Alireza Ariafard

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8322170/publications.pdf

Version: 2024-02-01

155 papers	5,244 citations	136950 32 h-index	98798 67 g-index
163 all docs	163 docs citations	163 times ranked	5878 citing authors

#	Article	IF	Citations
1	Degradation of chlorophenols by means of advanced oxidation processes: a general review. Applied Catalysis B: Environmental, 2004, 47, 219-256.	20.2	1,874
2	Connecting Binuclear Pd(III) and Mononuclear Pd(IV) Chemistry by Pdâ€“Pd Bond Cleavage. Journal of the American Chemical Society, 2012, 134, 12002-12009.	13.7	148
3	Understanding the Relative Easiness of Oxidative Addition of Aryl and Alkyl Halides to Palladium(0). Organometallics, 2006, 25, 4030-4033.	2.3	140
4	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.	13.8	99
5	Î²-Heteroatom versus Î²-Hydrogen Elimination:Â A Theoretical Study. Organometallics, 2006, 25, 812-819.	2.3	87
6	Nickel(IV)-Catalyzed Câ€“H Trifluoromethylation of (Hetero)arenes. Journal of the American Chemical Society, 2019, 141, 12872-12879.	13.7	82
7	DFT Studies on the Mechanism of Allylative Dearomatization Catalyzed by Palladium. Journal of the American Chemical Society, 2006, 128, 13010-13016.	13.7	76
8	Subtle Balance of Ligand Steric Effects in Stille Transmetalation. Journal of the American Chemical Society, 2009, 131, 13981-13991.	13.7	76
9	Borane-Catalyzed Stereoselective Câ€“H Insertion, Cyclopropanation, and Ring-Opening Reactions. CheM, 2020, 6, 2364-2381.	11.7	70
10	A Theoretical Study on the Protodeauration Step of the Gold(I)-Catalyzed Organic Reactions. Organometallics, 2015, 34, 3186-3195.	2.3	68
11	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.	2.3	67
12	DFT Study on the Mechanism of the Activation and Cleavage of CO₂ by (NHC)CuEPh₃ (E = Si, Ge, Sn). Organometallics, 2011, 30, 1340-1349.	2.3	66
13	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.	11.2	66
14	Oxidatively Induced Câ€“H Activation at High Valent Nickel. Journal of the American Chemical Society, 2017, 139, 6058-6061.	13.7	62
15	Experimental and Computational Studies of High-Valent Nickel and Palladium Complexes. Organometallics, 2017, 36, 4382-4393.	2.3	55
16	Mechanism of Pd-Catalyzed Arâ€“Ar Bond Formation Involving Ligand-Directed Câ€“H Arylation and Diaryliodonium Oxidants: Computational Studies of Orthopalladation at Binuclear Pd(II) Centers, Oxidation To Form Binuclear Palladium(III) Species, and ArÂ·Â·Â·Ar Reductive Coupling. Organometallics, 2013, 32, 544-555.	2.3	52
17	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.	1.8	48
18	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.	11.2	47

#	Article	IF	Citations
19	Theoretical Investigation into the Mechanism of Reductive Elimination from Bimetallic Palladium Complexes. Inorganic Chemistry, 2011, 50, 6449-6457.	4.0	46
20	Understanding the Highly Regioselective Cyanothiolation of 1-Alkynes Catalyzed by Palladium Phosphine Complexes. Organometallics, 2008, 27, 246-253.	2.3	43
21	Cleavage of Carbon Dioxide by an Iridium-Supported Fischer Carbene. A DFT Investigation. Journal of the American Chemical Society, 2009, 131, 5800-5808.	13.7	43
22	Experimental and Theoretical Investigation into the Gold-Catalyzed Reactivity of Cyclopropenylmethyl Acetates. Organic Letters, 2010, 12, 4768-4771.	4.6	43
23	Isomerism of Cp-Containing Transition Metal Allyl Complexes. Organometallics, 2005, 24, 680-686.	2.3	39
24	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.	13.7	39
25	DFT Studies on the Carboxylation of the Câ€“H Bond of Heteroarenes by Copper(I) Complexes. Organometallics, 2011, 30, 6218-6224.	2.3	38
26	Activation of CS2 and CS by ML3 Complexes. Journal of the American Chemical Society, 2008, 130, 11928-11938.	13.7	37
27	In-depth insight into the electronic and steric effects of phosphine ligands on the mechanism of the Râ€“R reductive elimination from (PR3)2PdR2. Journal of Organometallic Chemistry, 2009, 694, 2075-2084.	1.8	37
28	Ligand Effects in Bimetallic High Oxidation State Palladium Systems. Inorganic Chemistry, 2010, 49, 11249-11253.	4.0	37
29	Arylâ€“Fluoride Bond-Forming Reductive Elimination from Nickel(IV) Centers. Journal of the American Chemical Society, 2019, 141, 13261-13267.	13.7	37
30	Mechanism of Endoâ^'Exo Interconversion in Î·3-Allyl Cp Complexes:â€‰ A Longstanding Unresolved Issue. Organometallics, 2005, 24, 2241-2244.	2.3	36
31	Formation of Ethane from Mono-Methyl Palladium(II) Complexes. Journal of the American Chemical Society, 2014, 136, 8237-8242.	13.7	35
32	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.	13.7	33
33	Gas-Phase Ionâ€“Molecule Reactions of Copper Hydride Anions [CuH₂]^{â^'} and [Cu₂H₃]^{â^'}. Inorganic Chemistry, 2017, 56, 2387-2399.	4.0	32
34	Triarylboraneâ€Catalyzed Alkenylation Reactions of Aryl Esters with Diazo Compounds. Angewandte Chemie - International Edition, 2020, 59, 15492-15496.	13.8	32
35	Theoretical Investigation into the Mechanism of 3â€²-dGMP Oxidation by [Pt^{IV}Cl₄(dach)]. Inorganic Chemistry, 2013, 52, 707-717.	4.0	31
36	Insight into the Mechanism of Râ^'R Reductive Elimination from the Six-Coordinate d⁶ Complexes L₂Pt(R)₄ (R = vinyl, Me). Organometallics, 2011, 30, 422-432.	2.3	29

#	Article	IF	Citations
37	DFT mechanistic investigation into phenol dearomatization mediated by an iodine(<scp>iii</scp>) reagent. Organic and Biomolecular Chemistry, 2019, 17, 3521-3528.	2.8	29
38	Hydrogen peroxide decomposition over La0.9Sr0.1Ni1â˜'Cr O3 perovskites. Catalysis Communications, 2003, 4, 561-566.	3.3	28
39	Mechanistic Elucidation of the Arylation of Non-Spectator N-Heterocyclic Carbenes at Copper Using a Combined Experimental and Computational Approach. Organometallics, 2015, 34, 3497-3507.	2.3	28
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.	3.3	28
41	Dual Goldâ€Catalyzed Cycloaromatization of Unconjugated (E)â€Enediynes. Angewandte Chemie - International Edition, 2019, 58, 2114-2119.	13.8	28
42	Copper-catalysed synthesis of Î±-alkylidene cyclic carbonates from propargylic alcohols and CO₂. Green Chemistry, 2021, 23, 889-897.	9.0	28
43	Site-Selective C_{sp³}â€“C_{sp}/C_{sp³}â€“C_{sp²} Cross-Coupling Reactions Using Frustrated Lewis Pairs. Journal of the American Chemical Society, 2021, 143, 4451-4464.	13.7	28
44	Assembly of Cyclometalated Platinum(II) Complexes via 1,1â€²-Bis(diphenylphosphino)ferrocene Ligand: Kinetics and Mechanisms. Organometallics, 2011, 30, 1466-1477.	2.3	27
45	Theoretical Studies of Cycloaddition Reactions of Cationic Aluminum Î²-Diketiminate Alkyl Complexes with Alkenes and Alkynes. Organometallics, 2005, 24, 5140-5146.	2.3	26
46	Synthesis of Double-End-Capped Polyethylene by a Cationic Tris(pyrazolyl)borate Zirconium Benzyl Complex. Organometallics, 2008, 27, 5867-5875.	2.3	26
47	Synthesis, structure and gas-phase reactivity of the mixed silver hydride borohydride nanocluster [Ag₃(Î¼₃-H)(Î¼₃-BH₄)L^{Ph}₃]BF₄(L^{Ph}	5.4	26
48	Computational study of C(sp³)â€“O bond formation at a Pd^{IV} centre. Dalton Transactions, 2017, 46, 3742-3748.	3.3	25
49	Gold-catalyzed domino cyclizationâ€“alkynylation reactions with EBX reagents: new insights into the reaction mechanism. Dalton Transactions, 2017, 46, 12257-12262.	3.3	25
50	Nickel(II/IV) Manifold Enables Room-Temperature C(sp³)â€“H Functionalization. Journal of the American Chemical Society, 2019, 141, 19513-19520.	13.7	25
51	Decarboxylative-Coupling of Allyl Acetate Catalyzed by Group 10 Organometallics, [(phen)M(CH₃)]⁺. Journal of Organic Chemistry, 2014, 79, 12056-12069.	3.2	24
52	A one-pot route to thioamides discovered by gas-phase studies: palladium-mediated CO₂ extrusion followed by insertion of isothiocyanates. Chemical Communications, 2017, 53, 3854-3857.	4.1	24
53	Computational Study of Intramolecular Arene Palladation at a Palladium(IV) Center. Organometallics, 2015, 34, 1085-1090.	2.3	23
54	Density Functional Theory Study on the Mechanism of the Reductive Cleavage of CO₂ by a Bis-Î²-Diketoiminatediiron Dinitrogen Complex. Inorganic Chemistry, 2010, 49, 7773-7782.	4.0	22

#	Article	IF	Citations
55	A Mechanistic Investigation of the Gold(III)-Catalyzed Hydrofurylation of Câ€“C Multiple Bonds. Journal of the American Chemical Society, 2016, 138, 14599-14608.	13.7	22
56	DFT Mechanistic Investigation into BF₃-Catalyzed Alcohol Oxidation by a Hypervalent Iodine(III) Compound. ACS Catalysis, 2019, 9, 6510-6521.	11.2	22
57	Density functional studies of influences of Ni triad metals and solvents on oxidative addition of MeI to [M(CH3)2(NH3)2] complexes and Câ€“C reductive elimination from [M(CH3)3(NH3)2I] complexes. Journal of Organometallic Chemistry, 2011, 696, 3351-3358.	1.8	21
58	Theoretical Study on the Ring-Opening Reactions of Cyclopropenes Mediated by a Au^I Complex. Journal of Organic Chemistry, 2013, 78, 9553-9559.	3.2	21
59	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.	11.2	21
60	Computational Mechanistic Study of Palladium(II)-Catalyzed Carboxyalkynylation of an Olefin Using an Iodine(III) Oxidant Reagent. Organometallics, 2014, 33, 7318-7324.	2.3	20
61	A transition-metal-free fast track to flavones and 3-arylcoumarins. Chemical Communications, 2017, 53, 10676-10679.	4.1	20
62	Synthetic and computational studies of the palladium(iv) system Pd(alkyl)(aryl)(alkynyl)(bidentate)(triflate) exhibiting selectivity in Câ€“C reductive elimination. Dalton Transactions, 2012, 41, 11820.	3.3	19
63	Experimental and computational evidence for KOt-Bu-promoted synthesis of oxopyrazino[1,2-a]indoles. RSC Advances, 2015, 5, 101353-101361.	3.6	19
64	Total Synthesis of (Â±)â€Dihydroisosubamol. Advanced Synthesis and Catalysis, 2017, 359, 866-874.	4.3	19
65	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.	4.1	19
66	Gold Catalyzed Cyclopropanation/[5+3] Cycloaddition of 1,4,9â€•and 1,4,10â€Allenenynes to Bicyclo[3.3.1]nonane Derivatives. Advanced Synthesis and Catalysis, 2020, 362, 1084-1095.	4.3	19
67	In-depth insight into metalâ€“alkene bonding interactions. Inorganica Chimica Acta, 2006, 359, 3527-3534.	2.4	18
68	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.	4.1	18
69	Different Selectivities in the Insertions into C(sp²)â^'H Bonds: Benzofulvenes by Dual Gold Catalysis Competition Experiments. Chemistry - A European Journal, 2018, 24, 10766-10772.	3.3	18
70	Mechanistic investigation into phenol oxidation by IBX elucidated by DFT calculations. Organic and Biomolecular Chemistry, 2020, 18, 1117-1129.	2.8	18
71	Tris(pentafluorophenyl)boraneâ€Catalyzed Carbenium Ion Generation and Autocatalytic Pyrazole Synthesisâ€”A Computational and Experimental Study. Angewandte Chemie - International Edition, 2021, 60, 24395-24399.	13.8	18
72	Reduction of a platinum(<scp>iv</scp>) prodrug model by sulfur containing biological reductants: computational mechanistic elucidation. Chemical Communications, 2018, 54, 10491-10494.	4.1	17

#	Article	IF	Citations
73	Gold-Catalyzed [5,5]-Rearrangement. ACS Catalysis, 2021, 11, 6510-6518.	11.2	17
74	Factors Dictating Carbene Formation at (PNP)Ir. Organometallics, 2010, 29, 4239-4250.	2.3	16
75	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.	2.3	16
76	Structure and Bonding of d8 Allyl Complexes M(Î·3-allyl)L3 (M = Co, Rh, Ir; L = Phosphine or Carbonyl). Organometallics, 2005, 24, 3800-3806.	2.3	14
77	Theoretical Investigation into the Palladium-Catalyzed Silaboration of Pyridines. Organometallics, 2012, 31, 1680-1687.	2.3	14
78	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.	3.3	14
79	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.	3.3	14
80	A Molecular Orbital Rationalization of Ligand Effects in N₂ Activation. Chemistry - A European Journal, 2008, 14, 6119-6124.	3.3	13
81	Reactivity of CO2 towards Mo[N(R)Ph]3. Dalton Transactions, 2009, , 9266.	3.3	13
82	Tuning the Laplaza-Cummins 3-coordinate M[N(R)Ph]3 catalyst to activate and cleave CO2. Dalton Transactions, 2011, 40, 5569.	3.3	12
83	Proton supplier role of binuclear gold complexes in promoting hydrofunctionalisation of nonactivated alkenes. Catalysis Science and Technology, 2019, 9, 1420-1426.	4.1	11
84	The role of hypervalent iodine(<scp>iii</scp>) reagents in promoting alkoxylation of unactivated C(sp³)â€“H bonds catalyzed by palladium(<scp>ii</scp>) complexes. Chemical Science, 2021, 12, 7185-7195.	7.4	11
85	Understanding the Influence of Donorâ€Acceptor Diazo Compounds on the Catalyst Efficiency of B(C₆F₅)₃ Towards Carbene Formation. Chemistry - A European Journal, 2022, 28, .	3.3	11
86	Titanium-mediated rearrangement of cyclopropenylmethyl acetates to (E)-halodienes. Organic and Biomolecular Chemistry, 2011, 9, 3359.	2.8	10
87	Density Functional Theory Studies on the Oxidation of 5â€²-dGMP and 5â€²-dAMP by a Platinum(IV) Complex. Inorganic Chemistry, 2012, 51, 8002-8013.	4.0	10
88	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.	4.1	10
89	A Modified Cationic Mechanism for PdCl2-Catalyzed Transformation of a Homoallylic Alcohol to an Allyl Ether. Organometallics, 2019, 38, 2953-2962.	2.3	10
90	Disclosure of Some Obscure Mechanistic Aspects of the Copper-Catalyzed Click Reactions Involving N₂ Elimination Promoted by the Use of Electron-Deficient Azides from a DFT Perspective. Organometallics, 2019, 38, 256-267.	2.3	10

#	Article	IF	Citations
91	Iron Triflate Salts as Highly Active Catalysts for the Solventâ€Free Oxidation of Cyclohexane. European Journal of Organic Chemistry, 2020, 2020, 3552-3559.	2.4	10
92	Copper(I)-catalysed site-selective C(sp3)â€“H bond chlorination of ketones, (E)-enones and alkylbenzenes by dichloramine-T. Nature Communications, 2021, 12, 4065.	12.8	10
93	Borane Catalyzed Selective Diazo Crossâ€Coupling Towards Pyrazoles. Advanced Synthesis and Catalysis, 2022, 364, 773-780.	4.3	10
94	Density functional theory study on structural isomers and bonding of model complexes M(CO)5(BH3Â·PH3) (M=Cr, Mo, W) and W(CO)5(BH3Â·AH3) (A=N, P, As, Sb). Journal of Organometallic Chemistry, 2005, 690, 1147-1156.	1.8	9
95	Theoretical Investigation into the Mechanism of Ethylene Polymerization by a Cationic Dinuclear Aluminum Complex: A Longstanding Unresolved Issue. Organometallics, 2013, 32, 1687-1693.	2.3	9
96	Computational Study of Carbostannylation Implicating Bimetallic Catalysis Involving â€œAu^Iâ€“Vinylâ€“Pd^{II}â€•Species. ACS Catalysis, 2014, 4, 860-869.	11.2	9
97	Prying open a Reactive Site for Allylic Arylation by Phosphine-Ligated Geminally Diaurated Aryl Complexes. Organometallics, 2015, 34, 3255-3263.	2.3	9
98	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.	2.3	9
99	Chiral Gold Complex Catalyzed Cycloisomerization/Regio- and Enantioselective Nitroso-Dielsâ€“Alder Reaction of 1,6-Diyne Esters with Nitrosobenzenes. ACS Catalysis, 2022, 12, 7288-7299.	11.2	9
100	Theoretical study on interaction of different coordination modes of BH4 ligand with transition metal in [TM(BH4)(CO)4]â^' (TM=Cr, Mo). Journal of Organometallic Chemistry, 2005, 690, 84-95.	1.8	8
101	Mechanistic Studies of Ligand Fluxionality in [M(Î·5-Cp)(Î·1-Cp)(L)2]n. Journal of Physical Chemistry A, 2009, 113, 2982-2989.	2.5	8
102	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.	13.7	8
103	DFT-Based Comparison between Mechanistic Aspects of Amine and Alcohol Oxidation Mediated by IBX. Journal of Organic Chemistry, 2020, 85, 515-525.	3.2	8
104	Triarylborane catalysedN-alkylation of amines with aryl esters. Catalysis Science and Technology, 2020, 10, 7523-7530.	4.1	8
105	Bidentate Nitrogen-Ligated I(V) Reagents, Bi(N)-HVIs: Preparation, Stability, Structure, and Reactivity. Journal of Organic Chemistry, 2021, 86, 6566-6576.	3.2	8
106	DFT study of metalâ€“tetrahydroborato ligand interactions in [Ti(CO)4(BH4)]â^'. Computational and Theoretical Chemistry, 2003, 625, 305-314.	1.5	7
107	DFT studies of structural preference of coordinated ethylene in W(CO)3(PX3)2(CH2˜...CH2) (X=H, CH3, F,) Tj ETQq1 1 0.784314 rgB	1.8	7
108	Scission of Carbon Monoxide Using TaR₃, R=(N(tBu)Ph) or OSi(tBu)₃: A DFT Investigation. Chemistry - A European Journal, 2010, 16, 8117-8132.	3.3	7

#	Article	IF	Citations
109	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.	2.8	7
110	Understanding the mechanism of CuI-catalyzed Nâ€“H carboxylation of heterocyclic rings with CO2 from a theoretical point of view. Journal of Organometallic Chemistry, 2013, 748, 89-97.	1.8	7
111	Dual Goldâ€Catalyzed Cycloaromatization of Unconjugated (E)â€Enediynes. Angewandte Chemie, 2019, 131, 2136-2141.	2.0	7
112	Theoretical studies of rotational barriers of dithiocarbamate ligands in the square planar complexes TM(L)(Lâ€²)(H2dtc) (TM=Ir, Rh). Computational and Theoretical Chemistry, 2003, 636, 49-56.	1.5	6
113	Does type of phosphine affect rotational barrier of vinylidene in the complexes OsHCl(CCH2)(L)2 (L=phosphine)?. Inorganic Chemistry Communication, 2004, 7, 999-1002.	3.9	6
114	Sulfur Dioxide Activation: A Theoretical Investigation into Dual Sâ•O Bond Cleavage by Three-Coordinate Molybdenum(III) Complexes. Inorganic Chemistry, 2015, 54, 534-543.	4.0	6
115	Ïƒ-Alkenyl endo-palladacycle formation via regiospecific functionalisation of an unreactive NHC-tethered C(sp²)â€“H bond. Chemical Communications, 2015, 51, 5513-5515.	4.1	6
116	Computational study of selectivity in the [Pt^{II}Cl₄]^{2â^'}-catalysed arylation of arenes by diaryliodonium reagents: arene activation at Pt^{IV} centres. Dalton Transactions, 2017, 46, 15480-15486.	3.3	6
117	Substituent effects in the decarboxylation reactions of coordinated arylcarboxylates in dinuclear copper complexes, [(napy)Cu₂(O₂CC₆H₄X)]⁺. European Journal of Mass Spectrometry, 2017, 23, 351-358.	1.0	6
118	Nazarov cyclisations initiated by DDQ-oxidised pentadienyl ether: a mechanistic investigation from the DFT perspective. Organic and Biomolecular Chemistry, 2018, 16, 9021-9029.	2.8	6
119	Accessing Chelating Extended Linker Bis(NHC) Palladium(II) Complexes: Sterically Triggered Divergent Reaction Pathways. Organometallics, 2019, 38, 3032-3038.	2.3	6
120	Computational Analysis of Mesomerism in paraâ€Substituted merâ€NCN Pincer Platinum(II) Complexes, Including its Relationships with Hammett Ïƒ_p Substituent Parameters. Chemistry - A European Journal, 2020, 26, 15629-15635.	3.3	6
121	Goldâ€Catalyzed Annulation of 1,8â€Dialkynylnaphthalenes: Synthesis and Photoelectric Properties of Indenophenaleneâ€Based Derivatives. Chemistry - A European Journal, 2021, 27, 3552-3559.	3.3	6
122	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.	11.2	6
123	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.	3.2	6
124	Exploring Cyclization Strategies to Access Stemona Alkaloids: Subtle Effects Influencing Reactivity in Intramolecular Michael Additions. Organic Letters, 2021, 23, 8494-8498.	4.6	6
125	Stability of Heavier Group 14 Analogues of Vinylidene Complexes:â€‰ A Theoretical Study. Organometallics, 2005, 24, 6283-6286.	2.3	5
126	Theoretical studies on the protonation behavior of tropone and its metal complexes. Journal of Organometallic Chemistry, 2006, 691, 4545-4555.	1.8	5

#	Article	IF	Citations
127	Phosphine-Scavenging Role of Gold(I) Complexes from Pd(P^tBu₃)₂ in the Bimetallic Catalysis of Carbostannylation of Alkynes. Organometallics, 2017, 36, 2014-2019.	2.3	5
128	How the combination of PhIO and I₂ provides a species responsible for conducting organic reactions through radical mechanisms. Organic and Biomolecular Chemistry, 2020, 18, 8103-8108.	2.8	5
129	Triarylboranâ€katalysierte Alkenylierungen von Arylestern mit Diazoverbindungen. Angewandte Chemie, 2020, 132, 15621-15626.	2.0	5
130	Catalytic Role of Lewis Acids in ArIOâ€Mediated Oxidative Fluorination Reactions Revealed by DFT Calculations. European Journal of Organic Chemistry, 2020, 2020, 2251-2259.	2.4	5
131	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.	3.7	5
132	Rhodium-catalysed tetradehydro-Dielsâ€“Alder reactions of enediynes via a rhodium-stabilized cyclic allene. Chemical Science, 2020, 11, 10945-10950.	7.4	4
133	Catalytic role of amines in activation of PhICl₂ from a computational point of view. Chemical Communications, 2021, 57, 9108-9111.	4.1	4
134	Photochemical Activation of a Hydroxyquinone-Derived Phenyliodonium Ylide by Visible Light: Synthetic and Mechanistic Investigations. Journal of Organic Chemistry, 2021, 86, 1758-1768.	3.2	4
135	Two-Stage Catalysis in the Pd-Catalyzed Formation of 2,2,2-Trifluoroethyl-Substituted Acrylamides: Oxidative Alkylation of PdII by an IIII Reagent and Roles for Acetate, Triflate, and Triflic Acid. Organometallics, 0, , .	2.3	4
136	A Rare Alderâ€ene Cycloisomerization of 1,6â€Allenynes. Chemistry - A European Journal, 2022, 28, .	3.3	4
137	NO2bond cleavage by MoL3complexes. Dalton Transactions, 2014, 43, 1620-1629.	3.3	3
138	Phosphine-Scavenging Cationic Gold(I) Complexes: Alternative Applications of Gold Cocatalysis in Fundamental Palladium-Catalyzed Cross-Couplings. Organometallics, 2019, 38, 2683-2688.	2.3	3
139	Computational Investigation into the Mechanistic Features of Bromide-Catalyzed Alcohol Oxidation by PhIO in Water. Journal of Organic Chemistry, 2021, 86, 2998-3007.	3.2	3
140	Computational Study of Intramolecular Coordination Enhanced Oxidative Addition to form PdIV-Pincer Complexes, and Selectivity in Aryloxide Attack at PdIVCH2CRRâ€² Motifs in Palladium-Mediated Organic Synthesis. Organometallics, 2021, 40, 1262-1269.	2.3	3
141	Role of BrÃ¸nsted Acids in Promoting Pd(OAc)2-Catalyzed Chlorination of Phenol Carbamates Using N-Chlorosuccinimide. ACS Catalysis, 0, , 2681-2693.	11.2	3
142	Lewis Acid Assisted BrÃ¸nsted Acid Catalysed Decarbonylation of Isocyanates: A Combined DFT and Experimental Study. Chemistry - A European Journal, 2022, , .	3.3	3
143	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.	3.3	3
144	Comparison of rotational barriers of dithiocarbamate ligand in the four- and five-coordinate complexes Ir(PH3)(CO)(H2dtc) and Ir(PH3)2(CO)(H2dtc): a theoretical viewpoint. Computational and Theoretical Chemistry, 2004, 672, 141-150.	1.5	2

#	Article	IF	Citations
145	Theoretical Study of the Mechanism of CO and Acetylene Migratory Insertions into Ptâ€“Cp* Bonds. Organometallics, 2014, 33, 2384-2387.	2.3	2
146	Rationale for the reactivity differences between main group and d0 transition metal complexes toward olefin polymerisation. Dalton Transactions, 2019, 48, 6997-7005.	3.3	2
147	Tris(pentafluorophenyl)borane Catalyzed Carbenium Ion Generation and Autocatalytic Pyrazole Synthesis â€" A Computational and Experimental Study. Angewandte Chemie, 0, , .	2.0	2
148	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.	1.8	1
149	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.	1.8	1
150	Formation and reactions of the 1, 8-naphthyridine (napy) ligated geminally dimetallated phenyl complexes [(napy)Cu₂(Ph)]⁺, [(napy)Ag₂(Ph)]⁺ and [(napy)CuAg(Ph)]⁺. European Journal of Mass Spectrometry, 2019, 25, 30-43.	1.0	1
151	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.	3.3	1
152	Bismuth(III)-catalysed hydroalkylation of styrene with acetylacetone: a DFT-Based mechanistic study. Molecular Physics, 0, , .	1.7	1
153	Titelbild: Dual Gold-Catalyzed Cycloaromatization of Unconjugated (E)-Enediynes (Angew. Chem.) Tj ETQq1 1 0.784314 rgBT /Overlo	2.0	0
154	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.	3.3	0
155	Discovery of Redox-Promoted BrÃ¸nsted Acid Catalysis in the Gold(III)-Catalyzed Annulation of Phenol and Cyclohexadiene. ACS Catalysis, 0, , 7918-7925.	11.2	0