

The life of Brian

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This special issue of the *Australian Journal of Chemistry* celebrates the career and scientific achievements of Professor Brian Yates, an eminent Australian computational chemist who retired from the University of Tasmania in 2022. Prof. Yates' immense contributions to computational chemistry and chemical education in Australia, and his unwavering support for others in the Australian scientific community are worthy of this celebration. Thanks to all the authors who contributed to this special issue.

Brian Francis Yates is an interesting man, and always has been. One of us (Peter M. W. Gill) has known and admired him for more than 40 years and considers him to be a splendid example of a multidimensional scientist, a polymath whose skillset transcends the boundaries that confine most of us who have followed traditional academic careers. He completed a Bachelors degree, a PhD and a postdoc, accepted a lectureship at his *alma mater* and rose to become the Executive Dean of its College of Sciences and Engineering. But it is much more illuminating to discover what he did along the way, for our side-hustles often reveal our personalities in much sharper relief than our careers.

Brian studied chemistry and mathematics during his BSc at the University of Tasmania and won named prizes for the top science or chemistry student in each of his undergraduate years. But, even in those early days, there were signs that he was cut from uncommon cloth. His was not the stereotypical path, burning the candle at both ends, memorising lecture notes and rehearsing previous exams. He was a naturally gifted learner who could absorb and organise scientific ideas with ease but this was not enough. A life of isolated nerdiness was far too monochromatic to satisfy his desire to understand and help his fellow human being. And so, barely out of his teens, he had already been elected the secretary of the Tasmania University Students' Union and, shortly thereafter, the Student Representative on the University Council. This was a young man who achieved a Merkleian shape-shift, morphing effortlessly from an optimiser of molecular structures to an optimiser of university structures, eager to ensure that the latter function properly and for the good of all.

Having made his mark on the Taswegian tertiary education system and garnered a Diploma of Education to boot, Brian migrated north to join Leo Radom's group at the Australian National University (ANU) in Canberra and it was there that I (PMWG) first met him. We were both PhD students, but Brian was 1 year ahead of me and, in many ways, my role model and mentor. By the second year of his PhD, he had already ascended to the presidency of the ANU Research Students' Association and I (PMWG) was struck by his consistently unselfish willingness to help wherever he could, both inside Leo's lab on matters quantum mechanical and, more broadly, on issues that affected the lives of other students. A young inorganic PhD student who was negotiating difficulties with her residential college was one of the many beneficiaries of Brian's tireless support for the underdog and has never forgotten his kindness (she is now my wife).

One might have thought that unlocking the secrets of gas-phase ion chemistry (Brian had published 13 papers by the end of his PhD) and providing pastoral care to numerous students would have left very little time for anything else. But, no. Brian was a talented tenor and one of the lynchpins of SCUNA, the inaptly named ANU Choral Society, throughout his postgraduate years. By day, he revealed the wonders of distonic radical cations to

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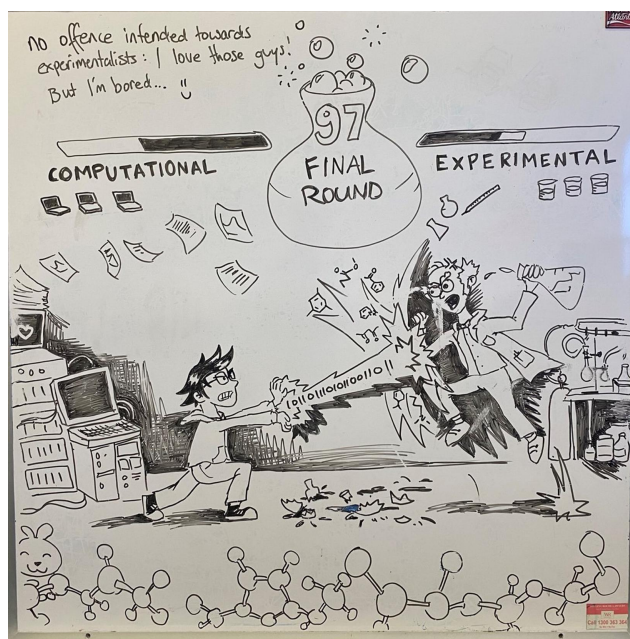


Fig. 1. A whiteboard sketch from a 2011 group meeting by Dr Miranda Shaw (who completed both theoretical and experimental studies during her PhD).

mass spectrometrists; by night, he unveiled the extraordinary soundscape of Palestrina to cultured Canberrans.

Brian completed his PhD with characteristic aplomb and, without further ado, sallied forth to postdoc with Fritz Schaefer at the University of California—Berkeley and, later, the University of Georgia. His enviable productivity continued unabated in the hothouse of a top US research group and, as one would anticipate, the sirens of Tasmania wasted no time in luring him back to his roots. This proved to be a major coup for the university, for Brian subsequently not only produced a continuous stream of high-quality graduate students and research papers but also received university teaching awards almost every year. Academics of such breadth and depth cannot hide for long and, by 2006, he had become Head of the School of Chemistry, a natural leader who set an admirable example as both a world-class researcher and outstanding pedagogue.

Our paths crossed many times at international conferences, where he would invariably present beautifully polished lectures on the application of quantum chemistry to pressing problems in catalysis and elsewhere. His name was internationally recognised and almost universally respected. The only exception that I recall was a meeting at which the organisers engaged the services of a registration computer that printed his badge using the anagrammatically reasonable but anatomically disturbing *nom de plume* 'Brain Yeast'.

With a chair at his *alma mater*, a throng of adoring students and an established international research reputation, most academics would relax, comfortable in the knowledge that their trajectory had been a successful one and

satisfied that, thenceforth, the status quo would suffice. But not the manifestly inexhaustible Brian! Never one to rest on his laurels, he actively pursued even greater challenges. After first becoming the Chair of the Physics, Chemistry and Earth Sciences panel of the Australian Research Council (ARC), his redoubtable talent was recognised and he was catapulted into the position of Executive Director of the ARC where he developed new policy initiatives to support Australia's scientific research and oversaw the complex processes of grant awarding. Though three decades had past, Brian was still Brian, continuously striving to ensure that the bureaucracies did their jobs efficiently and fairly. His service within the ARC has left an enduring legacy, the fruits of which we are now beginning to enjoy.

With the ARC rectified and on course, Brian returned once again to the University of Tasmania to accept the Deanship of the Faculty of Science, Engineering and Technology and, inevitably perhaps, proceeding to become the Executive Dean of the College of Sciences and Engineering. He provided executive leadership to that College for a turbulent period of academic restructuring and redirection that included most of the COVID years.

Brian's main research interests focus on using density functional theory and quantum chemical methods to solve challenging reaction and catalytic mechanisms used in organic synthesis. By understanding the fundamental mechanisms of reactions, guidance can be provided to synthetic chemists to assist in the targeted production of novel chemical compounds such as anti-cancer drugs and other pharmaceuticals, and new materials which might be used in frontier technologies. Specific areas of interest in which Brian made significant contributions include distonic radical cations, Pd and Pt complexes of *N*-heterocyclic carbenes for catalysis, accurate calculation of the basicity of carbenes, activation of N_2 , CO and CO_2 , catalytic reactions with Au complexes, and oxidation with hypervalent iodine reagents. A whiteboard sketch from a 2011 group meeting captures the lively spirit and collaborative atmosphere of Brian's research group at the University of Tasmania (Fig. 1). Brian has published over 200 papers, which have been cited over 5000 times in the scientific literature. Most of these publications were published in highly reputable journals such as the *Journal of the American Chemical Society*, *Organometallics*, *Dalton Transactions* and *Chemistry – A European Journal*. It should be noted that Brian made significant contributions to the *Australian Journal of Chemistry*, including 10 research publications, one of which has been cited more than 100 times in the scientific literature.¹ Brian also served as an Associate Editor of the journal in 2008–10.

Brian has made outstanding contributions to the teaching and learning of chemistry in Australia. Together with Susan Jones, he has led the development of national Threshold Learning Outcomes (TLOs) for undergraduate science degrees. These have informed curriculum design and accreditation practices in many institutions. The impact of this

work on tertiary science education in Australia is discussed in detail in a contribution to this special issue by Schultz *et al.*, entitled “‘Transformative’: the threshold learning outcomes for science”.² Brian’s significant contributions to teaching and learning in Australia were recognised through the award of numerous prizes, including the Carrick National Teaching Excellence Award for the Physical Sciences (2006), RACI Divisional Medal for the Chemical Education Division (2007), RACI Citation for contributions to chemical education, computational chemistry and the RACI (2007), UTAS Vice-Chancellor’s Individual Citation for Outstanding Contribution to Student Learning (2010) and the RACI Fensham medal for outstanding contribution to chemical education (2015).

Apart from serving as the Executive Director of the ARC, as mentioned above, Brian has made significant contributions to chemistry in Australia through additional top-level appointments, including the Chair of the Australian Partnership for Advanced Computing (APAC) and National Computational Infrastructure (NCI) National Merit Allocation Committee (2006–12), Australian Learning and Teaching Council National Discipline Scholar in Science (2010–11) and President of the Australian Council of Deans of Science (2016–20). Through these roles, Brian made extensive

contributions to strategies and policies supporting excellence in research and teaching in Australia.

Perhaps more important than all of the numerous contributions above are Brian’s human qualities and concern for students and collaborators, which are listed in [Appendix A1](#) to this Foreword. Throughout his career, Brian has mentored and guided many students and colleagues with invaluable wisdom and advice that shaped their professional careers. And somehow, during a lifetime that included so many contributions on so many fronts, Brian managed to find time to meet and marry Jennifer and to father three remarkable children, Patrick, Mark and Alison, each of whom has blossomed into a confident and caring adult. Brian will be celebrated for many things but, above all, for his faithful representation of science with a human face.

Peter Gill and Amir Karton

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Conflicts of interest. P. M. W. Gill and A. Karton are Guest Editors of this special issue and A. Karton is an Associate Editor of *Australian Journal of Chemistry*, but they did not at any stage have editor-level access to this manuscript or any other in the issue they authored while in peer review, as is the standard practice when handling manuscripts submitted by an editor to this journal. *Australian Journal of Chemistry* encourages its editors to publish in the journal and they are kept totally separate from the decision-making processes for their manuscripts. The authors have no further conflicts of interest to declare.

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Appendix A1 Students and collaborators of Brian Yates

Summer students and visiting students: Matt Addicoat, Christine Hawkins, Henrietta Headlam, Kara Johns, Rachael Madden, Jane Moran, Nicole Rijs, Nadja Saendig and Jack Sleigh.

Honours students: Mark Abraham, Ruth Amos, Paul Anderson, Clive Brettingham-Moore, Raimondo Bruno, Antony Chipman, Andrew Clippingdale, Andrew Dick, Ed Doddridge, Katrina Frankcombe, Adam Friend, David Graham, Karina Groenewoud, Adam James, Bryce Lockhart-Gillet, Mark Mackey, Rachael Madden, Alison Magill, Lynsey Maher, Chris Marks, Robert Martin, Reyne Pullen, Rhitu Rao, Bruce Reardon, Shane Seabrook, Tell Tuttle, Trent Wale, Michaela Wegman, Adele Wilson and Lauren Wise.

PhD students: Ruth Amos, Rasool Babaahmadi, Vicky Barnett, Nigel Brookes, Elzbieta Chelkowska, Katrina Frankcombe, Yos Ginting, Ali Gouranourimi, David Graham, Kirsty Hawkes, George Heard, Mona Jalali, Adam James, Morteza Jamshidi, Bryce Lockhart-Gillet, Alison Magill, Doug McLean, Peter Molesworth, Reyne Pullen, Miranda Shaw, Damien Stringer, Yan-Ping Sun, Adele Wilson and Lauren Wise.

Postdocs and research fellows: Alireza Ariafard, Robert O’Reilly and Robert Robinson.

Sabbatical visitors: Peter Boyd, Agusti Lledos and Toshiaki Saitoh.

Other scientific collaborators: John Abbot, Wesley Allen, Lou Allinger, Jon Baker, Paul Banham, Harold Basch, Hossein Batebi, Greg Beran, Michael Bermingham, Maria Besora, Nathan Bindoff, Alex Bissember, Adrian Blackman, Chuck Blahous, Willem Bouma, John Bremner, George Britovsek, Elaine Browne, Mark Buntine, Allan Canty, Kingsley Cavell, Germán

Cavigliasso, Bun Chan, Chen-Loung Chen, Gemma Christian, Allen Clabo, Geoffrey Cloke, Eric Clot, Kit Cummins, Stefan Dapprich, Ayan Dasgupta, Randy Davy, Roger DeKock, Allan East, Alison Edwards, Moris Eisen, Odile Eisenstein, Kaveh Farshadfar, Larry Forbes, Gernot Frenking, Alistair Frey, Michael Gardiner, Adrian George, Frank Gerhards, Narges Ghohe, Peter Gill, Robert Gossage, Christophe Gourlaouen, Brendon Gourlay, Mel Green, Roger Grev, Renate Griffith, Robert Grubbs, Nina Gunawan, Paul Haddad, Trevor Hambley, Stephen Hashmi, Martin Head-Gordon, Roland Hertwig, Curtis Ho, James Howard, Mark Humphrey, Chris Hyland, Naoko Ichiishi, Curt Janssen, Roderick Jones, Meredith Jordan, Scott Kable, Sam Karpiniec, Andrew Katsifis, Robert Knott, Wolfram Koch, Frank Larkins, Tim Lee, Trevor Lewis, John MacLeod, Feliu Maseras, David McGuinness, Rebecca Melen, Greg Metha, Keiji Morokuma, Djamal Musaev, David Nielsen, Ross Nobes, Adrien Normand, Richard O'Hair, Angus Olding, Jim Patel, Evan Peacock, Simon Petrie, Stephen Pyne, Geoff Quelch, Leo Radom, Nasir Rajabi, Anung Riapanitra, Julia Rice, Des Richardson, Tobias Ritter, Melanie Sanford, Fritz Schaefer, Andy Scheiner, Carl Schiesser, Gustavo Scuseria, Ed Seidel, Manab Sharma, Brian Skelton, Jason Smith, Karen Stack, Rob Stranger, Elham Tabatabaie, Mohammad Talebi, Brenda Thiess, Vicki-Anne Tolhurst, Ashley Townsend, Jamal Uddin, Andaravaas Vaas, Dave Vercoe, Krista Vikse, Adrian Wallis, Jun Wang, Roland Warner, Sarah Wengryniuk, Allan White, Matthew Whited, Alan Williams, Richard Wong, Matthew Woolley, Yaoming Xie, Yukio Yamaguchi and Fatemeh Zarkoob.

Education research collaborators: Stephanie Beames, Dan Bedgood, Adam Bridgeman, Mark Buntine, Andrea Crampton, Graham Cross, Julian Dermoudy, Greg Dicoski, Chris Evans, Michael Gardiner, Greg Hannan, Jason Harper, Sally James, Liz Johnson, Jo Kelder, Gwen Lawrie, Brett Lidbury, Kieran Lim, Ted Lloyd, Kelly Matthews, Danielle Meyrick, Mauro Mocerino, Gayle Morris, Glennys O'Brien, Barry O'Grady, Jon Osborn, Simon Pyke, John Rice, Will Rifkin, John Rodger, Brian Salter-Duke, Sigg Schmid, Jurgen Schulte, Madeleine Schultz, Manju Sharma, Jason Smith, Daniel Southam, Cristina Varsavsky, Ute Wille, Margaret Wong, Marjan Zadnik and Felicia Zhang.

Australian Learning and Teaching Council discipline scholars: Ian Cameron, Christine Ewan, Mark Freeman, Roger Hadgraft, Iain Hay, Greg Heath, Amanda Henderson, Jonathan Holmes, Sue Jones, Sally Kift, Sid Newton, Maree O'Keefe and Susan Savage.