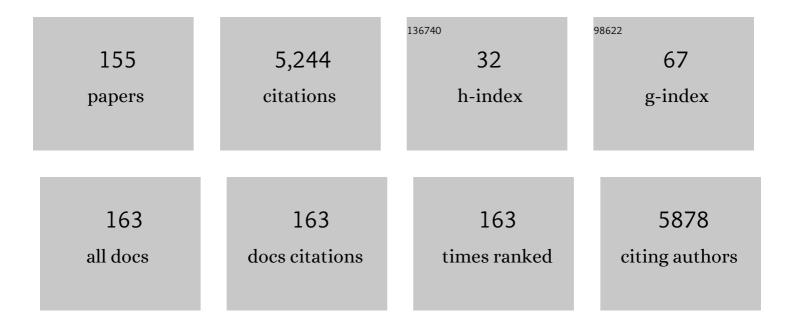
Alireza Ariafard

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Borane Catalyzed Selective Diazo Crossâ€Coupling Towards Pyrazoles. Advanced Synthesis and Catalysis, 2022, 364, 773-780.	2.1	10
2	Understanding the Influence of Donorâ€Acceptor Diazo Compounds on the Catalyst Efficiency of B(C ₆ F ₅) ₃ Towards Carbene Formation. Chemistry - A European Journal, 2022, 28, .	1.7	11
3	A Rare Alderâ€ene Cycloisomerization of 1,6â€Allenynes. Chemistry - A European Journal, 2022, 28, .	1.7	4
4	Lewis Acid Assisted BrÃ,nsted Acid Catalysed Decarbonylation of Isocyanates: A Combined DFT and Experimental Study. Chemistry - A European Journal, 2022, , .	1.7	3
5	DFT characterisation of a Pd ^{II} â†' I ^{III} adduct, and a Pd ^{II} complex formed after oxidative alkenylation of Pd ^{II} by [Ph(alkenyl)I ^{III}] ⁺ , in Pd-mediated synthesis of benzofurans involving Pd ^{IV} , annulation and chain-walking. Dalton Transactions. 2022. 51. 9377-9384.	1.6	3
6	Chiral Gold Complex Catalyzed Cycloisomerization/Regio- and Enantioselective Nitroso-Diels–Alder Reaction of 1,6-Diyne Esters with Nitrosobenzenes. ACS Catalysis, 2022, 12, 7288-7299.	5.5	9
7	Goldâ€Catalyzed Annulation of 1,8â€Dialkynylnaphthalenes: Synthesis and Photoelectric Properties of Indenophenaleneâ€Based Derivatives. Chemistry - A European Journal, 2021, 27, 3552-3559.	1.7	6
8	Copper-catalysed synthesis of \hat{l} ±-alkylidene cyclic carbonates from propargylic alcohols and CO ₂ . Green Chemistry, 2021, 23, 889-897.	4.6	28
9	How a Bismuth(III) Catalyst Achieves Greatest Activation of Organic Lewis Bases in a Catalytic Reaction: Insights from DFT Calculations. ChemCatChem, 2021, 13, 975-980.	1.8	5
10	Computational Investigation into the Mechanistic Features of Bromide-Catalyzed Alcohol Oxidation by PhIO in Water. Journal of Organic Chemistry, 2021, 86, 2998-3007.	1.7	3
11	Catalytic role of amines in activation of PhICl ₂ from a computational point of view. Chemical Communications, 2021, 57, 9108-9111.	2.2	4
12	The role of hypervalent iodine(<scp>iii</scp>) reagents in promoting alkoxylation of unactivated C(sp ³)–H bonds catalyzed by palladium(<scp>ii</scp>) complexes. Chemical Science, 2021, 12, 7185-7195.	3.7	11
13	Site-Selective C _{sp³} –C _{sp} /C _{sp³} –C _{sp²< Cross-Coupling Reactions Using Frustrated Lewis Pairs. Journal of the American Chemical Society, 2021, 143, 4451-4464.}	/sub>	28
14	Hydroalkylation of Alkenes with 1,3-Diketones via Gold(III) or Silver(I) Catalysis: Divergent Mechanistic Pathways Revealed by a DFT-Based Investigation. ACS Catalysis, 2021, 11, 5795-5807.	5.5	6
15	Bidentate Nitrogen-Ligated I(V) Reagents, Bi(<i>N</i>)-HVIs: Preparation, Stability, Structure, and Reactivity. Journal of Organic Chemistry, 2021, 86, 6566-6576.	1.7	8
16	Computational Study of Intramolecular Coordination Enhanced Oxidative Addition to form PdIV-Pincer Complexes, and Selectivity in Aryloxide Attack at PdIVCH2CRR′ Motifs in Palladium-Mediated Organic Synthesis. Organometallics, 2021, 40, 1262-1269.	1.1	3
17	Gold-Catalyzed [5,5]-Rearrangement. ACS Catalysis, 2021, 11, 6510-6518.	5.5	17
18	Copper(I)-catalysed site-selective C(sp3)–H bond chlorination of ketones, (E)-enones and alkylbenzenes by dichloramine-T. Nature Communications, 2021, 12, 4065.	5.8	10

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19	Oxidation of Electron-Deficient Phenols Mediated by Hypervalent Iodine(V) Reagents: Fundamental Mechanistic Features Revealed by a Density Functional Theory-Based Investigation. Journal of Organic Chemistry, 2021, 86, 12237-12246.	1.7	6
20	Computational study of bridgeâ€splitting, aryl halide oxidative addition to PtII, and reductive elimination from PtIV: a route to pincerâ€PtII reagents with chemical and biological applications. Chemistry - A European Journal, 2021, 27, 15426-15433.	1.7	0
21	Tris(pentafluorophenyl)borane atalyzed Carbenium Ion Generation and Autocatalytic Pyrazole Synthesis—A Computational and Experimental Study. Angewandte Chemie - International Edition, 2021, 60, 24395-24399.	7.2	18
22	Photochemical Activation of a Hydroxyquinone-Derived Phenyliodonium Ylide by Visible Light: Synthetic and Mechanistic Investigations. Journal of Organic Chemistry, 2021, 86, 1758-1768.	1.7	4
23	Exploring Cyclization Strategies to Access Stemona Alkaloids: Subtle Effects Influencing Reactivity in Intramolecular Michael Additions. Organic Letters, 2021, 23, 8494-8498.	2.4	6
24	Acyl Migration versus Epoxidation in Gold Catalysis: Facile, Switchable, and Atomâ€Economic Synthesis of Acylindoles and Quinoline Derivatives. Angewandte Chemie - International Edition, 2020, 59, 471-478.	7.2	99
25	DFT-Based Comparison between Mechanistic Aspects of Amine and Alcohol Oxidation Mediated by IBX. Journal of Organic Chemistry, 2020, 85, 515-525.	1.7	8
26	Gold Catalyzed Cyclopropanation/[5+3] Cycloaddition of 1,4,9―and 1,4,10â€Allenenynes to Bicyclo[3.3.1]nonane Derivatives. Advanced Synthesis and Catalysis, 2020, 362, 1084-1095.	2.1	19
27	Borane-Catalyzed Stereoselective C–H Insertion, Cyclopropanation, and Ring-Opening Reactions. CheM, 2020, 6, 2364-2381.	5.8	70
28	Computational Analysis of Mesomerism in <i>para</i> ‣ubstituted <i>mer</i> â€NCN Pincer Platinum(II) Complexes, Including its Relationships with Hammett σ _p Substituent Parameters. Chemistry - A European Journal, 2020, 26, 15629-15635.	1.7	6
29	How the combination of PhIO and I ₂ provides a species responsible for conducting organic reactions through radical mechanisms. Organic and Biomolecular Chemistry, 2020, 18, 8103-8108.	1.5	5
30	DFT studies of two-electron oxidation, photochemistry, and radical transfer between metal centres in the formation of platinum(<scp>iv</scp>) and palladium(<scp>iv</scp>) selenolates from diphenyldiselenide and metal(<scp>ii</scp>) reactants. Dalton Transactions, 2020, 49, 13566-13572.	1.6	1
31	Triarylborane catalysed <i>N</i> -alkylation of amines with aryl esters. Catalysis Science and Technology, 2020, 10, 7523-7530.	2.1	8
32	Rhodium-catalysed tetradehydro-Diels–Alder reactions of enediynes <i>via</i> a rhodium-stabilized cyclic allene. Chemical Science, 2020, 11, 10945-10950.	3.7	4
33	Triarylboranâ€katalysierte Alkenylierungen von Arylestern mit Diazoverbindungen. Angewandte Chemie, 2020, 132, 15621-15626.	1.6	5
34	Triarylboraneâ€Catalyzed Alkenylation Reactions of Aryl Esters with Diazo Compounds. Angewandte Chemie - International Edition, 2020, 59, 15492-15496.	7.2	32
35	Iron Triflate Salts as Highly Active Catalysts for the Solventâ€Free Oxidation of Cyclohexane. European Journal of Organic Chemistry, 2020, 2020, 3552-3559.	1.2	10
36	Mechanistic investigation into phenol oxidation by IBX elucidated by DFT calculations. Organic and Biomolecular Chemistry, 2020, 18, 1117-1129.	1.5	18

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37	Catalytic Role of Lewis Acids in ArIOâ€Mediated Oxidative Fluorination Reactions Revealed by DFT Calculations. European Journal of Organic Chemistry, 2020, 2020, 2251-2259.	1.2	5
38	Aryl–Fluoride Bond-Forming Reductive Elimination from Nickel(IV) Centers. Journal of the American Chemical Society, 2019, 141, 13261-13267.	6.6	37
39	Nickel(IV)-Catalyzed C–H Trifluoromethylation of (Hetero)arenes. Journal of the American Chemical Society, 2019, 141, 12872-12879.	6.6	82
40	Goldâ€Catalyzed Regiospecific Annulation of Unsymmetrically Substituted 1,5â€Diynes for the Precise Synthesis of Bispentalenes. Chemistry - A European Journal, 2019, 25, 12180-12186.	1.7	28
41	Accessing Chelating Extended Linker Bis(NHC) Palladium(II) Complexes: Sterically Triggered Divergent Reaction Pathways. Organometallics, 2019, 38, 3032-3038.	1.1	6
42	A Modified Cationic Mechanism for PdCl2-Catalyzed Transformation of a Homoallylic Alcohol to an Allyl Ether. Organometallics, 2019, 38, 2953-2962.	1.1	10
43	Phosphine-Scavenging Cationic Gold(I) Complexes: Alternative Applications of Gold Cocatalysis in Fundamental Palladium-Catalyzed Cross-Couplings. Organometallics, 2019, 38, 2683-2688.	1.1	3
44	DFT Mechanistic Investigation into BF ₃ -Catalyzed Alcohol Oxidation by a Hypervalent Iodine(III) Compound. ACS Catalysis, 2019, 9, 6510-6521.	5.5	22
45	Rationale for the reactivity differences between main group and d0 transition metal complexes toward olefin polymerisation. Dalton Transactions, 2019, 48, 6997-7005.	1.6	2
46	Revisiting the mechanism of acetylenic amine N-Oxide rearrangement catalysed by Gold(I) complexes from a DFT perspective. Journal of Organometallic Chemistry, 2019, 889, 45-52.	0.8	1
47	DFT mechanistic investigation into phenol dearomatization mediated by an iodine(<scp>iii</scp>) reagent. Organic and Biomolecular Chemistry, 2019, 17, 3521-3528.	1.5	29
48	Formation and reactions of the 1, 8-naphthyridine (napy) ligated geminally dimetallated phenyl complexes [(napy)Cu ₂ (Ph)] ⁺ , [(napy)Ag ₂ (Ph)] ⁺ and [(napy)CuAg(Ph)] ⁺ . European Journal of Mass Spectrometry, 2019, 25, 30-43.	0.5	1
49	Proton supplier role of binuclear gold complexes in promoting hydrofunctionalisation of nonactivated alkenes. Catalysis Science and Technology, 2019, 9, 1420-1426.	2.1	11
50	Nickel(II/IV) Manifold Enables Room-Temperature C(sp ³)–H Functionalization. Journal of the American Chemical Society, 2019, 141, 19513-19520.	6.6	25
51	Disclosure of Some Obscure Mechanistic Aspects of the Copper-Catalyzed Click Reactions Involving N ₂ Elimination Promoted by the Use of Electron-Deficient Azides from a DFT Perspective. Organometallics, 2019, 38, 256-267.	1.1	10
52	Synthesis of Amidines by Palladium-Mediated CO2 Extrusion Followed by Insertion of Carbodiimides: Translating Mechanistic Studies to Develop a One-Pot Method. Organometallics, 2019, 38, 424-435.	1.1	16
53	Mechanistic Elucidation of Gold(I)-Catalyzed Oxidation of a Propargylic Alcohol by a N-Oxide in the Presence of an Imine Using DFT Calculations. Organometallics, 2019, 38, 489-497.	1.1	9

54 Titelbild: Dual Gold-Catalyzed Cycloaromatization of Unconjugated (E)-Enediynes (Angew. Chem.) Tj ETQq0 0 0 rgBT/Overlock 10 Tf 50

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55	Dual Goldâ€Catalyzed Cycloaromatization of Unconjugated (<i>E</i>)â€Enediynes. Angewandte Chemie - International Edition, 2019, 58, 2114-2119.	7.2	28
56	Dual Gold atalyzed Cycloaromatization of Unconjugated (E)â€Enediynes. Angewandte Chemie, 2019, 131, 2136-2141.	1.6	7
57	A Computational Mechanistic Investigation into Reduction of Gold(III) Complexes by Amino Acid Glycine: A New Variant for Amine Oxidation. Chemistry - A European Journal, 2018, 24, 8361-8368.	1.7	14
58	Chiral BrÃ,nsted Acid Catalyzed Enantioselective Dehydrative Nazarov-Type Electrocyclization of Aryl and 2-Thienyl Vinyl Alcohols. Journal of the American Chemical Society, 2018, 140, 5834-5841.	6.6	33
59	Nazarov cyclisations initiated by DDQ-oxidised pentadienyl ether: a mechanistic investigation from the DFT perspective. Organic and Biomolecular Chemistry, 2018, 16, 9021-9029.	1.5	6
60	Different Selectivities in the Insertions into C(sp ²)â^'H Bonds: Benzofulvenes by Dual Gold Catalysis Competition Experiments. Chemistry - A European Journal, 2018, 24, 10766-10772.	1.7	18
61	DFT studies of isomerization in palladium(IV) chemistry and alkyl halide transfer from palladium(IV) to palladium(II). Journal of Organometallic Chemistry, 2018, 872, 110-113.	0.8	1
62	Reduction of a platinum(<scp>iv</scp>) prodrug model by sulfur containing biological reductants: computational mechanistic elucidation. Chemical Communications, 2018, 54, 10491-10494.	2.2	17
63	A one-pot route to thioamides discovered by gas-phase studies: palladium-mediated CO ₂ extrusion followed by insertion of isothiocyanates. Chemical Communications, 2017, 53, 3854-3857.	2.2	24
64	Computational study of C(sp ³)–O bond formation at a Pd ^{IV} centre. Dalton Transactions, 2017, 46, 3742-3748.	1.6	25
65	Gas-Phase Ion–Molecule Reactions of Copper Hydride Anions [CuH ₂] ^{â^'} and [Cu ₂ H ₃] ^{â^'} . Inorganic Chemistry, 2017, 56, 2387-2399.	1.9	32
66	Oxidatively Induced C–H Activation at High Valent Nickel. Journal of the American Chemical Society, 2017, 139, 6058-6061.	6.6	62
67	Phosphine-Scavenging Role of Gold(I) Complexes from Pd(P ^t Bu ₃) ₂ in the Bimetallic Catalysis of Carbostannylation of Alkynes. Organometallics, 2017, 36, 2014-2019.	1.1	5
68	Total Synthesis of (±)â€Dihydroisosubamol. Advanced Synthesis and Catalysis, 2017, 359, 866-874.	2.1	19
69	A computational mechanistic investigation into the reduction of Pt(<scp>iv</scp>) prodrugs with two axial chlorides by biological reductants. Chemical Communications, 2017, 53, 1413-1416.	2.2	19
70	Experimental and Computational Studies of High-Valent Nickel and Palladium Complexes. Organometallics, 2017, 36, 4382-4393.	1.1	55
71	A transition-metal-free fast track to flavones and 3-arylcoumarins. Chemical Communications, 2017, 53, 10676-10679.	2.2	20
72	Gold-catalyzed domino cyclization–alkynylation reactions with EBX reagents: new insights into the reaction mechanism. Dalton Transactions, 2017, 46, 12257-12262.	1.6	25

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73	Computational study of selectivity in the [Pt ^{II} Cl ₄] ^{2â^'} -catalysed arylation of arenes by diaryliodonium reagents: arene activation at Pt ^{IV} centres. Dalton Transactions, 2017, 46, 15480-15486.	1.6	6
74	Substituent effects in the decarboxylation reactions of coordinated arylcarboxylates in dinuclear copper complexes, [(napy)Cu ₂ (O ₂ CC ₆ H ₄ X)] ⁺ . European Journal of Mass Spectrometry, 2017, 23, 351-358.	0.5	6
75	A Mechanistic Investigation of the Gold(III)-Catalyzed Hydrofurylation of C–C Multiple Bonds. Journal of the American Chemical Society, 2016, 138, 14599-14608.	6.6	22
76	The different roles of a cationic gold(<scp>i</scp>) complex in catalysing hydroarylation of alkynes and alkenes with a heterocycle. Chemical Communications, 2016, 52, 9422-9425.	2.2	18
77	Theoretical rationalisation for the mechanism of N-heterocyclic carbene-halide reductive elimination at Cu ^{III} , Ag ^{III} and Au ^{III} . Chemical Communications, 2016, 52, 5057-5060.	2.2	10
78	Theoretical Investigation into the Mechanism of Cyanomethylation of Aldehydes Catalyzed by a Nickel Pincer Complex in the Absence of Base Additives. ACS Catalysis, 2016, 6, 60-68.	5.5	21
79	Sulfur Dioxide Activation: A Theoretical Investigation into Dual Sâ•O Bond Cleavage by Three-Coordinate Molybdenum(III) Complexes. Inorganic Chemistry, 2015, 54, 534-543.	1.9	6
80	σ-Alkenyl endo-palladacycle formation via regiospecific functionalisation of an unreactive NHC-tethered C(sp ²)–H bond. Chemical Communications, 2015, 51, 5513-5515.	2.2	6
81	Mechanistic Elucidation of the Arylation of Non-Spectator <i>N</i> -Heterocyclic Carbenes at Copper Using a Combined Experimental and Computational Approach. Organometallics, 2015, 34, 3497-3507.	1.1	28
82	A Theoretical Study on the Protodeauration Step of the Gold(I)-Catalyzed Organic Reactions. Organometallics, 2015, 34, 3186-3195.	1.1	68
83	Prying open a Reactive Site for Allylic Arylation by Phosphine-Ligated Geminally Diaurated Aryl Complexes. Organometallics, 2015, 34, 3255-3263.	1.1	9
84	Computational Study of Intramolecular Arene Palladation at a Palladium(IV) Center. Organometallics, 2015, 34, 1085-1090.	1.1	23
85	Gas-Phase and Computational Study of Identical Nickel- and Palladium-Mediated Organic Transformations Where Mechanisms Proceeding via M ^{II} or M ^{IV} Oxidation States Are Determined by Ancillary Ligands. Journal of the American Chemical Society, 2015, 137, 13588-13593.	6.6	8
86	Synthesis, structure and gas-phase reactivity of the mixed silver hydride borohydride nanocluster [Ag ₃ (μ ₃ -H)(μ ₃ -BH ₄)L ^{Ph} ₃]BF	<sub2x84< s<="" td=""><td>ub>2(ts^P</td></sub2x84<>	ub>2(ts ^P
87	Experimental and computational evidence for KOt-Bu-promoted synthesis of oxopyrazino[1,2-a]indoles. RSC Advances, 2015, 5, 101353-101361.	1.7	19
88	Computational Mechanistic Study of Palladium(II)-Catalyzed Carboxyalkynylation of an Olefin Using an Iodine(III) Oxidant Reagent. Organometallics, 2014, 33, 7318-7324.	1.1	20
89	Highly Selective Liquid-Phase Oxidation of Cyclohexane to KA Oil over Ti-MWW Catalyst: Evidence of Formation of Oxyl Radicals. ACS Catalysis, 2014, 4, 53-62.	5.5	66
90	Decarboxylative-Coupling of Allyl Acetate Catalyzed by Group 10 Organometallics, [(phen)M(CH ₃)] ⁺ . Journal of Organic Chemistry, 2014, 79, 12056-12069.	1.7	24

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91	Mechanistic Insights into the Oxidative Coupling of Nâ€Heterocyclic Carbenes within the Coordination Sphere of Copper Complexes. Chemistry - A European Journal, 2014, 20, 12729-12733.	1.7	14
92	NO2bond cleavage by MoL3complexes. Dalton Transactions, 2014, 43, 1620-1629.	1.6	3
93	Computational Study of Carbostannylation Implicating Bimetallic Catalysis Involving "Au ^I –Vinyl–Pd ^{II} ―Species. ACS Catalysis, 2014, 4, 860-869.	5.5	9
94	A Density Functional Theory (DFT) Mechanistic Study of Gold(I)-Catalyzed Alkynylation of the Indole and Pyrrole Substrates, Using a Hypervalent Iodine Reagent. ACS Catalysis, 2014, 4, 2896-2907.	5.5	47
95	Theoretical Study of the Mechanism of CO and Acetylene Migratory Insertions into Pt–Cp* Bonds. Organometallics, 2014, 33, 2384-2387.	1.1	2
96	Formation of Ethane from Mono-Methyl Palladium(II) Complexes. Journal of the American Chemical Society, 2014, 136, 8237-8242.	6.6	35
97	Theoretical Study on the Ring-Opening Reactions of Cyclopropenes Mediated by a Au ^I Complex. Journal of Organic Chemistry, 2013, 78, 9553-9559.	1.7	21
98	Mechanism of Pd-Catalyzed Ar–Ar Bond Formation Involving Ligand-Directed C–H Arylation and Diaryliodonium Oxidants: Computational Studies of Orthopalladation at Binuclear Pd(II) Centers, Oxidation To Form Binuclear Palladium(III) Species, and Ar··Àr Reductive Coupling. Organometallics, 2013, 32, 544-555.	1.1	52
99	Understanding the mechanism of Cul-catalyzed N–H carboxylation of heterocyclic rings with CO2 from a theoretical point of view. Journal of Organometallic Chemistry, 2013, 748, 89-97.	0.8	7
100	Theoretical Investigation into the Mechanism of 3′-dGMP Oxidation by [Pt ^{IV} Cl ₄ (dach)]. Inorganic Chemistry, 2013, 52, 707-717.	1.9	31
101	Theoretical Investigation into the Mechanism of Ethylene Polymerization by a Cationic Dinuclear Aluminum Complex: A Longstanding Unresolved Issue. Organometallics, 2013, 32, 1687-1693.	1.1	9
102	Synthetic and computational studies of the palladium(iv) system Pd(alkyl)(aryl)(alkynyl)(bidentate)(triflate) exhibiting selectivity in C–C reductive elimination. Dalton Transactions, 2012, 41, 11820.	1.6	19
103	Theoretical Investigation into the Palladium-Catalyzed Silaboration of Pyridines. Organometallics, 2012, 31, 1680-1687.	1.1	14
104	Oxo iron(iv) as an oxidative active intermediate of p-chlorophenol in the Fenton reaction: a DFT study. Physical Chemistry Chemical Physics, 2012, 14, 3766.	1.3	7
105	Density Functional Theory Studies on the Oxidation of 5′-dGMP and 5′-dAMP by a Platinum(IV) Complex. Inorganic Chemistry, 2012, 51, 8002-8013.	1.9	10
106	Connecting Binuclear Pd(III) and Mononuclear Pd(IV) Chemistry by Pd–Pd Bond Cleavage. Journal of the American Chemical Society, 2012, 134, 12002-12009.	6.6	148
107	Theoretical Investigation into the Mechanism of Au(I)-Catalyzed Reaction of Alcohols with 1,5 Enynes. Journal of the American Chemical Society, 2012, 134, 16882-16890.	6.6	39
108	Tuning the Laplaza-Cummins 3-coordinate M[N(R)Ph]3 catalyst to activate and cleave CO2. Dalton Transactions, 2011, 40, 5569.	1.6	12

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109	Titanium-mediated rearrangement of cyclopropenylmethyl acetates to (E)-halodienes. Organic and Biomolecular Chemistry, 2011, 9, 3359.	1.5	10
110	Insight into the Mechanism of Râ^'R Reductive Elimination from the Six-Coordinate d ⁶ Complexes L ₂ Pt(R) ₄ (R = vinyl, Me). Organometallics, 2011, 30, 422-432.	1.1	29
111	Assembly of Cyclometalated Platinum(II) Complexes via 1,1′-Bis(diphenylphosphino)ferrocene Ligand: Kinetics and Mechanisms. Organometallics, 2011, 30, 1466-1477.	1.1	27
112	Theoretical Investigation into the Mechanism of Reductive Elimination from Bimetallic Palladium Complexes. Inorganic Chemistry, 2011, 50, 6449-6457.	1.9	46
113	DFT Study on the Mechanism of the Activation and Cleavage of CO ₂ by (NHC)CuEPh ₃ (E = Si, Ge, Sn). Organometallics, 2011, 30, 1340-1349.	1.1	66
114	DFT Studies on the Carboxylation of the C–H Bond of Heteroarenes by Copper(I) Complexes. Organometallics, 2011, 30, 6218-6224.	1.1	38
115	Density functional studies of influences of Ni triad metals and solvents on oxidative addition of Mel to [M(CH3)2(NH3)2] complexes and C–C reductive elimination from [M(CH3)3(NH3)2I] complexes. Journal of Organometallic Chemistry, 2011, 696, 3351-3358.	0.8	21
116	Scission of Carbon Monoxide Using TaR ₃ , R=(N(<i>t</i> Bu)Ph) or OSi(<i>t</i> Bu) ₃ : A DFT Investigation. Chemistry - A European Journal, 2010, 16, 8117-8132.	1.7	7
117	Factors Dictating Carbene Formation at (PNP)Ir. Organometallics, 2010, 29, 4239-4250.	1.1	16
118	Ligand Effects in Bimetallic High Oxidation State Palladium Systems. Inorganic Chemistry, 2010, 49, 11249-11253.	1.9	37
119	Density Functional Theory Study on the Mechanism of the Reductive Cleavage of CO ₂ by a Bis-β-Diketoiminatediiron Dinitrogen Complex. Inorganic Chemistry, 2010, 49, 7773-7782.	1.9	22
120	Experimental and Theoretical Investigation into the Gold-Catalyzed Reactivity of Cyclopropenylmethyl Acetates. Organic Letters, 2010, 12, 4768-4771.	2.4	43
121	In-depth insight into the electronic and steric effects of phosphine ligands on the mechanism of the R–R reductive elimination from (PR3)2PdR2. Journal of Organometallic Chemistry, 2009, 694, 2075-2084.	0.8	37
122	Mechanistic Studies of Ligand Fluxionality in [M(η5-Cp)(η1-Cp)(L)2]n. Journal of Physical Chemistry A, 2009, 113, 2982-2989.	1.1	8
123	Cleavage of Carbon Dioxide by an Iridium-Supported Fischer Carbene. A DFT Investigation. Journal of the American Chemical Society, 2009, 131, 5800-5808.	6.6	43
124	Subtle Balance of Ligand Steric Effects in Stille Transmetalation. Journal of the American Chemical Society, 2009, 131, 13981-13991.	6.6	76
125	Reactivity of CO2 towards Mo[N(R)Ph]3. Dalton Transactions, 2009, , 9266.	1.6	13
126	A Molecular Orbital Rationalization of Ligand Effects in N ₂ Activation. Chemistry - A European Journal, 2008, 14, 6119-6124.	1.7	13

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127	Activation of CS2 and CS by ML3 Complexes. Journal of the American Chemical Society, 2008, 130, 11928-11938.	6.6	37
128	Synthesis of Double-End-Capped Polyethylene by a Cationic Tris(pyrazolyl)borate Zirconium Benzyl Complex. Organometallics, 2008, 27, 5867-5875.	1.1	26
129	Understanding the Highly Regioselective Cyanothiolation of 1-Alkynes Catalyzed by Palladium Phosphine Complexes. Organometallics, 2008, 27, 246-253.	1.1	43
130	Theoretical studies of the oxidative addition of PhBr to Pd(PX3)2 and Pd(X2PCH2CH2PX2) (X=Me, H, Cl). Journal of Organometallic Chemistry, 2007, 692, 3984-3993.	0.8	48
131	β-Heteroatom versus β-Hydrogen Elimination: A Theoretical Study. Organometallics, 2006, 25, 812-819.	1.1	87
132	Effect of the Leaving Ligand X on Transmetalation of Organostannanes (vinylSnR3) with LnPd(Ar)(X) in Stille Cross-Coupling Reactions. A Density Functional Theory Study. Organometallics, 2006, 25, 5788-5794.	1.1	67
133	DFT Studies on the Mechanism of Allylative Dearomatization Catalyzed by Palladium. Journal of the American Chemical Society, 2006, 128, 13010-13016.	6.6	76
134	In-depth insight into metal–alkene bonding interactions. Inorganica Chimica Acta, 2006, 359, 3527-3534.	1.2	18
135	Theoretical studies on the protonation behavior of tropone and its metal complexes. Journal of Organometallic Chemistry, 2006, 691, 4545-4555.	0.8	5
136	Understanding the Relative Easiness of Oxidative Addition of Aryl and Alkyl Halides to Palladium(0). Organometallics, 2006, 25, 4030-4033.	1.1	140
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138	Density functional theory study on structural isomers and bonding of model complexes M(CO)5(BH3·PH3) (M=Cr, Mo, W) and W(CO)5(BH3·AH3) (A=N, P, As, Sb). Journal of Organometallic Chemistry, 2005, 690, 1147-1156.	0.8	9
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