Claire L Mcmullin

List of Publications by Year
in descending order

80 papers	3,618 citations	159358 30 h-index	143772 57 g-index
85 all docs	85 docs citations	85 times ranked	3485 citing authors

#	Article	IF	Citations
1	Computational Studies of Carboxylate-Assisted Câ€“H Activation and Functionalization at Group 8â€“10 Transition Metal Centers. Chemical Reviews, 2017, 117, 8649-8709.	23.0	472
2	Accurate modelling of Pd(0) + PhX oxidative addition kinetics. Dalton Transactions, 2010, 39, 10833.	1.6	179
3	Reaction of Cu^I with Dialkyl Peroxides: Cu^{II}-Alkoxides, Alkoxy Radicals, and Catalytic Câ€“H Etherification. Journal of the American Chemical Society, 2012, 134, 17350-17353.	6.6	143
4	Remote C6-Selective Ruthenium-Catalyzed Câ€“H Alkylation of Indole Derivatives via Ïƒ-Activation. ACS Catalysis, 2017, 7, 2616-2623.	5.5	141
5	Azulene-Derived Fluorescent Probe for Bioimaging: Detection of Reactive Oxygen and Nitrogen Species by Two-Photon Microscopy. Journal of the American Chemical Society, 2019, 141, 19389-19396.	6.6	125
6	Câ€“H Functionalization Reactivity of a Nickelâ€“Imide. Journal of the American Chemical Society, 2012, 134, 10114-10121.	6.6	122
7	A Stable Calcium Alumanyl. Angewandte Chemie - International Edition, 2020, 59, 3928-3932.	7.2	117
8	Experimental and DFT Studies Explain Solvent Control of Câ€“H Activation and Product Selectivity in the Rh(III)-Catalyzed Formation of Neutral and Cationic Heterocycles. Journal of the American Chemical Society, 2015, 137, 9659-9669.	6.6	108
9	Rutheniumâ€Catalyzed <i>para</i>â€Selective Câˆ’H Alkylation of Aniline Derivatives. Angewandte Chemie - International Edition, 2017, 56, 15131-15135.	7.2	108
10	Computed ligand effects on the oxidative addition of phenyl halides to phosphine supported palladium(0) catalysts. Dalton Transactions, 2014, 43, 13545-13556.	1.6	100
11	Copper(II) Anilides in sp³ C-H Amination. Journal of the American Chemical Society, 2014, 136, 10930-10940.	6.6	99
12	Ruthenium(II)-Catalyzed Câ€“H Functionalization Using the Oxazolidinone Heterocycle as a Weakly Coordinating Directing Group: Experimental and Computational Insights. ACS Catalysis, 2016, 6, 5520-5529.	5.5	87
13	Easy access to nucleophilic boron through diborane to magnesium boryl metathesis. Nature Communications, 2017, 8, 15022.	5.8	87
14	Combined Experimental and Computational Investigations of Rhodium- and Ruthenium-Catalyzed Câ€“H Functionalization of Pyrazoles with Alkynes. Journal of Organic Chemistry, 2014, 79, 1954-1970.	1.7	75
15	The Challenge of Palladium-Catalyzed Aromatic Azidocarbonylation: From Mechanistic and Catalyst Deactivation Studies to a Highly Efficient Process. Organometallics, 2014, 33, 736-752.	1.1	68
16	Dehydrogenative Boron Homocoupling of an Amineâ€Borane. Angewandte Chemie - International Edition, 2013, 52, 9776-9780.	7.2	66
17	The Importance of Kinetic and Thermodynamic Control when Assessing Mechanisms of Carboxylate-Assisted Câ€“H Activation. Journal of the American Chemical Society, 2019, 141, 8896-8906.	6.6	66
18	Azuleneâ€“boronate esters: colorimetric indicators for fluoride in drinking water. Chemical Communications, 2017, 53, 12580-12583.	2.2	65

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19	A Stable Calcium Alumanyl. Angewandte Chemie, 2020, 132, 3956-3960.	1.6	60
20	A ligand knowledge base for carbenes (LKB-C): maps of ligand space. Dalton Transactions, 2009, , 8183.	1.6	59
21	Organometallic reactivity: the role of metalâ€"ligand bond energies from a computational perspective. Dalton Transactions, 2011, 40, 11184.	1.6	57
22	Ligand effects in chromium diphosphine catalysed olefin co-trimerisation and diene trimerisation. Dalton Transactions, 2010, 39, 560-567.	1.6	47
23	Î±-Halo carbonyls enable meta selective primary, secondary and tertiary Câ€"H alkylations by ruthenium catalysis. Organic and Biomolecular Chemistry, 2017, 15, 5993-6000.	1.5	47
24	Stable Fluorophosphines: Predicted and Realized Ligands for Catalysis. Angewandte Chemie - International Edition, 2012, 51, 118-122.	7.2	46
25	Ambiphilic Alâˆ'Cu Bonding. Angewandte Chemie - International Edition, 2021, 60, 14390-14393.	7.2	44
26	Catalytic Hydroarylation of Ethylene Using TpRu(L)(NCMe)Ph (L =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 472 Td (2,6,7-Trioxa-1-phospha 2012, 31, 6851-6860.	1.1	43
27	<i>N</i>,<i>N</i>â€²-Bis(diphenylphosphino)diaminophenylphosphine Ligands for Chromium-Catalyzed Selective Ethylene Oligomerization Reactions. Organometallics, 2011, 30, 935-941.	1.1	39
28	Carbonâ€"Carbon Bond Forming Reactions Promoted by Aluminyl and Alumoxane Anions: Introducing the Ethenetetraolate Ligand. Angewandte Chemie - International Edition, 2020, 59, 12806-12810.	7.2	37
29	Magnesium Boryl Reactivity with 9â€BBN and Ph₃B: Rational Bâˆ'Bâ€² Bond Formation and Diborane Isomerization. Angewandte Chemie - International Edition, 2017, 56, 16363-16366.	7.2	36
30	Dihydrogen Activation by Lithiumâ€•and Sodiumâ€Aluminyls. Angewandte Chemie - International Edition, 2021, 60, 22289-22292.	7.2	33
31	Reductive Dimerization of CO by a Na/Mg(I) Diamide. Journal of the American Chemical Society, 2021, 143, 17851-17856.	6.6	31
32	Rubidium and caesium aluminyls: synthesis, structures and reactivity in Câ€"H bond activation of benzene. Chemical Communications, 2022, 58, 1390-1393.	2.2	31
33	Coordination Chemistry of 4-Methyl-2,6,7-trioxa-1-phosphabicyclo[2,2,1]heptane: Preparation and Characterization of Ru(II) Complexes. Inorganic Chemistry, 2012, 51, 4791-4801.	1.9	30
34	Diphosphanes derived from phobane and phosphatrioxa-adamantane: similarities, differences and anomalies. Dalton Transactions, 2011, 40, 7137.	1.6	28
35	<i>N</i>,<i>N</i>â€Diphospholylaminesâ€"A New Family of Ligands for Highly Active, Chromiumâ€Based, Selective Ethene Oligomerisation Catalysts. ChemCatChem, 2013, 5, 2946-2954.	1.8	28
36	Rutheniumâ€Catalyzed <i>para</i>â€Selective Câˆ'H Alkylation of Aniline Derivatives. Angewandte Chemie, 2017, 129, 15327-15331.	1.6	28

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37	Combined Experimental and Computational Investigations of Rhodiumâ€Catalysed Cï£¿H Functionalisation of Pyrazoles with Alkenes. Chemistry - A European Journal, 2015, 21, 3087-3096.	1.7	27
38	The first ring-expanded NHCâ€"copper(<scp>i</scp>) phosphides as catalysts in the highly selective hydrophosphination of isocyanates. Chemical Communications, 2020, 56, 13359-13362.	2.2	27
39	Computational study of PtBu3 as ligand in the palladium-catalysed amination of phenylbromide with morpholineâ˜†. Journal of Molecular Catalysis A, 2010, 324, 48-55.	4.8	26
40	Subtleties in asymmetric catalyst structure: the resolution of a 6-phospha-2,4,8-trioxa-adamantane and its applications in asymmetric hydrogenation catalysis. Chemical Communications, 2010, 46, 100-102.	2.2	26
41	Cage Phosphinites: Ligands for Efficient Nickel-Catalyzed Hydrocyanation of 3-Pentenenitrile. Organometallics, 2011, 30, 974-985.	1.1	26
42	Diborane heterolysis and P(<scp>v</scp>) reduction by Ph₃Pî€O coordination to magnesium. Chemical Communications, 2019, 55, 9035-9038.	2.2	25
43	Understanding electronic effects on carboxylate-assisted Câ€"H activation at ruthenium: the importance of kinetic and thermodynamic control. Faraday Discussions, 2019, 220, 386-403.	1.6	23
44	On the reactivity of Al-group 11 (Cu, Ag, Au) bonds. Dalton Transactions, 2022, 51, 3913-3924.	1.6	23
45	Cobalt PCP Pincer Complexes via an Unexpected Sequence of Ortho Metalations. Organometallics, 2014, 33, 5686-5692.	1.1	21
46	Complete methane-to-methanol catalytic cycle: A DFT study of oxygen atom transfer from N2O to late-row (MNi, Cu, Zn) Î²-diketiminate CH activation catalysts. Polyhedron, 2013, 52, 945-956.	1.0	20
47	Magnesium-Mediated Nucleophilic Borylation of Carbonyl Electrophiles. Organometallics, 2018, 37, 4457-4464.	1.1	20
48	Sevenâ€Membered Cyclic Potassium Diamidoalumanyls. Chemistry - A European Journal, 2021, 27, 14971-14980.	1.7	20
49	Is restricted Mâ€"P rotation a common feature of enantioselective monophos catalysts? An example of restricted Rhâ€"P rotation in a secondary phosphine complex. Tetrahedron: Asymmetry, 2010, 21, 1206-1209.	1.8	19
50	Snapshots of magnesium-centred diborane heterolysis by an outer sphere S_N2 process. Chemical Science, 2019, 10, 6672-6682.	3.7	19
51	Potassium Aluminyl Promoted Carbonylation of Ethene. Angewandte Chemie - International Edition, 2022, 61, .	7.2	19
52	Large, weakly basic bis(carboranyl)phosphines: an experimental and computational study. Dalton Transactions, 2017, 46, 5218-5228.	1.6	18
53	Rhodium Complexes of Cyclopropenylidene Carbene Ligands: Synthesis, Structure, and Hydroformylation Catalysis. Organometallics, 2009, 28, 1476-1479.	1.1	17
54	Magnesium Boryl Reactivity with 9â€BBN and Ph₃B: Rational Bâˆ'Bâ€² Bond Formation and Diborane Isomerization. Angewandte Chemie, 2017, 129, 16581-16584.	1.6	17

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55	Cyclopropenylidene carbene ligands in palladium catalysed coupling reactions: carbene ligand rotation and application to the Stille reaction. Dalton Transactions, 2011, 40, 5316.	1.6	15
56	Azulenes with aryl substituents bearing pentafluorosulfanyl groups: synthesis, spectroscopic and halochromic properties. New Journal of Chemistry, 2019, 43, 992-1000.	1.4	15
57	[BO₂]^{âˆ’} as a Synthon for the Generation of Boronâ€Centered Carbamate and Carboxylate Isosteres. Angewandte Chemie - International Edition, 2020, 59, 13628-13632.	7.2	15
58	Double insertion of CO₂ into an Alâ€“Te multiple bond. Chemical Communications, 2021, 57, 2673-2676.	2.2	15
59	Calcium stannyl formation by organostannane dehydrogenation. Chemical Communications, 2019, 55, 12964-12967.	2.2	14
60	Tuning ligand structure in chiral bis(phosphite) and mixed phosphiteâ€“phosphinite PCP-palladium pincer complexes. Dalton Transactions, 2011, 40, 9034.	1.6	13
61	Modelling and Rationalizing Organometallic Chemistry with Computation: Where Are We?. Structure and Bonding, 2015, , 1-37.	1.0	13
62	Ambiphilic Alâˆ'Cu Bonding. Angewandte Chemie, 2021, 133, 14511-14514.	1.6	13
63	Carbonâ€“Carbon Bond Forming Reactions Promoted by Aluminyl and Alumoxane Anions: Introducing the Ethenetetraolate Ligand. Angewandte Chemie, 2020, 132, 12906-12910.	1.6	12
64	Controlling Alâ€“M Interactions in Group 1 Metal Aluminyls (M = Li, Na, and K). Facile Conversion of Dimers to Monomeric and Separated Ion Pairs. Inorganic Chemistry, 2021, 60, 18423-18431.	1.9	12
65	Chiral palladacycles based on resorcinol monophosphite ligands: the role of the meta-hydroxyl in ligand Câ€“H activation and catalysis. Dalton Transactions, 2011, 40, 9042.	1.6	10
66	Phosphinoborane interception at magnesium by borane-assisted phosphine-borane dehydrogenation. Dalton Transactions, 2020, 49, 14584-14591.	1.6	10
67	Carbonâ€“chalcogen bond formation initiated by [Al(NON^{Dipp})(E)]^{âˆ’}anions containing Alâ€“E{16} (E{16} = S, Se) multiple bonds. Chemical Science, 2022, 13, 4635-4646.	3.7	10
68	Dihydrogen Activation by Lithiumâ€•and Sodiumâ€Aluminyls. Angewandte Chemie, 2021, 133, 22463-22466.	1.6	9
69	Computational Studies on Heteroatom-Assisted Câ€“H Activation and Functionalisation at Group 8 and 9 Metal Centres. Topics in Organometallic Chemistry, 2015, , 53-76.	0.7	7
70	[BO 2] âˆ’ as a Synthon for the Generation of Boronâ€Centered Carbamate and Carboxylate Isosteres. Angewandte Chemie, 2020, 132, 13730-13734.	1.6	7
71	Synthesis and reactivity of alkaline-earth stannanide complexes by hydride-mediated distannane metathesis and organostannane dehydrogenation. Dalton Transactions, 2020, 49, 10523-10534.	1.6	6
72	Nucleophilic Magnesium Silanide and Silaamidinate Derivatives. Inorganic Chemistry, 2020, 59, 13679-13689.	1.9	6

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73	Reductive dehydrocoupling of diphenyltin dihydride with LiAlH4: selective synthesis and structures of the first bicyclo[2.2.1]heptastannane-1,4-diide and bicyclo[2.2.2]octastannane-1,4-diide. Chemical Communications, 2020, 56, 336-339.	2.2	5
74	Isocyanate deoxygenation by a molecular magnesium silanide. Dalton Transactions, 2021, 51, 136-144.	1.6	4
75	Unexpectedly High Barriers to Mâ€"P Rotation in Tertiary Phobane Complexes: PhobPR Behavior That Is Commensurate with tBu2PR. Organometallics, 2014, 33, 702-714.	1.1	3
76	A computational study on the identity of the active catalyst structure for Ru(ii) carboxylate assisted Câ€"H activation in acetonitrile. Organic and Biomolecular Chemistry, 2019, 17, 6678-6686.	1.5	3
77	Correlations of the Structural Properties of a Complete R₂PX Series (X = Hydrogen or) Tj ETQq1 1 0.784314 rgBT /Overlo	1.0	2
78	A Terphenyl Supported Dioxophosphorane Dimer: the Light Congener of Lawesson's and Woollinsâ€™ Reagents. Chemistry - A European Journal, 2022, , .	1.7	2
79	DFT calculations bring insight to internal alkyne-to-vinylidene transformations at rhodium PNP- and PONOP-pincer complexes. RSC Advances, 2021, 11, 11793-11803.	1.7	1
80	Potassium Aluminyl Promoted Carbonylation of Ethene. Angewandte Chemie, 2022, 134, .	1.6	0