

# Claire L McMullin

## List of Publications by Citations

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76  
papers

2,660  
citations

28  
h-index

50  
g-index

85  
ext. papers

3,190  
ext. citations

7.9  
avg, IF

5.52  
L-index

| #  | Paper  | IF   | Citations |
|----|--|------|-----------|
| 76 | Computational Studies of Carboxylate-Assisted C-H Activation and Functionalization at Group 8-10 Transition Metal Centers. <i>Chemical Reviews</i> , <b>2017</b> , 117, 8649-8709  | 68.1 | 343       |
| 75 | Accurate modelling of Pd(0) + PhX oxidative addition kinetics. <i>Dalton Transactions</i> , <b>2010</b> , 39, 10833-6  | 4.3  | 163       |
| 74 | Reaction of Cu(I) with dialkyl peroxides: Cu(II)-alkoxides, alkoxy radicals, and catalytic C-H etherification. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 17350-3  | 16.4 | 121       |
| 73 | C-H functionalization reactivity of a nickel-imide. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 10114-21  | 16.4 | 112       |
| 72 | Remote C6-Selective Ruthenium-Catalyzed C-H Alkylation of Indole Derivatives via $\pi$ Activation. <i>ACS Catalysis</i> , <b>2017</b> , 7, 2616-2623   | 13.1 | 111       |
| 71 | Experimental and DFT Studies Explain Solvent Control of C-H Activation and Product Selectivity in the Rh(III)-Catalyzed Formation of Neutral and Cationic Heterocycles. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 9659-69 | 16.4 | 90        |
| 70 | Computed ligand effects on the oxidative addition of phenyl halides to phosphine supported palladium(0) catalysts. <i>Dalton Transactions</i> , <b>2014</b> , 43, 13545-56   | 4.3  | 80        |
| 69 | Copper(II) anilides in sp <sup>2</sup> C-H amination. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 10930-40  | 16.4 | 76        |
| 68 | Azulene-Derived Fluorescent Probe for Bioimaging: Detection of Reactive Oxygen and Nitrogen Species by Two-Photon Microscopy. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 19389-19396                                       | 16.4 | 73        |
| 67 | Ruthenium-Catalyzed para-Selective C-H Alkylation of Aniline Derivatives. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 15131-15135   | 16.4 | 72        |
| 66 | A Stable Calcium Alumanyl. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 3928-3932  | 16.4 | 72        |
| 65 | Ruthenium(II)-Catalyzed C-H Functionalization Using the Oxazolidinone Heterocycle as a Weakly Coordinating Directing Group: Experimental and Computational Insights. <i>ACS Catalysis</i> , <b>2016</b> , 6, 5520-5529                               | 13.1 | 69        |
| 64 | Easy access to nucleophilic boron through diborane to magnesium boryl metathesis. <i>Nature Communications</i> , <b>2017</b> , 8, 15022  | 17.4 | 68        |
| 63 | Combined experimental and computational investigations of rhodium- and ruthenium-catalyzed C-H functionalization of pyrazoles with alkynes. <i>Journal of Organic Chemistry</i> , <b>2014</b> , 79, 1954-70  | 4.2  | 68        |
| 62 | Dehydrogenative boron homocoupling of an amine-borane. <i>Angewandte Chemie - International Edition</i> , <b>2013</b> , 52, 9776-80  | 16.4 | 62        |
| 61 | The Challenge of Palladium-Catalyzed Aromatic Azidocarbonylation: From Mechanistic and Catalyst Deactivation Studies to a Highly Efficient Process. <i>Organometallics</i> , <b>2014</b> , 33, 736-752   | 3.8  | 56        |
| 60 | Azulene-boronate esters: colorimetric indicators for fluoride in drinking water. <i>Chemical Communications</i> , <b>2017</b> , 53, 12580-12583  | 5.8  | 55        |

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|----|--|---------|
| 59 | A ligand knowledge base for carbenes (LKB-C): maps of ligand space. <i>Dalton Transactions</i> , <b>2009</b> , 8183-964.3  | 51      |
| 58 | Organometallic reactivity: the role of metal-ligand bond energies from a computational perspective. <i>Dalton Transactions</i> , <b>2011</b> , 40, 11184-91  | 4.3 48  |
| 57 | Ligand effects in chromium diphosphine catalysed olefin co-trimerisation and diene trimerisation. <i>Dalton Transactions</i> , <b>2010</b> , 560-7   | 4.3 41  |
| 56 | The Importance of Kinetic and Thermodynamic Control when Assessing Mechanisms of Carboxylate-Assisted C-H Activation. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 8896-8906   | 16.4 40 |
| 55 | Catalytic Hydroarylation of Ethylene Using TpRu(L)(NCMe)Ph (L = 2,6,7-Trioxa-1-phospha-bicyclo[2,2,1]heptane): Comparison to TpRu(L')(NCMe)Ph Systems (L' = CO, PMe <sub>3</sub> , P(pyr) <sub>3</sub> , or P(OCH <sub>2</sub> ) <sub>3</sub> CEt). <i>Organometallics</i> , <b>2012</b> , 31, 6851-6860 | 3.8 40  |
| 54 | Stable fluorophosphines: predicted and realized ligands for catalysis. <i>Angewandte Chemie - International Edition</i> , <b>2012</b> , 51, 118-22   | 16.4 38 |
| 53 | Halo carbonyls enable meta selective primary, secondary and tertiary C-H alkylations by ruthenium catalysis. <i>Organic and Biomolecular Chemistry</i> , <b>2017</b> , 15, 5993-6000   | 3.9 38  |
| 52 | A Stable Calcium Alumanyl. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 3956-3960   | 3.6 38  |
| 51 | N,N'-Bis(diphenylphosphino)diaminophenylphosphine Ligands for Chromium-Catalyzed Selective Ethylene Oligomerization Reactions. <i>Organometallics</i> , <b>2011</b> , 30, 935-941  | 3.8 36  |
| 50 | Magnesium Boryl Reactivity with 9-BBN and Ph B: Rational B-B Bond Formation and Diborane Isomerization. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 16363-16366   | 16.4 29 |
| 49 | Coordination chemistry of 4-methyl-2,6,7-trioxa-1-phospha-bicyclo[2,2,1]heptane: preparation and characterization of Ru(II) complexes. <i>Inorganic Chemistry</i> , <b>2012</b> , 51, 4791-801   | 5.1 29  |
| 48 | Combined experimental and computational investigations of rhodium-catalysed C - H functionalisation of pyrazoles with alkenes. <i>Chemistry - A European Journal</i> , <b>2015</b> , 21, 3087-96   | 4.8 26  |
| 47 | N,N-Diphospholylamines: A New Family of Ligands for Highly Active, Chromium-Based, Selective Ethene Oligomerisation Catalysts. <i>ChemCatChem</i> , <b>2013</b> , 5, 2946-2954   | 5.2 25  |
| 46 | Ruthenium-Catalyzed para-Selective C-H Alkylation of Aniline Derivatives. <i>Angewandte Chemie</i> , <b>2017</b> , 129, 15327-15331  | 3.6 24  |
| 45 | Cage Phosphinites: Ligands for Efficient Nickel-Catalyzed Hydrocyanation of 3-Pentenenitrile. <i>Organometallics</i> , <b>2011</b> , 30, 974-985   | 3.8 24  |
| 44 | Subtleties in asymmetric catalyst structure: the resolution of a 6-phospha-2,4,8-trioxa-adamantane and its applications in asymmetric hydrogenation catalysis. <i>Chemical Communications</i> , <b>2010</b> , 46, 100-2  | 5.8 23  |
| 43 | Diphosphanes derived from phobane and phosphatrioxa-adamantane: similarities, differences and anomalies. <i>Dalton Transactions</i> , <b>2011</b> , 40, 7137-46  | 4.3 22  |
| 42 | Computational study of PtBu <sub>3</sub> as ligand in the palladium-catalysed amination of phenylbromide with morpholine. <i>Journal of Molecular Catalysis A</i> , <b>2010</b> , 324, 48-55   | 22      |

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|----|--|------|----|
| 41 | Complete methane-to-methanol catalytic cycle: A DFT study of oxygen atom transfer from N <sub>2</sub> O to late-row (MNi, Cu, Zn) Ediketimate CH activation catalysts. <i>Polyhedron</i> , <b>2013</b> , 52, 945-956                   | 2.7  | 19 |
| 40 | Carbon-Carbon Bond Forming Reactions Promoted by Aluminyl and Alumoxane Anions: Introducing the Ethenetetraolate Ligand. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 12806-12810                              | 16.4 | 18 |
| 39 | Dehydrogenative Boron Homocoupling of an Amine-Borane. <i>Angewandte Chemie</i> , <b>2013</b> , 125, 9958-9962   | 3.6  | 18 |
| 38 | Is restricted M $\sigma$ rotation a common feature of enantioselective monophos catalysts? An example of restricted Rh $\sigma$ rotation in a secondary phosphine complex. <i>Tetrahedron: Asymmetry</i> , <b>2010</b> , 21, 1206-1209 |      | 18 |
| 37 | Diborane heterolysis and P(v) reduction by PhP[double bond, length as m-dash]O coordination to magnesium. <i>Chemical Communications</i> , <b>2019</b> , 55, 9035-9038   | 5.8  | 17 |
| 36 | Cobalt PCP Pincer Complexes via an Unexpected Sequence of Ortho Metalations. <i>Organometallics</i> , <b>2014</b> , 33, 5686-5692  | 3.8  | 17 |
| 35 | Large, weakly basic bis(carboranyl)phosphines: an experimental and computational study. <i>Dalton Transactions</i> , <b>2017</b> , 46, 5218-5228   | 4.3  | 16 |
| 34 | Rhodium Complexes of Cyclopropenylidene Carbene Ligands: Synthesis, Structure, and Hydroformylation Catalysis. <i>Organometallics</i> , <b>2009</b> , 28, 1476-1479  | 3.8  | 16 |
| 33 | Magnesium Boryl Reactivity with 9-BBN and Ph <sub>3</sub> B: Rational B-B $\sigma$ Bond Formation and Diborane Isomerization. <i>Angewandte Chemie</i> , <b>2017</b> , 129, 16581-16584  | 3.6  | 15 |
| 32 | Snapshots of magnesium-centred diborane heterolysis by an outer sphere S <sub>2</sub> process. <i>Chemical Science</i> , <b>2019</b> , 10, 6672-6682   | 9.4  | 14 |
| 31 | Ambiphilic Al-Cu Bonding. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 14390-14393   | 16.4 | 14 |
| 30 | Tuning ligand structure in chiral bis(phosphite) and mixed phosphite-phosphinite PCP-palladium pincer complexes. <i>Dalton Transactions</i> , <b>2011</b> , 40, 9034-41  | 4.3  | 13 |
| 29 | Azulenenes with aryl substituents bearing pentafluorosulfanyl groups: synthesis, spectroscopic and halochromic properties. <i>New Journal of Chemistry</i> , <b>2019</b> , 43, 992-1000  | 3.6  | 12 |
| 28 | Understanding electronic effects on carboxylate-assisted C-H activation at ruthenium: the importance of kinetic and thermodynamic control. <i>Faraday Discussions</i> , <b>2019</b> , 220, 386-403                                     | 3.6  | 12 |
| 27 | Modelling and Rationalizing Organometallic Chemistry with Computation: Where Are We?. <i>Structure and Bonding</i> , <b>2015</b> , 1-37  | 0.9  | 12 |
| 26 | Cyclopropenylidene carbene ligands in palladium catalysed coupling reactions: carbene ligand rotation and application to the Stille reaction. <i>Dalton Transactions</i> , <b>2011</b> , 40, 5316-23                                   | 4.3  | 12 |
| 25 | Magnesium-Mediated Nucleophilic Borylation of Carbonyl Electrophiles. <i>Organometallics</i> , <b>2018</b> , 37, 4457-4464   | 3.4  | 12 |
| 24 | The first ring-expanded NHC-copper(i) phosphides as catalysts in the highly selective hydrophosphination of isocyanates. <i>Chemical Communications</i> , <b>2020</b> , 56, 13359-13362  | 5.8  | 11 |

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| 23 | Chiral palladacycles based on resorcinol monophosphite ligands: the role of the meta-hydroxyl in ligand C-H activation and catalysis. <i>Dalton Transactions</i> , <b>2011</b> , 40, 9042-50  | 4.3  | 10 |
| 22 | [BO] as a Synthon for the Generation of Boron-Centered Carbamate and Carboxylate Isosteres. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 13628-13632  | 16.4 | 9  |
| 21 | Carbon-Carbon Bond Forming Reactions Promoted by Alumanyl and Alumoxane Anions: Introducing the Ethenetetraolate Ligand. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 12906-12910  | 3.6  | 9  |
| 20 | Calcium stannyl formation by organostannane dehydrogenation. <i>Chemical Communications</i> , <b>2019</b> , 55, 12964-12967   | 5.8  | 8  |
| 19 | Computational Studies on Heteroatom-Assisted C-H Activation and Functionalisation at Group 8 and 9 Metal Centres. <i>Topics in Organometallic Chemistry</i> , <b>2015</b> , 53-76   | 0.6  | 6  |
| 18 | Stable Fluorophosphines: Predicted and Realized Ligands for Catalysis. <i>Angewandte Chemie</i> , <b>2012</b> , 124, 122-126  | 3.6  | 6  |
| 17 | Reductive Dimerization of CO by a Na/Mg(I) Diamide. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 17851-17856  | 16.4 | 5  |
| 16 | Dihydrogen Activation by Lithium- and Sodium-Aluminyls. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 22289-22292  | 16.4 | 5  |
| 15 | [BO <sub>2</sub> ] as a Synthon for the Generation of Boron-Centered Carbamate and Carboxylate Isosteres. <i>Angewandte Chemie</i> , <b>2020</b> , 132, 13730-13734   | 3.6  | 4  |
| 14 | Ambiphilic Al-Cu Bonding. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 14511-14514   | 3.6  | 4  |
| 13 | Seven-Membered Cyclic Potassium Diamidoalumanyls. <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 14971-14980   | 4.8  | 4  |
| 12 | Double insertion of CO into an Al-Te multiple bond. <i>Chemical Communications</i> , <b>2021</b> , 57, 2673-2676  | 5.8  | 4  |
| 11 | Unexpectedly High Barriers to M <sup>II</sup> Rotation in Tertiary Phobane Complexes: PhobPR Behavior That Is Commensurate with tBu <sub>2</sub> PR. <i>Organometallics</i> , <b>2014</b> , 33, 702-714   | 3.8  | 3  |
| 10 | Controlling Al- Interactions in Group 1 Metal Aluminyls (= Li, Na, and K). Facile Conversion of Dimers to Monomeric and Separated Ion Pairs. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 18423-18431   | 5.1  | 3  |
| 9  | Reductive dehydrocoupling of diphenyltin dihydride with LiAlH: selective synthesis and structures of the first bicyclo[2.2.1]heptastannane-1,4-diide and bicyclo[2.2.2]octastannane-1,4-diide. <i>Chemical Communications</i> , <b>2020</b> , 56, 336-339 | 5.8  | 3  |
| 8  | Synthesis and reactivity of alkaline-earth stannanide complexes by hydride-mediated distannane metathesis and organostannane dehydrogenation. <i>Dalton Transactions</i> , <b>2020</b> , 49, 10523-10534  | 4.3  | 3  |
| 7  | Correlations of the Structural Properties of a Complete R <sub>2</sub> PX Series (X = Hydrogen or Halogen). <i>European Journal of Inorganic Chemistry</i> , <b>2014</b> , 2014, 1843-1849  | 2.3  | 2  |
| 6  | Phosphinoborane interception at magnesium by borane-assisted phosphine-borane dehydrogenation. <i>Dalton Transactions</i> , <b>2020</b> , 49, 14584-14591   | 4.3  | 2  |

- 5 Nucleophilic Magnesium Silanide and Silaamidinate Derivatives. *Inorganic Chemistry*, **2020**, 59, 13679-13689 2
- 4 Computational Studies of Heteroatom-Assisted C-H Activation at Ru, Rh, Ir, and Pd as a Basis for Heterocycle Synthesis and Derivatization **2016**, 1-44 2
- 3 DFT calculations bring insight to internal alkyne-to-vinylidene transformations at rhodium PNP- and PONOP-pincer complexes.. *RSC Advances*, **2021**, 11, 11793-11803 3.7 1
- 2 Dihydrogen Activation by Lithium- and Sodium-Aluminyls. *Angewandte Chemie*, **2021**, 133, 22463-22466 3.6 1
- 1 A computational study on the identity of the active catalyst structure for Ru(ii) carboxylate assisted C-H activation in acetonitrile. *Organic and Biomolecular Chemistry*, **2019**, 17, 6678-6686 3.9 0