Brian F Yates

List of Publications by Year
in descending order

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187	5,910	81743	95083
papers	citations	39 h-index	68 g-index

193	193	193	4697
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Basicity of Nucleophilic Carbenes in Aqueous and Nonaqueous SolventsTheoretical Predictions. Journal of the American Chemical Society, 2004, 126, 8717-8724.	6.6	426
2	Detection of the prototype phosphonium (CH2PH3), sulfonium (CH2SH2) and chloronium (CH2ClH) ylides by neutralization-reionization mass spectrometry: a theoretical prediction. Journal of the American Chemical Society, 1984, 106, 5805-5808.	6.6	261
3	Oxidative Addition of the Imidazolium Cation to Zerovalent Ni, Pd, and Pt:Â A Combined Density Functional and Experimental Study. Journal of the American Chemical Society, 2001, 123, 8317-8328.	6.6	242
4	Kinetic and Density Functional Studies on Alkyl-Carbene Elimination from PdIIHeterocylic Carbene Complexes:Â A New Type of Reductive Elimination with Clear Implications for Catalysis. Journal of the American Chemical Society, 2001, 123, 4029-4040.	6.6	232
5	Distonic radical cations. Tetrahedron, 1986, 42, 6225-6234.	1.0	170
6	Cu-Catalyzed Fluorination of Diaryliodonium Salts with KF. Organic Letters, 2013, 15, 5134-5137.	2.4	162
7	Connecting Binuclear Pd(III) and Mononuclear Pd(IV) Chemistry by Pdâ€“Pd Bond Cleavage. Journal of the American Chemical Society, 2012, 134, 12002-12009.	6.6	148
8	Ylides and ylidions: a comparative study of unusual gas-phase structures. Journal of the American Chemical Society, 1987, 109, 2250-2263.	6.6	137
9	Unprecedented Câ€“H bond oxidative addition of the imidazolium cation to Pt0: a combined density functional analysis and experimental study. Chemical Communications, 2001, , 355-356.	2.2	122
10	A theoretical approach to gas-phase ion chemistry. Pure and Applied Chemistry, 1984, 56, 1831-1842.	0.9	91
11	The Mechanism of the Stetter Reaction â€“ A DFT Study. European Journal of Organic Chemistry, 2008, 2008, 5563-5570.	1.2	91
12	Atom-Efficient Catalytic Coupling of Imidazolium Salts with Ethylene Involving Niâˆ’NHC Complexes as Intermediates:â€‰ A Combined Experimental and DFT Study. Organometallics, 2007, 26, 5352-5363.	1.1	88
13	An Assessment of Theoretical Protocols for Calculation of the pKa Values of the Prototype Imidazolium Cation. Australian Journal of Chemistry, 2004, 57, 1205.	0.5	85
14	Subtle Balance of Ligand Steric Effects in Stille Transmetalation. Journal of the American Chemical Society, 2009, 131, 13981-13991.	6.6	76
15	Ligand design for Î± 1 adrenoceptor subtype selective antagonists. Bioorganic and Medicinal Chemistry, 2000, 8, 201-214.	1.4	71
16	Borane-Catalyzed Stereoselective Câ€“H Insertion, Cyclopropanation, and Ring-Opening Reactions. CheM, 2020, 6, 2364-2381.	5.8	70
17	A Theoretical Study on the Protodeauration Step of the Gold(I)-Catalyzed Organic Reactions. Organometallics, 2015, 34, 3186-3195.	1.1	68
18	Infrared spectrum of F.hivin..cntdot.H2O. Journal of the American Chemical Society, 1988, 110, 6327-6332.	6.6	67

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19	Organoactinides Promote the Dimerization of Aldehydes: Scope, Kinetics, Thermodynamics, and Calculation Studies. Journal of the American Chemical Society, 2011, 133, 1341-1356.	6.6	66
20	DFT Study on the Mechanism of the Activation and Cleavage of CO₂ by (NHC)CuEPh₃ (E = Si, Ge, Sn). Organometallics, 2011, 30, 1340-1349.	1.1	66
21	The syn rotational barrier in butane. Journal of the American Chemical Society, 1990, 112, 114-118.	6.6	64
22	Experimental and computational study of a reductive elimination mechanism in a methylâ€“Pd(ii)â€“CNC carbene complex. Chemical Communications, 2002, , 2500-2501.	2.2	64
23	Intramolecular hydrogen migration in ionized amines: a theoretical study of the gas-phase analogs of the Hofmann-Loeffler and related rearrangements. Journal of the American Chemical Society, 1987, 109, 2910-2915.	6.6	63
24	Symmetry breaking in the NO2 Ïƒ radical: Construction of the 2A1 and 2B2 states with Cs symmetry complete active space selfâ€consistentâ€field wave functions. Journal of Chemical Physics, 1990, 93, 8105-8109.	1.2	62
25	Mechanistic Investigations of Cu-Catalyzed Fluorination of Diaryliodonium Salts: Elaborating the Cu^I/Cu^{III} Manifold in Copper Catalysis. Organometallics, 2014, 33, 5525-5534.	1.1	60
26	Nature of the Metalâ^'Alkene Bond in Platinum Complexes of Strained Olefins. Organometallics, 1999, 18, 457-465.	1.1	59
27	The influence of N-substitution on the reductive elimination behaviour of hydrocarbylâ€“palladiumâ€“carbene complexesâ€”a DFT study. Dalton Transactions, 2006, , 1768.	1.6	57
28	Dimerization mechanisms of heterocyclic carbenes. Journal of Physical Organic Chemistry, 2005, 18, 298-309.	0.9	52
29	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.	1.1	52
30	Phosphine and solvent effects on oxidative addition of CH3Br to Pd(PR3) and Pd(PR3)2 complexes. Dalton Transactions, 2011, 40, 11089.	1.6	50
31	Theoretical Investigation into the Mechanism of Reductive Elimination from Bimetallic Palladium Complexes. Inorganic Chemistry, 2011, 50, 6449-6457.	1.9	46
32	Influence of geometry on reductive elimination of hydrocarbylâ€“palladiumâ€“carbene complexes. Dalton Transactions, 2005, , 1093-1100.	1.6	44
33	Oxidative addition of 2-substituted azolium salts to Group-10 metal zero complexesâ€”A DFT study. Dalton Transactions, 2007, , 4650.	1.6	43
34	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
35	Experimental and Theoretical Investigation into the Gold-Catalyzed Reactivity of Cyclopropenylmethyl Acetates. Organic Letters, 2010, 12, 4768-4771.	2.4	43
36	Role of the Metal, Ligand, and Alkyl/Aryl Group in the Hydrolysis Reactions of Group 10 Organometallic Cations [(L)M(R)]⁺. Organometallics, 2013, 32, 6931-6944.	1.1	43

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37	Ylide dications: an examination of first- and second-row systems. Journal of the American Chemical Society, 1986, 108, 6545-6554.	6.6	42
38	Reduction of a Chelating Bis(NHC) Palladium(II) Complex to [{Î¼â€bis(NHC)}₂Pd₂H]⁺: A Terminal Hydride in a Binuclear Palladium(I) Species Formed under Catalytically Relevant Conditions. Angewandte Chemie - International Edition, 2010, 49, 6315-6318.	7.2	41
39	Nitrogen Activation via Three-Coordinate Molybdenum Complexes: Comparison of Density Functional Theory Performance with Wave Function Based Methods. Journal of Physical Chemistry A, 2005, 109, 6762-6772.	1.1	40
40	Cationic methylpalladium(II) complexes containing bidentate Nâ€“O ligands as catalysts for the copolymerisation of CO and ethylene. Identification and isolation of intermediates from the stepwise insertion reactions, and subsequent detailed mechanistic interpretationâ€Šâ€¡. Journal of the Chemical Society Dalton Transactions, 1998, , 1137-1144.	1.1	39
41	Rhodium-Catalyzed Câ^'C Coupling Reactions: Mechanistic Considerations. Organometallics, 2008, 27, 4758-4771.	1.1	39
42	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
43	A mechanistic study on the oxidation of hydrazides: application to the tuberculosis drug isoniazid. Chemical Communications, 2008, , 1695.	2.2	38
44	DFT Studies on the Carboxylation of the Câ€“H Bond of Heteroarenes by Copper(I) Complexes. Organometallics, 2011, 30, 6218-6224.	1.1	38
45	Activation of CS2 and CS by ML3 Complexes. Journal of the American Chemical Society, 2008, 130, 11928-11938.	6.6	37
46	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.	0.8	37
47	Dimethylcuprate Undergoes a Dyotropic Rearrangement. Chemistry - A European Journal, 2010, 16, 2674-2678.	1.7	37
48	Ligand Effects in Bimetallic High Oxidation State Palladium Systems. Inorganic Chemistry, 2010, 49, 11249-11253.	1.9	37
49	NO2 radical spectroscopy: Vibrational frequencies, dipole moment, and the energy difference between the bent and linear stationary points on the ground state potential surface. Chemical Physics, 1989, 135, 179-186.	0.9	36
50	Formation of Ethane from Mono-Methyl Palladium(II) Complexes. Journal of the American Chemical Society, 2014, 136, 8237-8242.	6.6	35
51	Substituted methylene dications (HCX2+): some remarkably short bonds to carbon. Journal of the American Chemical Society, 1987, 109, 3181-3187.	6.6	34
52	Cyclic isomers of singlet Si4H4 related to tetrasilacyclobutadiene. Chemical Physics Letters, 1988, 143, 421-427.	1.2	34
53	The Mechanism of Ethylene Dimerization with the Ti(ORâ€²)₄/AlR₃ Catalytic System: DFT Studies Comparing Metallacycle and Cossee Proposals. ACS Catalysis, 2013, 3, 3006-3015.	5.5	34
54	Competing Reaction Mechanisms for the Carbonylation of Neutral Palladium(II) Complexes Containing Bidentate Ligands:Â A Theoretical Study. Organometallics, 1997, 16, 3199-3206.	1.1	31

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55	Theoretical Investigation into the Mechanism of 3â€²-dGMP Oxidation by [Pt^{IV}Cl₄(dach)]. Inorganic Chemistry, 2013, 52, 707-717.	1.9	31
56	Synthesis of N-heterocyclic carbene palladium(ii) bis-phosphine complexes and their decomposition in the presence of aryl halides. Dalton Transactions, 2007, , 3398.	1.6	30
57	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.	1.1	29
58	Tetrasilacyclobutadiylidene: The lowest energy cyclic isomer of singlet Si4H4?. Chemical Physics Letters, 1989, 155, 563-571.	1.2	28
59	Ethylene Trimerisation with Cr-PNP Catalysts: A Theoretical Benchmarking Study and Assessment of Catalyst Oxidation State. Australian Journal of Chemistry, 2014, 67, 1481.	0.5	28
60	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
61	Dual Goldâ€Catalyzed Cycloaromatization of Unconjugated (E)â€Enediynes. Angewandte Chemie - International Edition, 2019, 58, 2114-2119.	7.2	28
62	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.	6.6	28
63	Theoretical Study of Methyl-PdIIN-Heterocyclic Silylene and Germylene Complexes:Â Comparisons to N-Heterocyclic Carbene Reactivity. Organometallics, 2002, 21, 5408-5414.	1.1	27
64	The influence of peripheral ligand bulk on nitrogen activation by threeâ€coordinate molybdenum complexesâ€"A theoretical study using the ONIOM method. Journal of Computational Chemistry, 2009, 30, 2146-2156.	1.5	27
65	Solution, Structural and Catalytic Studies of Neutral MCl2 (M = Pd, Pt) Complexes of the N/E Mixed-Donor Ligands 2-(RECH2)C5H4N(RE = MeS, PhS, MeSe). European Journal of Inorganic Chemistry, 2005, 2005, 1048-1055.	1.0	26
66	Optimizing Small Molecule Activation and Cleavage in Three-Coordinate M[N(R)Ar]3Complexes. Inorganic Chemistry, 2006, 45, 6851-6859.	1.9	25
67	Computational study of C(sp³)â€“O bond formation at a Pd^{IV} centre. Dalton Transactions, 2017, 46, 3742-3748.	1.6	25
68	Breaking Chemistry's Strongest Bond: Can Three-Coordinate [M{N(R)Ar}3] Complexes Cleave Carbon Monoxide?. Chemistry - A European Journal, 2007, 13, 4264-4272.	1.7	24
69	Decarboxylative-Coupling of Allyl Acetate Catalyzed by Group 10 Organometallics, [(phen)M(CH₃)]⁺. Journal of Organic Chemistry, 2014, 79, 12056-12069.	1.7	24
70	Methylnitrene; theoretical predictions of its molecular structure and comparison with the conventional C-N single bond in methylamine. Journal of the American Chemical Society, 1989, 111, 5181-5185.	6.6	23
71	The dissociation mechanism of triplet formaldehyde. Journal of Chemical Physics, 1990, 93, 8798-8807.	1.2	23
72	Competing Rearrangements of Ammonium Ylides:Â A Quantum Theoretical Study. Journal of Organic Chemistry, 1996, 61, 7276-7284.	1.7	23

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73	Computational Study of Intramolecular Arene Palladation at a Palladium(IV) Center. Organometallics, 2015, 34, 1085-1090.	1.1	23
74	Ligand Substitution:â€‰ An Assessment of the Reliability of ab Initio Calculations. The Journal of Physical Chemistry, 1996, 100, 18363-18370.	2.9	22
75	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.	1.9	22
76	Mechanistic investigation of the oxidation of hydrazides: implications for the activation of the TB drug isoniazid. Organic and Biomolecular Chemistry, 2013, 11, 170-176.	1.5	22
77	A Mechanistic Investigation of the Gold(III)-Catalyzed Hydrofurylation of Câ€“C Multiple Bonds. Journal of the American Chemical Society, 2016, 138, 14599-14608.	6.6	22
78	DFT Mechanistic Investigation into BF₃-Catalyzed Alcohol Oxidation by a Hypervalent Iodine(III) Compound. ACS Catalysis, 2019, 9, 6510-6521.	5.5	22
79	The platinumâ€“ethylene binding energy in Pt(PL 3) 2 (C 2 H 4). Computational and Theoretical Chemistry, 2000, 506, 223-232.	1.5	21
80	Ligand rotation in [Ar(R)N]3M-N2-Mâ€²[N(R)Ar]3(M, Mâ€² = MoIII, NbIII; R =iPr andtBu) dimers. Dalton Transactions, 2005, , 962-968.	1.6	21
81	.pi.-Bonded complex between aluminum and ethylene. Journal of the American Chemical Society, 1989, 111, 6163-6167.	6.6	20
82	Lanthanide(II) and -(III) Porphyrinogensâ^' Rational Synthesis and Derivatisation of Mononuclear, Alkali-Metal-Free Lanthanide(II) and -(III)meso-Octaalkylporphyrinogen Complexes. European Journal of Inorganic Chemistry, 2004, 2004, 1992-1995.	1.0	20
83	Theoretical studies of the oxidative addition of azolium salts to a model Wilkinson's catalystElectronic supplementary information (ESI) available: Electronic energies, zero point vibrational energies and enthalpy corrections. See http://www.rsc.org/suppdata/dt/b4/b407088g/. Dalton Transactions, 2004, , 2505.	1.6	20
84	Structures and relative energies of gas-phase [C2H7N]+Ë™ radical cations. Organic Mass Spectrometry, 1987, 22, 430-436.	1.3	19
85	Synthesis, structure and optical limiting properties of organoruthenium–chalcogenide clusters. Journal of Organometallic Chemistry, 2005, 690, 1487-1497.	0.8	19
86	Pre-catalyst resting states: a kinetic, thermodynamic and quantum mechanical analyses of [PdCl2(2-oxazoline)2] complexes. Dalton Transactions, 2008, , 3115.	1.6	19
87	Activation and cleavage of the Nâ€“N bond in side-on bound [L2M-NN-ML2] (L = NH2, NMe2, NiPr2, C5H5,) Tj ETQq1 1 0.784314 rgB 2010, 39, 4529.	1.6	19
88	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.	1.6	19
89	Two Spin-State Reactivity in the Activation and Cleavage of CO2 by [ReO2]â^'. Journal of Physical Chemistry Letters, 2016, 7, 1934-1938.	2.1	19
90	Total Synthesis of (Â±)â€Dihydroisosubamol. Advanced Synthesis and Catalysis, 2017, 359, 866-874.	2.1	19

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91	Theoretical Evaluation of Alternative Pathways in the Stevens Rearrangement. Australian Journal of Chemistry, 1995, 48, 1413.	0.5	18
92	Competing mechanisms in the carbonylation of neutral palladium(II) complexes containing bidentate ligands: theoretical insights. Chemical Communications, 1996, , 781.	2.2	18
93	Investigating CNâ€“cleavage by three-coordinate M[N(R)Ar]3complexes. Dalton Transactions, 2008, , 338-344.	1.6	18
94	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.	1.7	18
95	Tris(pentafluorophenyl)boraneâ€Catalyzed Carbenium Ion Generation and Autocatalytic Pyrazole Synthesisâ€"A Computational and Experimental Study. Angewandte Chemie - International Edition, 2021, 60, 24395-24399.	7.2	18
96	On the structures and relative energies of CH3Fâ¨¥ isomers. Chemical Physics Letters, 1982, 92, 620-625.	1.2	17
97	The wealth of energetically low-lying isomers for very simple organometallic systems. The aluminum-acetylene (AlC2H2) system. Journal of the American Chemical Society, 1990, 112, 517-523.	6.6	17
98	Large Basis Set Calculations on Model Zerovalent Palladium Systems. The Journal of Physical Chemistry, 1995, 99, 14316-14322.	2.9	17
99	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
100	The methyleneammonium radical cation (CH2NH3+). Chemical Physics Letters, 1985, 116, 474-477.	1.2	16
101	Reaction of H2 with a Binuclear Zirconium Dinitrogen Complex â^' Evaluation of Theoretical Models and Hybrid Approaches. Journal of Chemical Theory and Computation, 2006, 2, 1298-1316.	2.3	16
102	Rationalizing the different products in the reaction of N2 with three-coordinate MoL3 complexes. Dalton Transactions, 2007, , 1939.	1.6	16
103	A Comparison of N₂ Cleavage in Schrock's Mo[N₃N] and Laplazaâ€“Cummins' Mo[N(R)Ar]₃ Systems. Chemistry - A European Journal, 2009, 15, 646-655.	1.7	16
104	Factors Dictating Carbene Formation at (PNP)Ir. Organometallics, 2010, 29, 4239-4250.	1.1	16
105	Steric and Electronic Effects on the Mechanism of the Stevens Rearrangementâ€"Large Organic Ylides of Unusually High Symmetry. Australian Journal of Chemistry, 1994, 47, 1685.	0.5	15
106	Buckling under Strain:â€‰ Relief of Steric Pressure Occurs Differently for Samarium(III) Porphyrinogen Complexes of the Ï€-Bound Auxiliary Ligands Cyclopentadienyl and Cyclooctatetraenediyl. Organometallics, 2007, 26, 1299-1302.	1.1	15
107	Cleavage of CO by Mo[N(R)Ar]3 Complexes. European Journal of Inorganic Chemistry, 2007, 2007, 3736-3741.	1.0	15
108	Theoretical Approaches To Estimating Homolytic Bond Dissociation Energies of Organocopper and Organosilver Compounds. Journal of Physical Chemistry A, 2012, 116, 8910-8917.	1.1	15

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109	Theoretical Investigation into the Palladium-Catalyzed Silaboration of Pyridines. Organometallics, 2012, 31, 1680-1687.	1.1	14
110	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
111	A Theoretical Study of the Stevens Rearrangement of Methylammonium Methylide and Methylammonium Formylmethylide. Australian Journal of Chemistry, 1993, 46, 1375.	0.5	13
112	A Molecular Orbital Rationalization of Ligand Effects in N₂ Activation. Chemistry - A European Journal, 2008, 14, 6119-6124.	1.7	13
113	Reactivity of CO2 towards Mo[N(R)Ph]3. Dalton Transactions, 2009, , 9266.	1.6	13
114	Electronic structure of the 3.SIGMA.- states of silicon-oxygen compounds, SiOSi and SiSiO. Inorganic Chemistry, 1989, 28, 1680-1684.	1.9	12
115	Associative versus dissociative binding of CO to 4d transition metal trimers: A density functional study. Journal of Computational Chemistry, 2008, 29, 1497-1506.	1.5	12
116	On the unprecedented level of dinitrogen activation in the calix[4]arene complex of Nb(iii). Dalton Transactions, 2011, 40, 11267.	1.6	12
117	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
118	Synthesis of Thieno[2,3-g][1,4]oxazonine and Thieno[2,3-h][1,5]oxazecine derivatives by cyanogen-bromide-induced ring expansion. Australian Journal of Chemistry, 1984, 37, 1043.	0.5	11
119	Achieving Câ€“N bond cleavage in dinuclear metal cyanide complexes. Dalton Transactions, 2011, 40, 7327.	1.6	11
120	Oxazoles revisited: On the nature of binding of benzoxazole and 2-methylbenzoxazole with the zinc and palladium halides. Dalton Transactions, 2011, 40, 1594.	1.6	11
121	Proton supplier role of binuclear gold complexes in promoting hydrofunctionalisation of nonactivated alkenes. Catalysis Science and Technology, 2019, 9, 1420-1426.	2.1	11
122	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, .	1.7	11
123	Oxidation of Lignin Model Compounds Containing an Î±-Carbonyl Group and a Ring-conjugated Double-bond by Hydrogen Peroxide-UV Photolysis. Holzforschung, 1996, 50, 226-232.	0.9	10
124	Olefin strain energies and platinum complexes of highly pyramidalised alkenes. Journal of Organometallic Chemistry, 2001, 635, 142-152.	0.8	10
125	Activation and cleavage of the Nâ€“O bond in dinuclear mixed-metal nitrosyl systems and comparative analysis of carbon monoxide, dinitrogen, and nitric oxideactivation. Dalton Transactions, 2009, , 956-964.	1.6	10
126	Titanium-mediated rearrangement of cyclopropenylmethyl acetates to (E)-halodienes. Organic and Biomolecular Chemistry, 2011, 9, 3359.	1.5	10

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127	Revisiting the Aufbau Reaction with Acetylene: Further Insights from Experiment and Theory. Organometallics, 2011, 30, 1569-1576.	1.1	10
128	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.	1.9	10
129	A Modified Cationic Mechanism for PdCl2-Catalyzed Transformation of a Homoallylic Alcohol to an Allyl Ether. Organometallics, 2019, 38, 2953-2962.	1.1	10
130	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.	1.1	10
131	Borane Catalyzed Selective Diazo Crossâ€Coupling Towards Pyrazoles. Advanced Synthesis and Catalysis, 2022, 364, 773-780.	2.1	10
132	Spontaneous intramolecular hydrogen migration in ionized ethane-1,2-diol. Journal of the Chemical Society Chemical Communications, 1987, , 204.	2.0	9
133	Mixing of electronic states in molybdenum complexes involved in nitrogen activation. Chemical Physics, 2006, 324, 202-209.	0.9	9
134	Dinitrogen Activation by Fryzukâ€™s [Nb(P₂N₂)] Complex and Comparison with the Laplazaâ€“Cummins [Mo{N(R)Ar}₃] and Schrock [Mo(N₃N)] Systems. Chemistry - A European Journal, 2009, 15, 11373-11383.	1.7	9
135	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
136	Computational Study of Carbostannylation Implicating Bimetallic Catalysis Involving â€œAu^Iâ€“Vinylâ€“Pd^{II}â€•Species. ACS Catalysis, 2014, 4, 860-869.	5.5	9
137	Prying open a Reactive Site for Allylic Arylation by Phosphine-Ligated Geminally Diaurated Aryl Complexes. Organometallics, 2015, 34, 3255-3263.	1.1	9
138	Theoretical study of the mechanism for the sequential Nâ€“O and Nâ€“N bond cleavage within N₂O adducts of N-heterocyclic carbenes by a vanadium(<scp>iii</scp>) complex. Dalton Transactions, 2016, 45, 1047-1054.	1.6	9
139	The HO2 + ion. Molecular Physics, 1989, 68, 1095-1109.	0.8	8
140	Acyl radical addition to pyridine: multiorbital interactions. Tetrahedron, 2009, 65, 7653-7657.	1.0	8
141	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.	1.1	8
142	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
143	The inversion barrier in NF+â‹…3. Journal of Chemical Physics, 1994, 100, 4459-4466.	1.2	7
144	ESR Study of Lignin Model Compounds Irradiated by UV (254 nm Photons) in the Presence of Hydrogen Peroxide. Holzforschung, 1996, 50, 233-236.	0.9	7

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145	A quantitative investigation of the transannular amine-ketone (NÂ·Â·Â·C=O) interaction in medium-sized heterocycles. Journal of Molecular Graphics and Modelling, 1997, 15, 91-99.	1.3	7
146	Structural and electronic characterisation of the organometallic distonic ion (C6H6)Fe+(p-C6H4)Â·. International Journal of Mass Spectrometry, 2000, 201, 297-305.	0.7	7
147	An Innovative Approach Characterising the Interactions Leading to Pitch Deposition. Journal of Wood Chemistry and Technology, 2005, 24, 115-137.	0.9	7
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