate pairing on transition metal hydride protonation. An IR and DFT study on proton transfer to CpRuH(CO)(PCy3). <i>Journal of the American Chemical Society</i> , 2003 , 125, 7715-25	16.4	68
340	A Density Functional Study on the Effect of the Trans Axial Ligand of Cobalamin on the Homolytic Cleavage of the Co-Cl Bond. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 7564-7571	3.4	68
339	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, 7303-9	4.2	67
338	Introducing copper as catalyst for oxidative alkane dehydrogenation. <i>Journal of the American Chemical Society</i> , 2013 , 135, 3887-96	16.4	66

- 337 Incorporation of manganese complexes into xylanase: new artificial metalloenzymes for enantioselective epoxidation. *ChemBioChem*, **2012**, 13, 240-51 3.8 65
- 336 Highly efficient redox isomerisation of allylic alcohols catalysed by pyrazole-based ruthenium(IV) complexes in water: mechanisms of bifunctional catalysis in water. *Chemistry - A European Journal*, **2012**, 18, 7749-65 4.8 65
- 335 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 3.8 65
- 334 Hydroamination of alkynes with ammonia: unforeseen role of the gold(I) catalyst. *Angewandte Chemie - International Edition*, **2011**, 50, 11147-51 16.4 64
- 333 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 4.8 63
- 332 Cationic intermediates in the Pd-catalyzed Negishi coupling. Kinetic and density functional theory study of alternative transmetalation pathways in the Me-Me coupling of ZnMe₂ and trans-[PdMeCl(PMePh₂)₂]. *Journal of the American Chemical Society*, **2011**, 133, 13519-26 16.4 60
- 331 Elongated Dihydrogen Complexes: A Combined Electronic DFT + Nuclear Dynamics Study of the [Ru(H₂)(C₅H₅)(H₂PCH₂PH₂)]⁺ Complex. *Journal of the American Chemical Society*, **1997**, 119, 9840-9847 16.4 60
- 330 Structural, kinetic, and docking studies of artificial imine reductases based on biotin-streptavidin technology: an induced lock-and-key hypothesis. *Journal of the American Chemical Society*, **2014**, 136, 15676-83 16.4 59
- 329 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 16.4 59
- 328 The importance of conformational search: a test case on the catalytic cycle of the Suzuki-Miyaura cross-coupling. *Theoretical Chemistry Accounts*, **2011**, 128, 639-646 1.9 57
- 327 Water-Assisted H-H Bond Splitting Mediated by [CpRu(PTA)₂Cl] (PTA=1,3,5-triaza-7-phosphaadamantane). A DFT Analysis. *Organometallics*, **2007**, 26, 3289-3296 3.8 57
- 326 Experimental and computational studies of hydrogen bonding and proton transfer to [Cp*Fe(dppe)H]. *Chemistry - A European Journal*, **2005**, 11, 873-88 4.8 57
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- 324 Design of an enantioselective artificial metallo-hydratase enzyme containing an unnatural metal-binding amino acid. *Chemical Science*, **2017**, 8, 7228-7235 9.4 55
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- 320 Theoretical study of reaction mechanisms for the ketonization of vinyl alcohol in gas phase and aqueous solution. *Theoretica Chimica Acta*, **1987**, 72, 175-195 55

319	Lactam/lactim tautomeric interconversion mechanism of 2-pyridone in aqueous solution. <i>Tetrahedron Letters</i> , 1981 , 22, 775-778	2	55
318	Two- and Four-Electron Alkyne Ligands in Osmium η -Cyclopentadienyl Chemistry: Consequences of the η -M Interaction. <i>Organometallics</i> , 2002 , 21, 305-314	3.8	53
317	First-Principles Molecular Dynamics Studies of Organometallic Complexes and Homogeneous Catalytic Processes. <i>Accounts of Chemical Research</i> , 2016 , 49, 1271-8	24.3	52
316	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	13.1	52
315	Why is the Suzuki-Miyaura cross-coupling of sp ³ carbons in alpha-bromo sulfoxide systems fast and stereoselective? A DFT study on the mechanism. <i>Journal of Organic Chemistry</i> , 2009 , 74, 4049-54	4.2	52
314	Concerted and stepwise mechanisms in metal-free and metal-assisted [4+3] cycloadditions involving allyl cations. <i>Chemistry - A European Journal</i> , 2010 , 16, 12147-57	4.8	52
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312	The Wacker process: inner- or outer-sphere nucleophilic addition? New insights from ab initio molecular dynamics. <i>Chemistry - A European Journal</i> , 2010 , 16, 8738-47	4.8	50
311	Crucial role of anions on the deprotonation of the cationic dihydrogen complex trans-[FeH(η -H ₂)(dppe) ₂] ⁺ . <i>Journal of the American Chemical Society</i> , 2007 , 129, 6608-18	16.4	50
310	Coordination and Rupture of Methyl C(sp ³) σ Bonds in OsmiumPolyhydride Complexes with σ Agostic Interaction. <i>Organometallics</i> , 2007 , 26, 5140-5152	3.8	50
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307	A versatile Ru catalyst for the asymmetric transfer hydrogenation of both aromatic and aliphatic sulfinylimines. <i>Chemistry - A European Journal</i> , 2012 , 18, 1969-83	4.8	49
306	True and masked three-coordinate T-shaped platinum(II) intermediates. <i>Beilstein Journal of Organic Chemistry</i> , 2013 , 9, 1352-82	2.5	49
305	Mechanism of Formation of Silver N-Heterocyclic Carbenes Using Silver Oxide: A Theoretical Study. <i>Organometallics</i> , 2007 , 26, 6170-6183	3.8	49
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303	Theoretical Study of the Hydrogen Exchange Coupling in the Metallocene Trihydride Complexes [(C ₅ H ₅) ₂ MH ₃] ⁿ⁺ (M = Mo, W, n = 1; M = Nb, Ta, n = 0). <i>Journal of the American Chemical Society</i> , 1996 , 118, 4617-4621	16.4	49
302	Diverse evolution of [[Ph ₂ P(CH ₂) _n PPH ₂] ₂ Pt(μ -S) ₂ Pt[Ph ₂ P(CH ₂) _n PPH ₂]] (n = 2, 3) metalloligands in CH ₂ Cl ₂ . <i>Inorganic Chemistry</i> , 2002 , 41, 3218-29	5.1	48

301	Palladium complexes of a phosphorus ylide with two stabilizing groups: synthesis, structure, and DFT study of the bonding modes. <i>Inorganic Chemistry</i> , 2006 , 45, 6803-15	5.1	47
300	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, 661-71	4.8	47
299	Bonding in Elongated Dihydrogen Complexes. Theoretical Analysis of the Electron Density in [MLn(H ₂)] Species. <i>Organometallics</i> , 1996 , 15, 2947-2953	3.8	47
298	Synthesis, structure, and catalytic applications for ortho- and meta-carboranyl based NBN pincer-Pd complexes. <i>Inorganic Chemistry</i> , 2014 , 53, 9284-95	5.1	46
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295	Mechanistic Comparison of Acid- and Gold(I)-Catalyzed Nucleophilic Addition Reactions to Olefins. <i>Organometallics</i> , 2010 , 29, 5919-5926	3.8	45
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293	When are tricoordinated PdII species accessible? Stability trends and mechanistic consequences. <i>Chemistry - A European Journal</i> , 2008 , 14, 8986-94	4.8	45
292	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, 3086-96	5.1	45
291	Influence of the Cis Ligand on the H ₂ 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	3.8	45
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289	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	3.5	44
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287	Selective B-H versus N-H Bond Activation in Ammonia Borane by [Ir(dppm) ₂ OTf]. <i>European Journal of Inorganic Chemistry</i> , 2009 , 2009, 3055-3059	2.3	44
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283	Chemical and constitutional influences in the self-assembly of functional supramolecular hydrogen-bonded nanoscopic fibres. <i>Chemistry - A European Journal</i> , 2006 , 12, 9161-75	4.8	43
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281	Toward the Computational Design of Artificial Metalloenzymes: From Protein-Ligand Docking to Multiscale Approaches. <i>ACS Catalysis</i> , 2015 , 5, 2469-2480	13.1	42
280	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, 13749-13753	16.4	42
279	Acid-base interaction between transition-metal hydrides: dihydrogen bonding and dihydrogen evolution. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 1367-70	16.4	42
278	Theoretical Analysis of the Hydrogen-Transfer Reaction to C \equiv N, C \equiv C, and C=C Bonds Catalyzed by Shvo's Ruthenium Complex. <i>Organometallics</i> , 2008 , 27, 4854-4863	3.8	42
277	Density Functional Study on the Effect of the trans Axial Ligand of B_{12} Cofactors on the Heterolytic Cleavage of the Co-C Bond. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 306-315	3.4	42
276	Selective Catalytic Deuterium Labeling of Alcohols during a Transfer Hydrogenation Process of Ketones Using D ₂ O as the Only Deuterium Source. Theoretical and Experimental Demonstration of a Ru \equiv D+ Exchange as the Key Step. <i>ACS Catalysis</i> , 2014 , 4, 1040-1053	13.1	41
275	Cobalt-catalyzed vinylation of aromatic halides using β -halostyrene: experimental and DFT studies. <i>Journal of Organic Chemistry</i> , 2012 , 77, 5056-62	4.2	41
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273	Synthesis and Spectroscopic and Theoretical Characterization of the Elongated Dihydrogen Complex OsCl(2)(eta(2)-H(2))(NH=CPh(2))(P(i)Pr(3))(2). <i>Inorganic Chemistry</i> , 1998 , 37, 5033-5035	5.1	41
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270	Hinge Distortion in Platinum(II) Dimers with a Pt(2)S(2) Ring. An ab Initio Molecular Orbital Study. <i>Inorganic Chemistry</i> , 1996 , 35, 490-497	5.1	41
269	AM1 study of hydrogen bonded complexes of water. <i>Computational and Theoretical Chemistry</i> , 1989 , 187, 55-68		41
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