

Brief Curriculum Vitae - Jason Brian Harper

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Professional Experience

- 2002 - Lecturer (2002-2007), Senior Lecturer (2007-2015) and Associate Professor (2016-),
School of Chemistry, University of New South Wales
(Also Visiting Positions at Queen's University, Belfast (2002/3), Australian National
University (2004), University of Melbourne (2004/5) and Boston College (2009))
- 2000-2002 National Health and Medical Research Council C. J. Martin Postdoctoral Research Fellow,
University Chemical Laboratory, University of Cambridge (with Prof. Anthony J. Kirby)
- 2001 Associate Lecturer, The Open University in East Anglia

Education

- 2000 Ph.D., Australian National University (with Prof. Christopher J. Easton)
- 1996 B.Sc.(Hons), Australian National University
- 1995 B.Sc., University of Adelaide

Research Record

- Total publications: 132 (including 126 journal articles and 6 book chapters)
- Total citations: 4400+ (Google Scholar)
- H-index: 36 (Google Scholar)
- Received >\$900K direct research funding and >\$1.5M infrastructure funding (ARC, UNSW)

Research Interests

- Understanding and predicting the outcome of processes in ionic liquids.
- Correlating structure, acidity and reactivity, particularly with respect to *N*-heterocyclic carbenes and polycyclic aromatic hydrocarbons.
- Developing novel methods, particularly using NMR spectroscopy, for following reaction outcomes.

Professional Activities

- Editor, *Chemical Physics* and Serial Co-Editor, *Advances in Physical Organic Chemistry*
- International Advisory Board, *ChemPlusChem*
- Guest Editor, *Physical Chemistry Chemical Physics* and *Organic and Biomolecular Chemistry* web based thematic issue (Non-Traditional Solvent Effects in Organic Reactions) and *Journal of Organic Chemistry* (Solvation effects in organic chemistry).
- Titular Member (2020-2021) and Associate Member (2018-2019), Division III (Organic), International Union of Pure and Applied Chemistry
- Committee Member, IUPAC Subcommittee on Structural and Mechanistic Chemistry
- Bid Developer and Co-Chair, 23rd IUPAC Conference on Physical Organic Chemistry (ICPOC23), July 3rd-8th 2016, Sydney
- Organising committee, 2014 Australasian Symposium on Ionic Liquids / Asia-Pacific Symposium on Ionic Liquids
- Assessor (ACS PRF, ARC (Australia), EPSRC (UK), Royal Society (UK), US Department of Defense, Romanian Ministry of National Education, Chilean National Science Commission, NSERC (Canada))
- Fellow, Royal Australian Chemical Institute; Member, American Chemical Society (ACS) and Royal Society of Chemistry (RSC)
- Postgraduate Examiner (Australia, India, New Zealand, Pakistan, South Africa and USA)

Publications (2017-, most recent first, remainder available on request)

Journal Articles

- 126) Barnett, C.*; Cole, M. L.; Harper, J. B.*: “Correlating electronic properties of *N*-heterocyclic carbenes with structure, and the implications of using different probes”, *ChemistrySelect*, accepted December 13th 2021.
- 125) Coney, M. D.; Morris, D. C.; Gilbert, A.; Prescott, S. W.; Haines, R. S.; Harper, J. B.*: “Effects of ionic liquids on the nucleofugality of chloride”, *Journal of Organic Chemistry*, accepted October 25th 2021. doi: 10.1021/acs.joc.1c02043.
- 124) Wang, J. E.; Gilbert, A.; Harper, J. B.*; Kim, D. J.: “Understanding the failure mechanism of rechargeable aluminum batteries: Metal anode perspective through X-ray tomography”, *Advanced Energy and Sustainability Research*, accepted October 15th 2021. doi: 10.1002/aesr.202100164.
- 123) Munavirov, B.; Black, J. J.; Shah, F. U.; Leckner, J.; Rutland, M. W.*; Harper, J. B.*; Glavatskih, S.*: "The effect of anion architecture on the lubrication chemistry of phosphonium orthoborate ionic liquids", *Scientific Reports*, **2021**, *11*, 24021. doi: 10.1038/s41598-021-02763-5.
- 122) Barnett, C.*; Cole, M. L.; Harper, J. B.*: “Steric properties of *N*-heterocyclic carbenes affect the performance of electronic probes”, *European Journal of Inorganic Chemistry*, **2021**, *47*, 4954-4958. doi: 10.1002/ejic.202100796.
- 121) Chen, J.; Kato, J.; Harper, J. B.; Shao, Y.; Ho, J.*: “On the Accuracy of QM/MM Models. A Systematic Study of Intramolecular Proton Transfer Reactions of Amino Acids in Water” *Journal of Physical Chemistry B*, **2021**, *125*, 9304-9316. doi: 10.1021/acs.jpcc.1c04876.
- 120) Barnett, C.*; Cole, M. L.; Harper, J. B.*: “A dual NMR probe approach to understanding the electronic properties of *N*-heterocyclic carbenes”, *Chemistry – Methods*, **2021**, *1*, 374-381. doi: 10.1002/cmtd.202100043.
- 119) Rohlmann, P.; Watanabe, S.; Shimpi, M.; Leckner, J.; Rutland, M. W.; Harper, J. B.; Glavatskih, S.*: “Boundary lubricity of phosphonium bisoxalato borate ionic liquids”, *Tribology International*, **2021**, *161*, 107075. doi: 10.1016/j.triboint.2021.107075.
- 118) Gilbert, A.; Haines, R. S.; Harper, J. B.*: “The effects of using an ionic liquid as a solvent for a reaction that proceeds through a phenonium ion”, *Journal of Physical Organic Chemistry*, **2021**, *34*, e4217. [COVER ARTICLE] doi: 10.1002/poc.4217.
- 117) Morris, D. C.; Prescott, S. W.*; Harper, J. B.*: “Rapid relaxation NMR measurements to predict rate coefficients in ionic liquid mixtures. An examination of reaction outcome changes in a homologous series of ionic liquids”, *Physical Chemistry Chemical Physics*, **2021**, *23*, 9878-9888. doi: 10.1039/d0cp06966f.
- 116) Greaves, T. L.*; Schaffarczyk McHale, K. S.; Burkart-Radke, R. F.; Harper, J. B.*; Le, T.*: “Machine learning approaches to understand and predict rate constants for organic processes in mixtures containing ionic liquids”, *Physical Chemistry Chemical Physics*, **2021**, *23*, 2742-2752. doi: 10.1039/d0cp04227g.
- 115) Sandler, I.; Harper, J. B.; Ho, J.*: “Explanation of Substituent Effects on Enolization of β -Diketones and β -Ketoesters”, *Journal of Chemical Education*, **2021**, *98*, 1043-1048. doi: 10.1021/acs.jchemed.0c01076.
- 114) Schindl, A.; Hawker, R. R.; Schaffarczyk McHale, K. S.; Liu, K. T.-C.; Morris, D. C.; Hsieh, A. Y.; Gilbert, A.; Prescott, S. W.; Haines, R. S.; Croft, A. K.*; Harper, J. B.*; Jäger, C. M.*: “Controlling the outcome of S_N2 reactions in ionic liquids: From rational data set design to predictive linear regression models”, *Physical Chemistry Chemical Physics*, **2020**, *22*, 23009-23018. [SELECTED AS A HOT ARTICLE] doi: 10.1039/d0cp04224b.
- 113) Liu, K. T.-C.; Haines, R. S.; Harper, J. B.*: “The effect of bisimidazolium based ionic liquids on a bimolecular substitution process. Are two head(group)s better than one?”, *Organic and Biomolecular Chemistry*, **2020**, *18*, 7388-7395. doi: 10.1039/d0ob01500h.

- 112) Gilbert, A.; Haines, R. S.; Harper, J. B.*: "Controlling the reactions of 1-bromogalactose acetate in methanol using ionic liquids as co-solvents", *Organic and Biomolecular Chemistry*, **2020**, *18*, 5442-5452. doi: 10.1039/d0ob01198c.
- 111) Konstandaras, N.; Dunn, M. H.; Luis, E. T.; Cole, M. L.; Harper, J. B.*: "The pK_a values of N-aryl imidazolium salts, their higher homologues, and formamidinium salts in dimethyl sulfoxide", *Organic and Biomolecular Chemistry*, **2020**, *18*, 1910-1917. doi: 10.1039/d0ob00036a.
- 110) Mallo, N.; Tron, A.; Andréasson, J.; Harper, J. B.; Jacob, L. S. D.; McClenaghan, N. D.; Jonusauskas, G.; Beves, J. E.*: "Hydrogen-bonding donor-acceptor Stenhouse adducts", *ChemPhotoChem*, **2020**, *4*, 407-412. doi: 10.1002/cptc.201900295.
- 109) Blake, S. A. P.*; Palmer, J. G.; Björklund, J.; Harper, J. B.; Tierney, C. S. M.: "Palaeoclimate potential of New Zealand *Manoao colensoi* (silver pine) tree rings using Blue-Intensity", *Dendrochronologia*, **2020**, *60*, Article 125644. doi: 10.1016/j.dendro.2020.125644.
- 108) Konstandaras, N.; Dunn, M. H.; Guerry, M. S.; Barnett, C. D.; Cole, M. L.; Harper, J. B.*: "The impact of cation structure upon the acidity of triazolium salts in dimethyl sulfoxide", *Organic and Biomolecular Chemistry*, **2020**, *18*, 66-75. doi: 10.1039/c9ob02258a.
- 107) Zheng, X.; Harper, J. B.; Hope, G.; Mooney, S. D.*: "A new preparation method for testate amoebae in minerogenic sediments", *Mires and Peat*, **2019**, *24*, Article 30. doi: 10.19189/MaP.2018.OMB.380.
- 106) Gilbert, A.; Bucher, G.; Haines, R. S.; Harper, J. B.*: "Correlating ionic liquid solvent effects with solvent parameters for a reaction that proceeds through a xanthylium intermediate", *Organic and Biomolecular Chemistry*, **2019**, *17*, 9336-9342. doi: 10.1039/C9OB01807G.
- 105) Schaffarczyk McHale, K. S.; Wong, M. J.; Evans, A. K.; Gilbert, A.; Haines, R. S.; Harper, J. B.*: "Understanding the effects of solvate ionic liquids as solvents on substitution processes", *Organic and Biomolecular Chemistry*, **2019**, *17*, 9243-9250. doi: 10.1039/c9ob01753d.
- 104) Schaffarczyk McHale, K. S.; Haines, R. S.; Harper, J. B.*: "Investigating variation of the pnictogen nucleophilic heteroatom on ionic liquid solvent effects in bimolecular nucleophilic substitution processes", *ChemPlusChem*, **2019**, *84*, 534-539. doi: 10.1002/cplu.201900188.
- 103) Schaffarczyk McHale, K. S.; Haines, R. S.; Harper, J. B.*: "Understanding the dependence of ionic liquid solvent effects on the nucleophilic heteroatom in S_NAr reactions. Highlighting the potential for control of selectivity", *ChemPlusChem*, **2019**, *84*, 465-473. doi: 10.1002/cplu.201900173.
- 102) Gilbert, A.; Haines, R. S.; Harper, J. B.*: "Understanding the effects of ionic liquids on a unimolecular substitution process: correlating solvent parameters with reaction outcome", *Organic and Biomolecular Chemistry*, **2019**, *17*, 675-682. doi:10.1039/c8ob02460j.
- 101) Clarke, C. J.*; Maxwell-Hogg, S.; Smith, E. F.; Hawker, R. R.; Harper, J. B.; Licence, P.*: "Resolving X-Ray Photoelectron Spectra of Ionic Liquids with Difference Spectroscopy", *Physical Chemistry Chemical Physics*, **2019**, *21*, 114-123. doi:10.1039/c8cp06701e.
- 100) Butler, B. J.; Harper, J. B.*: "The effect of the structure of the anion of an ionic liquid on the rate of reaction at a phosphorus centre", *Journal of Physical Organic Chemistry*, **2019**, *32*, e3819. doi:10.1002/poc.3819.
- 99) Schaffarczyk McHale, K. S.; Haines, R. S.; Harper, J. B.*: "Ionic liquids as solvents for S_N2 processes. Demonstration of the complex interplay of interactions resulting in the observed solvent effects", *ChemPlusChem*, **2018**, *83*, 1162-1168. doi:10.1002/cplu.201800510.
- 98) Keaveney, S. T.*; Harper, J. B.*; Croft, A. K.*: "Ion – reagent interactions contributing to ionic liquid solvent effects on a condensation reaction", *ChemPhysChem*, **2018**, *19*, 3279-3287. doi:10.1002/cphc.201800695.
- 97) Hawker, R. R.; Harper, J. B.*: "Organic reaction outcomes in ionic liquids", *Advances in Physical Organic Chemistry*, **2018**, *52*, 49-85. doi:10.1016/bs.apoc.2018.09.001.
- 96) Mallo, N.; Foley, E. D.; Iranmesh, H.; Kennedy, A. W. D.; Luis, E., Ho, J., Harper, J. B.; Beves, J. E.*: "Structure-Function Relationships of Donor-Acceptor Stenhouse Adduct Photochromic Switches", *Chemical Science*, **2018**, *9*, 8242-8252. doi:10.1039/c8sc03218a.
- 95) Black, J. J.; Dolan, A.; Harper, J. B.; Aldous, L.*: "Kamlet–Taft solvent parameters, NMR spectroscopic analysis and thermoelectrochemistry of lithium–glyme solvate ionic liquids and their

- dilute solutions", *Physical Chemistry Chemical Physics*, **2018**, *20*, 16558-16567. doi:10.1039/c8cp02527d.
- 94) Hawker, R. R.; Haines, R. S.; Harper, J. B.*: "Predicting solvent effects in ionic liquids: extension of a nucleophilic aromatic substitution reaction on a benzene to a pyridine", *Journal of Physical Organic Chemistry*, **2018**, *31*, e3862. doi:10.1002/poc.3862.
- 93) Hawker, R. R.; Haines, R. S.; Harper, J. B.*: "The effect of varying the anion of an ionic liquid on the solvent effects on a nucleophilic aromatic substitution reaction", *Organic and Biomolecular Chemistry*, **2018**, *16*, 3453-3463. doi:10.1039/c8ob00651b.
- 92) Hart, W. E. S.; Aldous, L.; Harper, J. B.*: "Nucleophilic cleavage of lignin model compounds under acidic conditions in an ionic liquid. A mechanistic study", *ChemPlusChem*, **2018**, *53*, 348-353. doi:10.1002/cplu.201700486.
- 91) Hawker, R. R.; Haines, R. S.; Harper, J. B.*: "Rational selection of the cation of an ionic liquid to control the reaction outcome of a substitution reaction", *Chemical Communications*, **2018**, *54*, 2296-2299. doi:10.1039/c8cc00241j.
- 90) Oss, G.; de Vos, S. D.; Luc, K. N. H.; Harper, J. B.; Nguyen, T. V.*: "Tropylium-Promoted Oxidative Functionalisation of Tetrahydroisoquinolines", *Journal of Organic Chemistry*, **2018**, *83*, 1000-1010. doi:10.1021/acs.joc.7b02584.
- 89) Black, J. J.; Harper, J. B.; Aldous, L.*: "Temperature effect upon the thermoelectrochemical potential generated between lithium metal and lithium ion intercalation electrodes in symmetric and asymmetric battery arrangement", *Electrochemistry Communications*, **2018**, *86*, 153-156. doi:10.1016/j.elecom.2017.12.005.
- 88) Konstandaras, N.; Matto, L.; Bhadbhade, M.; Hunter, L.; Harper, J. B.*: "Synthesis and determination of the pK_a values of a series of bis(anilino)furazano[3,4-b]pyrazines", *ChemistrySelect*, **2017**, *2*, 7018-7023. doi:10.1002/slct.201701674.
- 87) Hawker, R. R.; Wong, M. J.; Haines, R. S.; Harper, J. B.*: "Rationalising the effects of ionic liquids on a nucleophilic aromatic substitution reaction", *Organic and Biomolecular Chemistry*, **2017**, *15*, 6433-6440. doi:10.1039/c7ob01476g.
- 86) Dunn, M. H.; Konstandaras, N.; Cole, M. L.*; Harper, J. B.*: "A targeted and systematic approach to the study of pK_a values of imidazolium salts in DMSO", *Journal of Organic Chemistry*, **2017**, *82*, 7324-7331. doi:10.1021/acs.joc.7b00716.
- 85) Hart, W. E. S.; Aldous, L.; Harper, J. B.*: "Cleavage of ethers in an ionic liquid. Enhancement, selectivity and potential application", *Organic and Biomolecular Chemistry*, **2017**, *15*, 5556-5563. doi:10.1039/c7ob01096f.
- 84) Keaveney, S. T.*; Haines, R. S.; Harper, J. B.: "Ionic liquid solvents: the importance of microscopic interactions in predicting organic reaction outcomes", *Pure and Applied Chemistry*, **2017**, *89*, 745-757. doi:10.1515/pac-2016-1008.
- 83) Keaveney, S. T.; Haines, R. S.; Harper, J. B.*: "Investigating solvent effects of an ionic liquid on pericyclic reactions through kinetic analyses of simple rearrangements", *ChemPlusChem*, **2017**, *82*, 449-457. doi:10.1002/cplu.201600585.

Book Chapters

- 5) Gilbert, A.; Haines, R. S.; Harper, J. B.*: "Selecting ionic liquids to enhance and control reaction outcomes" in *Elsevier References Modules in Chemistry, Molecular Sciences and Chemical Engineering*, Reedijk, J., Ed.; Elsevier: Waltham, MA. 26-Jul-18 doi:10.1016/B978-0-12-409547-2.14212-X. [Invited Article]
- 4) Keaveney, S. T.; Haines, R. S.; Harper, J. B.*: "Reactions in Ionic Liquids" in *Encyclopedia of Physical Organic Chemistry, Volume 2* (Volume editor U. Wille), Wiley, 2017: Online ISBN: 9781118468586. [Invited Article]