

Benjamin Bede Kirk

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Research Interests

Mechanisms of organic radical reactions; free radicals in planetary atmospheres and combustion; oxidative aging in aerosols; mass spectrometric and photochemistry based techniques for analysis of free radical reactions; computational chemistry; developing software interfaces for scientific instruments.

Employment

2013 – Present **LAWRENCE BERKELEY NATIONAL LABORATORY, UNITED STATES**

Postdoctoral Fellow

Supervisor: Dr. Kevin R. Wilson

- Measured low-temperature rates and branching ratios of radical reactions relevant to Titan's atmosphere using a pulsed-Laval nozzle and slow-flow tube synchrotron-VUV photoionization mass spectrometer.
- Designed and manufactured a low-energy electron gun and LabView control software.
- Maintained high vacuum instrumentation, excimer lasers and mass spectrometers.
- Facilitated external user access to synchrotron-VUV beamlines at the Advanced Light Source.
- Developed safe working procedures and synthesized pyrophoric halogenated radical precursors.

2013 – 2013 **UNIVERSITY OF WOLLONGONG, AUSTRALIA**

Associate Research Fellow

Supervisors: Dr. Adam J. Trevitt; Dr. Gabriel da Silva

- Developed a low-energy (351 nm) hydroxyl radical generator for use with a laser photolysis flow tube reactors.
- Analysed experimental measurements of organic radical oxidation reactions by quantum chemical calculations of ionization potentials, photoionization spectra and potential energy schemes.
- Managed synthetic chemistry and laser laboratory, including user training, procurement and occupational health and safety.

2011 – 2012 **UNIVERSITY OF WOLLONGONG, AUSTRALIA**

Associate Research Fellow

Supervisors: Prof. Stephen J. Blanksby; Dr. Adam J. Trevitt

- Measured reaction rates and branching of distonic radical ion analogues of atmospherically relevant radical oxidation reactions.
- Developed mechanistic models of radical reactions based on analogous experimental measurements and quantum mechanical potential energy schemes derived from density functional theory and compound method calculations.
- Developed and maintained an ultraviolet photodissociation action spectroscopy experiment employing an Nd:YAG pumped OPO coupled to a linear ion-trap mass spectrometer, including development of LabView software to control the OPO laser and capture/process mass spectrometric data.
- Managed synthetic chemistry and laser laboratory, including user training, procurement and occupational health and safety.

2007 – 2013 **UNIVERSITY OF WOLLONGONG, AUSTRALIA**

Lab Leader 2nd/Demonstrator 3rd Year Physical Chemistry

- Led 2nd year physical chemistry laboratory classes.
- Aided in demonstration of 3rd year physical chemistry practical classes.
- Evaluated and amended laboratory course notes.
- Established marking criteria and assessed 2nd/3rd year physical chemistry assignments and exams.

2003 – 2012 **R.K.F ENGINEERING SERVICES**

Systems Administrator and Programming Contract

- Developed CARMS/SARMS software, including documentation and training for auditing civil works.
- System administrator and help desk support.

Education and Training

- 2007 – 2011 **UNIVERSITY OF WOLLONGONG, AUSTRALIA**
Doctor of Philosophy (Chemistry)
Project Title: Reactions of aryl and alkylperoxyl radicals in the gas phase
Supervisors: Prof. Stephen J. Blanksby, Dr. Adam. J. Trevitt
- 2002 – 2006 **UNIVERSITY OF WOLLONGONG, AUSTRALIA**
Bachelor of Computer Science with Distinction
Bachelor of Science (Chemistry Honours) 1st Class
Project Title: Synthesis, isolation and reactions of peroxyl radicals in the gas phase
Supervisor: Prof. Stephen J. Blanksby
- 2009 **LAWRENCE BERKELEY NATIONAL LABORATORY,
BERKELEY, CA, UNITED STATES**
Visiting Scholar (08/06/09 to 20/06/09)
Supervisor: Dr. Adam J. Trevitt
- 2008 **PURDUE UNIVERSITY, IN, UNITED STATES**
Visiting Scholar (09/06/08 to 01/08/08)
Supervisor: Prof. Hilikka Kenttämaa

Grants

- 2013 ISAP Australian Synchrotron Travel Scheme \$6400
2013 National Computing Infrastructure National Facility Merit Allocation Scheme
Computation Allocation (20000 Hours; \$2000; \$0.1/Hour)
2013 Intersect HPC Computation Allocation (20000 Hours; \$2000; \$0.1/Hour)
2011 Intersect HPC Computation Allocation (10000 Hours; \$1000; \$0.1/Hour)
2009 ISAP Australian Synchrotron Travel Scheme
2009 National Computing Infrastructure National Facility Merit Allocation Scheme
Computation Allocation

Fellowships/Honours

- Student Oral Presentation, Free Radical Spring Carnival, Monash University, 2010
- Larry Hick Award for The Best Research Paper by a HDR Student from the School of Chemistry, University of Wollongong, 2010
- Australian Postgraduate Award (APA), 2007-2010
- University of Wollongong, 2006 Honours Scholarship
- University of Wollongong, Faculty of Science, Dean's Merit List 2006
- University of Wollongong, Faculty of Informatics, Dean's Merit List - Voluntary Service Award 2005/2006
- University of Wollongong, Faculty of Informatics, Dean's Merit List 2005

References

Provided on request.

Publications

19. Richards-Henderson, N. K.; Pham, A.T.; **Kirk, B. B.**; Anastasio, C.; 'Secondary Organic Aerosol Formation from Aqueous Phase Reactions of Green Leaf Volatiles by Organic Triplet Excited States and Singlet Molecular Oxygen', *Environ. Sci. Tech.*, **Accepted**
18. Nah, T.; Zhang, H.; Worton, D.; Ruehl, C.; **Kirk, B.B.**; Goldstein, B.; Leone, S.; Wilson, K.; 'Isomeric Product Detection in the Heterogeneous Reaction of Hydroxyl Radicals with Aerosol Composed of Branched and Linear Unsaturated Organic Molecules', *J. Phys. Chem. A*, **In press**
17. So, S.; **Kirk, B. B.**; Trevitt, A. J.; Wille, U.; Blanksby, S. J.; da Silva, G.; 'Unimolecular reaction chemistry of a charge-tagged beta-hydroxyperoxyl radical', *Phys. Chem. Chem. Phys.*, **16** (45), 24954 - 24964 (2014)

16. Prendergast, M. B.; Cooper, P. A.; **Kirk, B. B.**; da Silva, G. R.; Blanksby, S. J.; Trevitt, A. J.; 'Hydroxyl Radical Formation in the Gas Phase Oxidation of Distonic 2-Methylphenyl Radical Cations', *Phys. Chem. Chem. Phys.*, **15**, 20577-20584 (2013)
15. Hansen, C. S.; **Kirk, B. B.**; Blanksby, S. J.; Trevitt, A. J.; 'Ultraviolet Photodissociation of the N-methylpyridinium Ion: Action Spectroscopy and Product Characterization', *J. Phys. Chem. A*, **117**(42), 10839-10846 (2013)
14. Thomas, M. C.; **Kirk, B. B.**; Altvater, J.; Blanksby, S. J.; Nette, G. W.; 'Formation and fragmentation of unsaturated fatty acid [M-2H+Na]⁻ ions: Stabilized carbanions for charge-directed fragmentation', *J. Am. Soc. Mass Spectrom.*, **25**(2), 237-247 (2014)
13. Poad, B. L. J.; **Kirk, B. B.**; Hettiarachchi, P. I.; Trevitt, A. J.; Blanksby, S. J.; Clark, T.; 'Direct Observation of a Persistent Carbonyloxyl Radical in the Gas Phase', *Angew. Chem. Int. Ed.*, **52** (35), 9301-9304 (2013)
12. **Kirk, B. B.**; Trevitt, A. J.; Poad, B. L. J.; Blanksby, S. J.; 'Characterisation of the ionic products arising from electron photodetachment of simple dicarboxylate dianions', *Int. J. Mass Spectrom.*, **351**, 81-94 (2013).
11. Maccarone, A. T.; **Kirk, B. B.**; Hansen, C. S.; Griffiths, T. M.; Olsen, S. Trevitt, A. J.; Blanksby, S. J.; 'Direct Observation of Photodissociation Products from Phenylperoxyl Radicals Isolated in the Gas Phase', *J. Am. Chem. Soc.*, **135**, 9010 (2013)
10. Hansen, C. S.; **Kirk, B. B.**; Blanksby, S. J.; O'Hair, R. A. J.; Trevitt, A. J.; 'UV Photodissociation Action Spectroscopy of Haloanilinium Ions in a Linear Quadrupole Ion Trap Mass Spectrometer', *J. Am. Soc. Mass Spectrom.*, **24**, 932 (2013)
9. **Kirk, B. B.**; Trevitt, A. J.; Blanksby, S. J.; 'Does addition of NO₂ to carbon-centered radicals yield RONO or RNO₂? An investigation using distonic radical ions', *J. Am. Soc. Mass Spectrom.*, **24**, 481 (2013)
8. Li, C. H.; Khairallah, G. N.; Lam, A. K. Y.; O'Hair, R. A. J.; **Kirk, B. B.**; Blanksby, S. J.; da Silva, G. R.; Wille, U.; 'Reaction of Aromatic Peroxyl Radicals with Alkynes: A Mass Spectrometric and Computational Study Using the Distonic Radical Ion Approach', *Chem. Asian J.*, **8**, 450 (2013)
7. **Kirk, B. B.**; Harman, D. G.; Kenttämaa, H. I.; Trevitt, A. J.; Blanksby, S. J.; 'Isolation of the phenylperoxyl radical and elucidation of degradation mechanisms using distonic radical ion models', *Phys. Chem. Chem. Phys.*, **14**, 16719 (2012)
6. **Kirk, B. B.**; Trevitt, A. J.; Blanksby, S. J.; Tao, Y.; Moore, B. N.; Julian, R. R.; 'Ultraviolet Action Spectroscopy of Iodine Labeled Peptides and Proteins in the Gas Phase', *J. Phys. Chem. A*, **117**, 1228 (2013)
5. da Silva, G.; **Kirk, B. B.**; Lloyd, C.; Trevitt, A. J.; Blanksby, S. J.; 'Concerted HO₂ Elimination from α-Aminoalkylperoxyl Free Radicals: Experimental and Theoretical Evidence from the Gas-Phase NH₂•CHCO₂ + O₂ Reaction', *J. Phys. Chem. Lett.*, **3**, 805-811 (2012)
4. Lam, A. K. Y.; Li, C. H.; Khairallah, G.; **Kirk, B. B.**; Blanksby, S. J.; Trevitt, A. J.; Wille, U.; O'Hair, R. A. J.; da Silva, G.; 'Gas-phase reactions of aryl radicals with 2-butyne: an experimental and theoretical investigation employing the N-methylpyridinium-4-yl radical cation', *Phys. Chem. Chem. Phys.*, **14**, 2417-2426 (2012)
3. Ly, T.; **Kirk, B. B.**; Hettiarachchi, P. I.; Poad, B. L. J.; Trevitt, A. J.; da Silva, G.; Blanksby, S. J.; 'Reactions of Simple and Peptidic alpha-Carboxylate Radical Anions with Dioxygen in the Gas Phase', *Phys. Chem. Chem. Phys.*, **13** (36), 16314 (2011)
2. **Kirk, B. B.**; Harman, D. G.; Blanksby, S. J.; 'Direct Observation of the Gas Phase Reaction of the Cyclohexyl Radical with Dioxygen Using a Distonic Radical Ion Approach', *J. Phys. Chem A*, **114** (3), 1446-1456 (2010)
1. Paine, M. R. L.; **Kirk, B. B.**; Ellis-Steinborner, S.; Blanksby, S. J.; 'Fragmentation pathways of 2,3-dimethyl-2,3-dinitrobutane cations in the gas phase', *Rapid Commun. Mass Spectrom.*, **23** (18), 2867-2877 (2009)

Oral Presentations

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| 2014 | Chemical Sciences Division Meeting, Lawrence Berkeley National Laboratory
Seminar: Isomer Specific Branching of Low Temperature Radical Reactions: Molecule growth in Titan's atmosphere |
| 2012 | UOW HPC User Group Meeting, Wollongong, Australia
Invited seminar: <i>Chemistry and High Performance Computing</i> |
| 2011 | 59th ASMS Conference on Mass Spectrometry and Allied Topics
Seminar: <i>Reactions of α-carboxylate radical anions with dioxygen</i> |

- 2010 **School of Chemistry, University of Wollongong, Australia**
Seminar: *Synthesis, isolation and characterisation of elusive radicals using distonic radical ions*
- 2010 **Free Radical Spring Carnival 2010, Monash University, Australia**
Seminar: *Characterising the elusive phenyl radical in the gas phase using distonic radical ions*
- 2009 **57th ASMS Conference on Mass Spectrometry and Allied Topics**
Seminar: *Direct observation of the reactions of the phenyl radical with dioxygen using distonic ions*
- 2007 **21st ANZSMS Conference, Christchurch, New Zealand**
Seminar: *Probing the reactions of alkyl peroxy radicals in the gas phase using distonic radical anions*
- 2006 **14th Annual RACI R&D Topics Conference, Wollongong, Australia**
Seminar: *Investigating the formation of atmospheric pollutants using mass spectrometry*

Poster Presentations

- 2013 **24th ANZSMS Conference, Melbourne, Australia**
Poster: *Identifying isomeric reaction products using CID and UVPD: the R + NO₂ reaction.*
- 2012 **Free Radical Spring Carnival 2012, Wollongong, Australia**
Poster: *UV action spectroscopy of peptides and proteins via photodissociation of iodine labelled tyrosine residues*
- 2012 **19th International Mass Spectrometry Conference, Kyoto, Japan**
Poster: *UV action spectroscopy of peptides and proteins via photodissociation of iodine labelled tyrosine residues*
- 2011 **BioPhysChem2011, University of Wollongong**
Poster: *Ph + NO₂ → PhONO or PhNO₂?*
- 2011 **Free Radical Spring Carnival 2011, Sydney**
Poster: *Ph + NO₂ → PhONO or PhNO₂?*
- 2011 **The 31st International Symposium on Free Radicals, Cairns, Australia**
Poster: *Investigating the stability of carboxylate radical anions*
- 2011 **23rd ANZSMS Conference, Fremantle, Australia**
Poster: *What makes a distonic radical anion? Gas-phase synthesis and characterisation of alkyl and arylperoxy radicals using distonic radical ions.*
- 2009 **22nd ANZSMS Conference, Sydney, Australia**
Poster: *Investigating the reactivity of strained carbon-centred radicals using distonic radical ions*
- 2008 **56th ASMS Conference on Mass Spectrometry and Allied Topics**
Poster: *Directly observing the gas-phase reactions of carbon-centred radicals using distonic anions*
- 2007 **55th ASMS Conference on Mass Spectrometry and Allied Topics**
Poster: *Directly observing the gas-phase reactions of alkyl and phenyl radicals with dioxygen using distonic anions*

Current Society Memberships

- Royal Australian Chemical Institute (MRACI CChem)
- American Chemical Society
- Australian and New Zealand Society for Mass Spectrometry
- American Society for Mass Spectrometry
- Golden Key International Honour Society