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	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(C₆F₅)₃ Towards Carbene Formation. Chemistry - A European Journal, 2022, 28, .	1.7	11
3	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
4	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
5	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
6	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
7	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
8	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
9	Borane-Catalyzed Stereoselective Câ€“H Insertion, Cyclopropanation, and Ring-Opening Reactions. CheM, 2020, 6, 2364-2381.	5.8	70
10	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
11	A Modified Cationic Mechanism for PdCl2-Catalyzed Transformation of a Homoallylic Alcohol to an Allyl Ether. Organometallics, 2019, 38, 2953-2962.	1.1	10
12	DFT Mechanistic Investigation into BF₃-Catalyzed Alcohol Oxidation by a Hypervalent Iodine(III) Compound. ACS Catalysis, 2019, 9, 6510-6521.	5.5	22
13	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
14	Proton supplier role of binuclear gold complexes in promoting hydrofunctionalisation of nonactivated alkenes. Catalysis Science and Technology, 2019, 9, 1420-1426.	2.1	11
15	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
16	Titelbild: Dual Gold-Catalyzed Cycloaromatization of Unconjugated (E)-Enediynes (Angew. Chem.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	1.6	0
17	Dual Goldâ€Catalyzed Cycloaromatization of Unconjugated (E)â€Enediynes. Angewandte Chemie - International Edition, 2019, 58, 2114-2119.	7.2	28
18	Dual Goldâ€Catalyzed Cycloaromatization of Unconjugated (E)â€Enediynes. Angewandte Chemie, 2019, 131, 2136-2141.	1.6	7

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19	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
20	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
21	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
22	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
23	Computational study of C(sp³)â€“O bond formation at a Pd^{IV} centre. Dalton Transactions, 2017, 46, 3742-3748.	1.6	25
24	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.	1.1	5
25	Total Synthesis of (Â±)â€Dihydroisosubamol. Advanced Synthesis and Catalysis, 2017, 359, 866-874.	2.1	19
26	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
27	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
28	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
29	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
30	A Theoretical Study on the Protodeauration Step of the Gold(I)-Catalyzed Organic Reactions. Organometallics, 2015, 34, 3186-3195.	1.1	68
31	Prying open a Reactive Site for Allylic Arylation by Phosphine-Ligated Geminally Diaurated Aryl Complexes. Organometallics, 2015, 34, 3255-3263.	1.1	9
32	Computational Study of Intramolecular Arene Palladation at a Palladium(IV) Center. Organometallics, 2015, 34, 1085-1090.	1.1	23
33	The development of teaching skills to support active learning in university science (ALIUS). Journal of Learning Design, 2015, 3, .	0.8	3
34	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
35	Decarboxylative-Coupling of Allyl Acetate Catalyzed by Group 10 Organometallics, [(phen)M(CH₃)]⁺. Journal of Organic Chemistry, 2014, 79, 12056-12069.	1.7	24
36	On the selective cleavage of nitrous oxide by metalâ€“amide complexes. Dalton Transactions, 2014, 43, 4631-4634.	1.6	6

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37	NO2bond cleavage by MoL3complexes. Dalton Transactions, 2014, 43, 1620-1629.	1.6	3
38	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
39	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
40	Theoretical Study of the Mechanism of CO and Acetylene Migratory Insertions into Ptâ€“Cp* Bonds. Organometallics, 2014, 33, 2384-2387.	1.1	2
41	Formation of Ethane from Mono-Methyl Palladium(II) Complexes. Journal of the American Chemical Society, 2014, 136, 8237-8242.	6.6	35
42	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
43	Cu-Catalyzed Fluorination of Diaryliodonium Salts with KF. Organic Letters, 2013, 15, 5134-5137.	2.4	162
44	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
45	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
46	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.	0.8	7
47	Theoretical Investigation into the Mechanism of 3â€²-dGMP Oxidation by [Pt^{IV}Cl₄(dach)]. Inorganic Chemistry, 2013, 52, 707-717.	1.9	31
48	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
49	Chemical Kinetics of a Bipalladium Complex. Journal of Physical Chemistry A, 2013, 117, 541-549.	1.1	0
50	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
51	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
52	Theoretical Investigation into the Palladium-Catalyzed Silaboration of Pyridines. Organometallics, 2012, 31, 1680-1687.	1.1	14
53	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
54	Dinitrogen metal complexes with a strongly activated Nâ€“N bond: a computational investigation of [(Cy2N)3Nb-(Î¼-NN)-Nb(NCy2)3] and related [Nb-(Î¼-NN)-Nb] systems. Dalton Transactions, 2012, 41, 13948.	1.6	4

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55	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
56	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
57	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
58	On the unprecedented level of dinitrogen activation in the calix[4]arene complex of Nb(iii). Dalton Transactions, 2011, 40, 11267.	1.6	12
59	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
60	Achieving Câ€“N bond cleavage in dinuclear metal cyanide complexes. Dalton Transactions, 2011, 40, 7327.	1.6	11
61	Titanium-mediated rearrangement of cyclopropenylmethyl acetates to (E)-halodienes. Organic and Biomolecular Chemistry, 2011, 9, 3359.	1.5	10
62	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
63	Revisiting the Aufbau Reaction with Acetylene: Further Insights from Experiment and Theory. Organometallics, 2011, 30, 1569-1576.	1.1	10
64	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
65	Theoretical Investigation into the Mechanism of Reductive Elimination from Bimetallic Palladium Complexes. Inorganic Chemistry, 2011, 50, 6449-6457.	1.9	46
66	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
67	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
68	DFT Studies on the Carboxylation of the Câ€“H Bond of Heteroarenes by Copper(I) Complexes. Organometallics, 2011, 30, 6218-6224.	1.1	38
69	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
70	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.	1.7	7
71	Dimethylcuprate Undergoes a Dyotropic Rearrangement. Chemistry - A European Journal, 2010, 16, 2674-2678.	1.7	37
72	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

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73	Acyl radical addition to benzene and related systemsâ€"a computational study. Tetrahedron, 2010, 66, 7600-7604.	1.0	4
74	Factors Dictating Carbene Formation at (PNP)Ir. Organometallics, 2010, 29, 4239-4250.	1.1	16
75	Ligand Effects in Bimetallic High Oxidation State Palladium Systems. Inorganic Chemistry, 2010, 49, 11249-11253.	1.9	37
76	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
77	Experimental and Theoretical Investigation into the Gold-Catalyzed Reactivity of Cyclopropenylmethyl Acetates. Organic Letters, 2010, 12, 4768-4771.	2.4	43
78	Activation and cleavage of the Nâ€"N bond in side-on bound [L2M-NN-ML2] (L = NH2, NMe2, NiPr2, C5H5,) Tj ETQq0 0 0 rgBT /Overlock 2010, 39, 4529.	1.6	19
79	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
80	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
81	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
82	Acyl radical addition to pyridine: multiorbital interactions. Tetrahedron, 2009, 65, 7653-7657.	1.0	8
83	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
84	Nucleophilic Acyl Substitution of Acyl Diimides. Journal of Organic Chemistry, 2009, 74, 5707-5710.	1.7	3
85	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
86	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
87	Subtle Balance of Ligand Steric Effects in Stille Transmetalation. Journal of the American Chemical Society, 2009, 131, 13981-13991.	6.6	76
88	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
89	Reactivity of CO2 towards Mo[N(R)Ph]3. Dalton Transactions, 2009, , 9266.	1.6	13
90	A Molecular Orbital Rationalization of Ligand Effects in N₂ Activation. Chemistry - A European Journal, 2008, 14, 6119-6124.	1.7	13

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91	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
92	The Mechanism of the Stetter Reaction â€“ A DFT Study. European Journal of Organic Chemistry, 2008, 2008, 5563-5570.	1.2	91
93	Activation of CS2 and CS by ML3 Complexes. Journal of the American Chemical Society, 2008, 130, 11928-11938.	6.6	37
94	A mechanistic study on the oxidation of hydrazides: application to the tuberculosis drug isoniazid. Chemical Communications, 2008, , 1695.	2.2	38
95	Pre-catalyst resting states: a kinetic, thermodynamic and quantum mechanical analyses of [PdCl2(2-oxazoline)2] complexes. Dalton Transactions, 2008, , 3115.	1.6	19
96	Rhodium-Catalyzed Câ^'C Coupling Reactions: Mechanistic Considerations. Organometallics, 2008, 27, 4758-4771.	1.1	39
97	Investigating CNâ€“cleavage by three-coordinate M[N(R)Ar]3complexes. Dalton Transactions, 2008, , 338-344.	1.6	18
98	Oxidative addition of 2-substituted azolium salts to Group-10 metal zero complexesâ€”A DFT study. Dalton Transactions, 2007, , 4650.	1.6	43
99	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
100	Rationalizing the different products in the reaction of N2 with three-coordinate MoL3 complexes. Dalton Transactions, 2007, , 1939.	1.6	16
101	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
102	Atom-Efficient Catalytic Coupling of Imidazolium Salts with Ethylene Involving Niâ^'NHC Complexes as Intermediates:â€‰ A Combined Experimental and DFT Study. Organometallics, 2007, 26, 5352-5363.	1.1	88
103	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
104	Cleavage of CO by Mo[N(R)Ar]3 Complexes. European Journal of Inorganic Chemistry, 2007, 2007, 3736-3741.	1.0	15
105	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
106	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
107	Computational organic chemistry. Annual Reports on the Progress of Chemistry Section B, 2006, 102, 219.	0.8	2
108	Optimizing Small Molecule Activation and Cleavage in Three-Coordinate M[N(R)Ar]3Complexes. Inorganic Chemistry, 2006, 45, 6851-6859.	1.9	25

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109	Mixing of electronic states in molybdenum complexes involved in nitrogen activation. Chemical Physics, 2006, 324, 202-209.	0.9	9
110	Synthesis, structure and optical limiting properties of organorutheniumâ€“chalcogenide clusters. Journal of Organometallic Chemistry, 2005, 690, 1487-1497.	0.8	19
111	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
112	Computational Organic Chemistry. ChemInform, 2005, 36, no.	0.1	0
113	Dimerization mechanisms of heterocyclic carbenes. Journal of Physical Organic Chemistry, 2005, 18, 298-309.	0.9	52
114	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
115	Influence of geometry on reductive elimination of hydrocarbylâ€“palladiumâ€“carbene complexes. Dalton Transactions, 2005, , 1093-1100.	1.6	44
116	Structural studies of Group 1 metal 4-azapentalenyl complexes. Dalton Transactions, 2005, , 1157.	1.6	6
117	An Innovative Approach Characterising the Interactions Leading to Pitch Deposition. Journal of Wood Chemistry and Technology, 2005, 24, 115-137.	0.9	7
118	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
119	10ÂÂComputational organic chemistry. Annual Reports on the Progress of Chemistry Section B, 2005, 101, 210.	0.8	3
120	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
121	Computational Organic Chemistry. ChemInform, 2004, 35, no.	0.1	0
122	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
123	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
124	Basicity of Nucleophilic Carbenes in Aqueous and Nonaqueous SolventsTheoretical Predictions. Journal of the American Chemical Society, 2004, 126, 8717-8724.	6.6	426
125	11ÂÂComputational organic chemistry. Annual Reports on the Progress of Chemistry Section B, 2004, 100, 251-283.	0.8	2
126	Increased Stability of NO and NS Heterocyclic Carbenes?. Australian Journal of Chemistry, 2004, 57, 359.	0.5	2

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127	Molecular Modelling and Design of Radiolabelled Complexes for Melanoma Diagnosis. Australian Journal of Chemistry, 2004, 57, 87.	0.5	0
128	Computational Chemistry and Spectroscopy. Australian Journal of Chemistry, 2004, 57, 1117.	0.5	0
129	Computational Organic Chemistry. ChemInform, 2003, 34, no.	0.1	0
130	9â€ƒâ€ƒComputational organic chemistry. Annual Reports on the Progress of Chemistry Section B, 2003, 99, 292.	0.8	2
131	Computational Quantum Chemistry Experiments via the Web. Lecture Notes in Computer Science, 2003, , 132-141.	1.0	0
132	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
133	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
134	13â€ƒâ€ƒComputational organic chemistry. Annual Reports on the Progress of Chemistry Section B, 2002, 98, 607-638.	0.8	2
135	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
136	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
137	Olefin strain energies and platinum complexes of highly pyramidalised alkenes. Journal of Organometallic Chemistry, 2001, 635, 142-152.	0.8	10
138	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
139	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
140	Ligand design for Î± 1 adrenoceptor subtype selective antagonists. Bioorganic and Medicinal Chemistry, 2000, 8, 201-214.	1.4	71
141	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
142	The Structure of a Methylpalladium(II) Complex of Pyridine-2-carboxylato (N - O) and Triphenylphosphine (PPh3), [Pd(CH3)(N - O)(PPh3)]. Australian Journal of Chemistry, 2000, 53, 805.	0.5	2
143	Nature of the Metalâ^'Alkene Bond in Platinum Complexes of Strained Olefins. Organometallics, 1999, 18, 457-465.	1.1	59
144	Economical treatments of relativistic effects and electron correlation in WH6. Journal of Computational Chemistry, 1998, 19, 1604-1611.	1.5	5

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145	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
146	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
147	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
148	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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