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	Beyond Continuum Solvent Models in Computational Homogeneous Catalysis. Topics in Catalysis, 2022, 65, 118-140.	1.3	24
2	Successes and Challenges in Multiscale Modelling of Artificial Metalloenzymes: the Case Study of POP-Rh2 Cyclopropanase. Faraday Discussions, 2022, , .	1.6	1
3	Copper(i) activation of Câ€“X bonds: bimolecular vs. unimolecular reaction mechanism. Chemical Communications, 2022, , .	2.2	3
4	Direct Benzene Hydroxylation with Dioxygen Induced by Copper Complexes: Uncovering the Active Species by DFT Calculations. Organometallics, 2022, 41, 1892-1904.	1.1	4
5	Reversible carbonâ€“boron bond formation at platinum centers through Ïƒ-BH complexes. Chemical Science, 2021, 12, 1647-1655.	3.7	10
6	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
7	Understanding the Use of Phosphine-(EWO) Ligands in Negishi Cross-Coupling: Experimental and Density Functional Theory Mechanistic Study. Organometallics, 2021, 40, 2272-2282.	1.1	8
8	Computational Organometallic Catalysis: Where We Are, Where We Are Going. European Journal of Inorganic Chemistry, 2021, 2021, 2547-2555.	1.0	17
9	Transmetalation Reactions Triggered by Electron Transfer between Organocopper Complexes. Inorganic Chemistry, 2021, 60, 11633-11639.	1.9	6
10	Ligand Effects in Carbonâ^'Boron Coupling Processes Mediated by Ïƒâ€BH Platinum Complexes. European Journal of Inorganic Chemistry, 2021, 2021, 3528-3539.	1.0	4
11	Design and evolution of chimeric streptavidin for protein-enabled dual gold catalysis. Nature Catalysis, 2021, 4, 643-653.	16.1	32
12	How acid can become a dihydrogen complex in water? A DFT study. Journal of Organometallic Chemistry, 2021, 949, 121957.	0.8	3
13	Ambiphilic boryl groups in a neutral Ni(<scp>ii</scp>) complex: a new activation mode of H₂. Chemical Science, 2021, 12, 2540-2548.	3.7	11
14	What Makes a Good (Computed) Energy Profile?. Topics in Organometallic Chemistry, 2020, , 1-38.	0.7	15
15	Aerobic intramolecular carbonâ€“hydrogen bond oxidation promoted by Cu(<scp>i</scp>) complexes. Dalton Transactions, 2020, 49, 14647-14655.	1.6	9
16	Comparative Mechanistic Study on the [Au(NHC)]⁺-Catalyzed Hydration of Alkynes, Alkenes, and Allenes. Organometallics, 2020, 39, 3469-3479.	1.1	14
17	Dynamic Pd^{II}/Cu^I Multimetallic Assemblies as Molecular Models to Study Metalâ€“Metal Cooperation in Sonogashira Coupling. Chemistry - A European Journal, 2020, 26, 12168-12179.	1.7	23
18	Molecular Modeling for Artificial Metalloenzyme Design and Optimization. Accounts of Chemical Research, 2020, 53, 896-905.	7.6	29

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19	Catalytic Regioselective Isomerization of 2,2â€Disubstituted Oxetanes to Homoallylic Alcohols. Angewandte Chemie, 2020, 132, 7591-7597.	1.6	1
20	Catalytic Regioselective Isomerization of 2,2â€Disubstituted Oxetanes to Homoallylic Alcohols. Angewandte Chemie - International Edition, 2020, 59, 7521-7527.	7.2	16
21	Skeletal diversity in Pt- and Au-catalyzed annulations of allenedienes: dissecting unconventional mechanistic pathways. Chemical Science, 2020, 11, 4209-4220.	3.7	1
22	Innerâ€Sphere Oxygen Activation Promoting Outerâ€Sphere Nucleophilic Attack on Olefins. Chemistry - A European Journal, 2019, 25, 14546-14554.	1.7	7
23	Ïƒâ€Silane Platinum(II) Complexes as Intermediates in Câ^'Si Bondâ€Coupling Processes. Chemistry - A European Journal, 2019, 25, 11346-11355.	1.7	17
24	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
25	The Effect of Cofactor Binding on the Conformational Plasticity of the Biological Receptors in Artificial Metalloenzymes: The Case Study of LmrR. Frontiers in Chemistry, 2019, 7, 211.	1.8	9
26	Integrated Computational Study of the Cu-Catalyzed Hydration of Alkenes in Water Solvent and into the Context of an Artificial Metallohydratase. ACS Catalysis, 2019, 9, 4616-4626.	5.5	10
27	Bonding rearrangements in organometallic reactions: from orbitals to curly arrows. Dalton Transactions, 2019, 48, 15740-15752.	1.6	14
28	Activating a Peroxo Ligand for Câ^'O Bond Formation. Angewandte Chemie - International Edition, 2019, 58, 3037-3041.	7.2	9
29	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
30	Activating a Peroxo Ligand for Câ^'O Bond Formation. Angewandte Chemie, 2019, 131, 3069-3073.	1.6	2
31	GARLEEK: Adding an extra flavor to ONIOM. Journal of Computational Chemistry, 2019, 40, 381-386.	1.5	6
32	Decoding Surface Interaction of V^{IV}O Metallodrug Candidates with Lysozyme. Inorganic Chemistry, 2018, 57, 4456-4469.	1.9	28
33	Well-Defined Î²-Diketiminatocobalt(II) Complexes for Alkene Cyclohydroamination of Primary Amines. ACS Catalysis, 2018, 8, 4446-4451.	5.5	16
34	Isolation of a Cationic Platinum(II) Ïƒâ€Silane Complex. Angewandte Chemie, 2018, 130, 3271-3275.	1.6	10
35	Isolation of a Cationic Platinum(II) Ïƒâ€Silane Complex. Angewandte Chemie - International Edition, 2018, 57, 3217-3221.	7.2	27
36	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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37	An Artificial Heme Enzyme for Cyclopropanation Reactions. Angewandte Chemie, 2018, 130, 7911-7915.	1.6	26
38	An Artificial Heme Enzyme for Cyclopropanation Reactions. Angewandte Chemie - International Edition, 2018, 57, 7785-7789.	7.2	98
39	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
40	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
41	Iridium-Catalyzed Isomerization of N-Sulfonyl Aziridines to Allyl Amines. Organic Letters, 2018, 20, 5747-5751.	2.4	25
42	Frontispiece: Selective Synthesis of Tetrasubstituted Olefins by Copperâ€Mediated Acetoxythiolation of Internal Alkynes: Scope and Mechanistic Studies. Chemistry - A European Journal, 2018, 24, .	1.7	0
43	Accurate prediction of vertical electronic transitions of Ni(II) coordination compounds via time dependent density functional theory. International Journal of Quantum Chemistry, 2018, 118, e25655.	1.0	16
44	Mechanistic Insights on the Hydration of Terminal and Internal Allenes Catalyzed by [(NHC)Au]⁺. Organometallics, 2018, 37, 3543-3551.	1.1	10
45	Selective Synthesis of Tetrasubstituted Olefins by Copperâ€Mediated Acetoxythiolation of Internal Alkynes: Scope and Mechanistic Studies. Chemistry - A European Journal, 2018, 24, 13124-13135.	1.7	13
46	Desulfinylation of Ag(I) Sulfinyl Mesoionic Carbenes: Preparation of C-Unsubstituted Au(I)â€“1,2,3-Triazole Carbene Complexes. Organic Letters, 2017, 19, 822-825.	2.4	14
47	Rhodium Complexes Promoting Câ€“O Bond Formation in Reactions with Oxygen: The Role of Superoxo Species. Chemistry - A European Journal, 2017, 23, 5232-5243.	1.7	9
48	Speciation of ZnMe₂, ZnMeCl, and ZnCl₂ in Tetrahydrofuran (THF), and Its Influence on Mechanism Calculations of Catalytic Processes. ACS Catalysis, 2017, 7, 3575-3583.	5.5	28
49	Frontispiece: Rhodium Complexes Promoting Câ€“O Bond Formation in Reactions with Oxygen: The Role of Superoxo Species. Chemistry - A European Journal, 2017, 23, .	1.7	0
50	Elucidation of Binding Site and Chiral Specificity of Oxidovanadium Drugs with Lysozyme through Theoretical Calculations. Inorganic Chemistry, 2017, 56, 12938-12951.	1.9	40
51	A competing, dual mechanism for catalytic direct benzene hydroxylation from combined experimental-DFT studies. Chemical Science, 2017, 8, 8373-8383.	3.7	30
52	Design of an enantioselective artificial metallo-hydratase enzyme containing an unnatural metal-binding amino acid. Chemical Science, 2017, 8, 7228-7235.	3.7	69
53	Computing the arrows of chemical reactions. ChemTexts, 2017, 3, 1.	1.0	9
54	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

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55	Silver(I)â€Catalyzed Addition of Phenols to Alkyne Cobalt Cluster Stabilized Carbocations. Chemistry - A European Journal, 2016, 22, 9015-9023.	1.7	8
56	Acid Activation in Phenyliodine Dicarboxylates: Direct Observation, Structures, and Implications. Journal of the American Chemical Society, 2016, 138, 12747-12750.	6.6	127
57	Platinum(0)-mediated Câ€“O bond activation of ethers via an SN2 mechanism. Dalton Transactions, 2016, 45, 18842-18850.	1.6	4
58	New Insights into the Reactivity of Cisplatin with Free and Restrained Nucleophiles: Microsolvation Effects and Base Selectivity in Cisplatinâ€“DNA Interactions. ChemPhysChem, 2016, 17, 3932-3947.	1.0	10
59	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
60	NHâ€Heterocyclic Aryliodonium Salts and their Selective Conversion into N1â€Arylâ€5â€iodoimidazoles. Angewandte Chemie - International Edition, 2016, 55, 7152-7156.	7.2	48
61	First-Principles Molecular Dynamics Studies of Organometallic Complexes and Homogeneous Catalytic Processes. Accounts of Chemical Research, 2016, 49, 1271-1278.	7.6	64
62	Chapter 15. Enzyme Design. RSC Theoretical and Computational Chemistry Series, 2016, , 481-521.	0.7	1
63	Realistic Simulation of Organometallic Reactivity in Solution by Means of First-Principles Molecular Dynamics. Structure and Bonding, 2015, , 81-106.	1.0	7
64	Mechanistic Insight into the Facilitation of Î²â€Lactam Fragmentation through Metal Assistance. Chemistry - A European Journal, 2015, 21, 16781-16785.	1.7	25
65	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
66	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
67	Rutheniumâ€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
68	Azole Assisted Câ€“H Bond Activation Promoted by an Osmium-Polyhydride: Discerning between N and NH. Organometallics, 2015, 34, 1898-1910.	1.1	29
69	Toward the Computational Design of Artificial Metalloenzymes: From Proteinâ€“Ligand Docking to Multiscale Approaches. ACS Catalysis, 2015, 5, 2469-2480.	5.5	51
70	Orbitalâ€Like Motion of Hydride Ligands around Lowâ€Coordinate Metal Centers. Angewandte Chemie - International Edition, 2014, 53, 14158-14161.	7.2	14
71	Palladium monophosphine Pd(PPh₃): is it really accessible in solution?. Chemical Communications, 2014, 50, 661-663.	2.2	34
72	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

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73	Reactivity of Coordinatively Unsaturated Bis(N-heterocyclic carbene) Pt(II) Complexes toward H₂. Crystal Structure of a 14-Electron Pt(II) Hydride Complex. Inorganic Chemistry, 2014, 53, 4257-4268.	1.9	25
74	Unravelling novel synergies between organometallic and biological partners: a quantum mechanics/molecular mechanics study of an artificial metalloenzyme. Journal of the Royal Society Interface, 2014, 11, 20140090.	1.5	10
75	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
76	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
77	A stable, mononuclear, cationic Pt(<scp>iii</scp>) complex stabilised by bulky N-heterocyclic carbenes. Chemical Communications, 2014, 50, 1299-1301.	2.2	21
78	Synthesis, Structure, and Catalytic Applications for ortho- and meta-Carboranyl Based NBN Pincer-Pd Complexes. Inorganic Chemistry, 2014, 53, 9284-9295.	1.9	57
79	On the Road to MMâ€²X Polymers: Redox Properties of Heterometallic NiÂ·Â·Â·Pt Paddlewheel Complexes. Inorganic Chemistry, 2014, 53, 10553-10562.	1.9	6
80	Counteranion-Dependent Reaction Pathways in the Protonation of Cationic Rutheniumâ€“Vinylidene Complexes. Organometallics, 2014, 33, 2549-2560.	1.1	8
81	Computational Insights on an Artificial Imine Reductase Based on the Biotinâ€“Streptavidin Technology. ACS Catalysis, 2014, 4, 833-842.	5.5	27
82	The use of localised orbitals for the bonding and mechanistic analysis of organometallic compounds. Dalton Transactions, 2014, 43, 11145.	1.6	42
83	Assessing protein-ligand docking for the binding of organometallic compounds to proteins. Journal of Computational Chemistry, 2014, 35, 192-198.	1.5	22
84	The Transmetalation Process in Suzukiâ€“Miyaura Reactions: Calculations Indicate Lower Barrier via Boronate Intermediate. ChemCatChem, 2014, 6, 3132-3138.	1.8	68
85	Coordinatively Unsaturated T-Shaped Platinum(II) Complexes Stabilized by Small N-Heterocyclic Carbene Ligands. Synthesis and Cyclometalation. Organometallics, 2014, 33, 3746-3756.	1.1	22
86	Computational Perspective on Pd-Catalyzed Câ€“C Cross-Coupling Reaction Mechanisms. Accounts of Chemical Research, 2013, 46, 2626-2634.	7.6	306
87	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
88	Speciation of [Cp*₂M₂O₅] in Polar and Donor Solvents. Chemistry - A European Journal, 2013, 19, 3969-3985.	1.7	3
89	Counteranion and Solvent Assistance in Ruthenium-Mediated Alkyne to Vinylidene Isomerizations. Inorganic Chemistry, 2013, 52, 8919-8932.	1.9	36
90	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

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91	Introducing Copper as Catalyst for Oxidative Alkane Dehydrogenation. Journal of the American Chemical Society, 2013, 135, 3887-3896.	6.6	89
92	Mechanistic Intricacies of Goldâ€Catalyzed Intermolecular Cycloadditions between Allenamides and Dienes. Chemistry - A European Journal, 2013, 19, 15248-15260.	1.7	57
93	True and masked three-coordinate T-shaped platinum(II) intermediates. Beilstein Journal of Organic Chemistry, 2013, 9, 1352-1382.	1.3	55
94	Mechanistic Exploration of the Pd-Catalyzed Copper-Free Sonogashira Reaction. ACS Catalysis, 2012, 2, 135-144.	5.5	103
95	PtII as a proton shuttle during Câ€“H bond activation in the Shilov process. Chemical Communications, 2012, 48, 1979.	2.2	26
96	Rearrangement of Tridentate [OSO]-Type Ligands and Migratory Insertion Reaction Mechanisms in Cyclopentadienyl Tantalum Complexes. Organometallics, 2012, 31, 7052-7062.	1.1	8
97	Cobalt-Catalyzed Vinylation of Aromatic Halides Using Î²-Halostyrene: Experimental and DFT Studies. Journal of Organic Chemistry, 2012, 77, 5056-5062.	1.7	49
98	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
99	Coordination Chemistry of New Chiral P,N Ferrocenyl Ligands with Half-Sandwich Ruthenium(II), Rhodium(III), and Iridium(III) Complexes. Organometallics, 2012, 31, 6669-6680.	1.1	25
100	Characterization of a Paramagnetic, Mononuclear Pt(III)â€“Alkyl Complex Intermediate in Carbonâ€“Halogen Bond Coupling Reactions. Journal of the American Chemical Society, 2012, 134, 15261-15264.	6.6	29
101	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
102	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
103	Hydrogenâ€“deuterium exchange in hydride chemistry: Dihydrogen bonded complexes as key intermediates. Computational and Theoretical Chemistry, 2012, 998, 129-140.	1.1	18
104	Computational insights on the possibility of tri-coordinated cisplatinated adducts with protein models. Journal of Inorganic Biochemistry, 2012, 117, 230-236.	1.5	4
105	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
106	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
107	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
108	Directionality of Dihydrogen Bonds: The Role of Transition Metal Atoms. ChemPhysChem, 2012, 13, 2677-2687.	1.0	22

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109	Incorporation of Manganese Complexes into Xylanase: New Artificial Metalloenzymes for Enantioselective Epoxidation. ChemBioChem, 2012, 13, 240-251.	1.3	72
110	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
111	Basic ancillary ligands promote Oâ€“O bond formation in iridium-catalyzed water oxidation: A DFT study. Dalton Transactions, 2011, 40, 11241.	1.6	45
112	Theoretical study on intramolecular allene-diene cycloadditions catalyzed by PtCl2 and Au(i) complexes. Dalton Transactions, 2011, 40, 11095.	1.6	19
113	Nature of Bonding in Terminal Borylene, Alylene, and Gallylene Complexes of Vanadium and Niobium [(Î·⁵-C₅H₅)(CO)₃M(ENR₂)] (M = V, Nb; E = B,) Tj ETQq1 1 0.784314 rg Inorganic Chemistry, 2011, 50, 1402-1410.	1.9	30
114	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
115	Gold-Catalyzed Cycloadditions Involving Allenes: Mechanistic Insights from Theoretical Studies. Topics in Current Chemistry, 2011, 302, 225-248.	4.0	33
116	What can molecular modelling bring to the design of artificial inorganic cofactors?. Faraday Discussions, 2011, 148, 137-159.	1.6	26
117	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
118	Theoretical Evaluation of Phosphine Effects in Cross-Coupling Reactions. Catalysis By Metal Complexes, 2011, , 57-84.	0.6	12
119	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
120	Gold versus Silverâ€Catalyzed Intermolecular Hydroaminations of Alkenes and Dienes. Advanced Synthesis and Catalysis, 2011, 353, 3451-3466.	2.1	44
121	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
122	Acidâ€“Base Interaction between Transitionâ€Metal Hydrides: Dihydrogen Bonding and Dihydrogen Evolution. Angewandte Chemie - International Edition, 2011, 50, 1367-1370.	7.2	50
123	Hydroamination of Alkynes with Ammonia: Unforeseen Role of the Gold(I) Catalyst. Angewandte Chemie - International Edition, 2011, 50, 11147-11151.	7.2	67
124	Solventâ€Dependent Dihydrogen/Dihydride Stability for [Mo(CO)(Cp*)H₂(PMe₃)₂]⁺[BF₄]^{â^'} Determined by Multiple Solventâ‹…â‹…â‹…Anionâ‹…â‹…â‹…Cation Nonâ€Covalent Interactions. Chemistry - A European Journal, 2010, 16, 189-201.	1.7	31
125	A Computational Study of the Olefin Epoxidation Mechanism Catalyzed by Cyclopentadienyloxidomolybdenum(VI) Complexes. Chemistry - A European Journal, 2010, 16, 2147-2158.	1.7	84
126	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

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127	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
128	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
129	Linear versus bent bonding in metal-phosphinidene complexes: Theoretical studies of the electrophilic Organometallic Chemistry, 2010, 695, 206-214.	0.8	15
130	Inner- and Outer-Sphere Hydrogenation Mechanisms: A Computational Perspective. Advances in Inorganic Chemistry, 2010, 62, 231-260.	0.4	34
131	Mechanistic Comparison of Acid- and Gold(I)-Catalyzed Nucleophilic Addition Reactions to Olefins. Organometallics, 2010, 29, 5919-5926.	1.1	46
132	Intramolecular Ïƒ-Bond Metathesis/Protonolysis on Zirconium(IV) and Hafnium(IV) Pyridylamido Olefin Polymerization Catalyst Precursors: Exploring Unexpected Reactivity Paths. Inorganic Chemistry, 2010, 49, 6811-6813.	1.9	21
133	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
134	Comparative DFT Analysis of Ligand and Solvent Effects on the Mechanism of H₂Activation in Water Mediated by Half-Sandwich Complexes [Cpâ€²Ru(PTA)₂Cl] (Cpâ€² =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 462 T Organometallics, 2010, 29, 5121-5131.	1.1	32
135	Mechanism for Hydride-Assisted Rearrangement from Ethylidene to Ethylene in Iridium Cationic Complexes. Organometallics, 2010, 29, 2040-2045.	1.1	28
136	Neutral Transition Metal Hydrides as Acids in Hydrogen Bonding and Proton Transfer: Media Polarity and Specific Solvation Effects. Journal of the American Chemical Society, 2010, 132, 11234-11246.	6.6	35
137	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
138	Dinuclear Dicyclopentadienyl Titanium Complexes with Bridging Cyclopentadienylsiloxo Ligands. Organometallics, 2010, 29, 642-655.	1.1	6
139	Mechanistic Studies on the Interaction of [(Î·³-P,P,P-NP₃)IrH₃] [NP₃= N(CH₂CH₂PPh₂)₃] with HBF₄and Fluorinated Alcohols by Combined NMR, IR, and DFT Techniques. Inorganic Chemistry, 2010, 49, 4343-4354.	1.9	18
140	Structural Analysis of Zincocenes with Substituted Cyclopentadienyl Rings. Chemistry - A European Journal, 2009, 15, 924-935.	1.7	18
141	Goldâ€Catalyzed [4C+3C] Intramolecular Cycloaddition of Allenedienes: Synthetic Potential and Mechanistic Implications. Chemistry - A European Journal, 2009, 15, 3336-3339.	1.7	138
142	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
143	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
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