

## Celebrating Professor Graham Chandler's 80th Birthday

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This special issue of the *Australian Journal of Chemistry* celebrates the 80th birthday and scientific achievements of Graham Chandler, an eminent Australian theoretical chemist who has had an enormous impact on the field of theoretical chemistry and whose lifelong support of others in the Australian milieu is worthy of celebration.

Graham Chandler was born in Adelaide in 1939. Following the completion of his BSc in Chemistry at the University of Adelaide, he obtained a PhD degree in 1964 under the supervision of Wolfgang Sasse, with a thesis entitled 'Substitution Reactions of Some Heterocyclic Compounds'. During his PhD research, Graham became fascinated by theory, having focused part of his research on the correlation of experimental results with theoretical activity parameters available at the time. After graduation, he was determined to pursue postdoctoral research in that area with David Craig, at University College London. As Craig was working on more abstruse spectroscopic problems at that time, Graham ended up working with T. Thirunamachandran on the nature of *d*-orbitals in phosphorus and sulfur, building on earlier work by Craig and others. Graham returned to Australia in 1967 as a research fellow, accompanying David Craig in his move to the Research School of Chemistry at the Australian National University. A chapter in *Rodd's Chemistry of Carbon Compounds*,<sup>†</sup> with David Craig, emerged from that period at ANU.

In 1970, Graham moved to the University of Western Australia. He arrived with his young family in February, immediately after the first Australian theoretical summer school held at ANU, and had to hurriedly prepare lecture material while accommodated in a flat near Steve's Hotel, a very popular student pub in the 1970s. The bulk of Graham's research has naturally been influenced by his interactions with colleagues and academic visitors throughout his nearly half-century at UWA. An enduring theme in his research concerns the use of *ab initio* computational quantum chemistry methods for the calculation of spin and charge density distributions in molecules and the comparison of these calculated properties with experimental X-ray data, and this can be traced to key collaborations with Doug McLean at IBM and Brian Figgis at UWA.

A. D. (Doug) McLean was a UWA chemistry graduate (BSc (Hons) in physical chemistry, 1951) who undertook postgraduate studies at the University of Chicago. He was an important

contributor to the development of pioneering programs for the computation of wave functions and spectroscopic properties of linear molecules. After a brief stint as a senior lecturer in the UWA Chemistry Department (1960–62), McLean returned to the United States, joining the IBM Research Laboratory in San Jose. A return visit by Doug McLean to UWA in early 1976 led to Graham spending six months of sabbatical leave at IBM San Jose later that year, as well as several shorter visits over Christmas holidays and subsequent study leaves. During one of those visits focusing on the structure and chemical properties of homonuclear diatomic molecules, Graham decided to familiarize himself with the details of constructing contracted Gaussian basis sets, and he ended up developing a hierarchy of new basis sets for first and second row atoms, as well as the first transition series. This was at a time when several groups were independently pursuing the optimization of basis sets for molecular calculations, and the basis sets developed for second row atoms were published in 1980.<sup>‡</sup> These 'McLean-Chandler' basis sets are used to this day, and that publication turned out to be influential in the history of basis-set development. It has been cited over 5,700 times in the scientific literature, is by far the most highly-cited paper by either author, and in 2013 was one of 80 articles chosen to highlight the '80 years of outstanding work' published in the *Journal of Chemical Physics*. Such is the serendipity of scientific research, and Graham's collaboration with Doug McLean lasted well into the 1990s.

The determination of electron densities from single crystal X-ray diffraction data was an important research focus of the Crystallography Centre at UWA throughout the 1970s, principally in the research group of E. N. (Ted) Maslen. Graham naturally became interested in the contributions to that research that could be made by theory, and this work commenced with the Honours and PhD research projects undertaken by Mark Spackman, supervised by Graham, during 1975–79. A period of sabbatical leave with Ron Mason's group in Sussex in the late 1970s alerted Brian Figgis to the considerable potential of polarized neutron diffraction experiments to reveal details of spin distributions in paramagnetic single crystals. Graham's productive collaboration with Brian Figgis spanned more than 25 years, with joint publications between 1981 and 2007. In most of those, Graham, along with a succession of postgraduate students and postdoctoral researchers funded by the Australian

<sup>†</sup>G. Chandler, D. P. Craig, Aromatic Character and the Benzene Nucleus, in *Rodd's Chemistry of Carbon Compounds* (Ed. S. Coffey) 1971, pp. 5–44 (Elsevier: Amsterdam).

<sup>‡</sup>A. D. McLean, G. S. Chandler, Contracted Gaussian basis sets for molecular calculations. I. Second row atoms, Z=11–18, *J. Chem. Phys.* 1980, 72, 5639.

Research Grants Scheme, provided *ab initio* calculations of charge and spin distributions of metal coordination complexes to complement the outcomes of polarized neutron and X-ray diffraction experiments by Figgis and Phillip Reynolds.

In parallel with this ongoing collaboration, Graham also published papers on atomic polarizabilities (with Robert Glass) and applications of a unitary group approach to several problems in quantum chemistry (with Mark Gould). Other productive collaborations were with Dylan Jayatilaka (a former Honours student, who returned to UWA in 2001), Patrick Cassam-Chenaï (Université Nice Sophia Antipolis, who spent a large part of his PhD research at UWA), and most recently with Dahbia Talbi (Université de Montpellier).

Graham, of course, is well known for his sense of humour, and we could fill many pages of this special issue with stories from his past. Graham entered the University of Adelaide in 1958 and became involved with Prosh, the University Union's fundraising event held annually, which whetted his appetite for having some fun during study. In 1959, during Prosh celebrations, he made the front page of *The Advertiser* dressed as a cowboy having a shoot-out with a slick gambler, and the following year he was involved in a stunt that left Rundle Street, after rain, glowing green with fluorescein, which was pictured in the *Australasian Post* of that year. However, it was his Honours graduation that provided the opportunity for a particularly memorable exploit. Graham found the usual Honours graduation ceremony to be overly serious and pompous and decided to add a lighter touch to his first ceremony in 1962. Fortunately, his brother had given him a whoopee cushion the previous Christmas, and at 7 a.m. the morning before the ceremony, he sneaked into Bonython Hall and placed this on the chair of the

Chancellor, Sir George Coutts Ligertwood. At the time, the hall was arranged with the staff in choir stalls parallel to the aisle, with the Chancellor in a chair at the head of the choir stalls. The ceremony commenced with organ music, the procession filed in and, as dictated by tradition, everyone – staff, graduands, and audience – waited in silence for the Chancellor to be seated. Eventually the Chancellor sat, emitting a flatulent noise in the process, a noise that wasn't particularly noticeable from the audience, but definitely audible to staff. Apparently, the entire staff turned and gazed at the Chancellor with looks of horror. Quite understandably, the Chancellor himself was shocked and struggled to get out of the chair, only to fall backwards and produce yet another loud flatulent sound. Apart from Graham, his brother and the few in on the joke, no one really knew what happened that day until 54 years later when Graham visited the University of Adelaide and confessed, on camera, to the then quite famous deed.<sup>§</sup>

Graham is certainly still fond of a good joke and has a love and knowledge of fine wine that he freely shares. More importantly, his human qualities set him apart and are most evident in his concern for students, colleagues and, poignantly, elderly retired colleagues. Graham has patiently guided new (and old) staff through the sea of academic icebergs with advice that has stayed with them throughout their careers. He continues to inspire while *Emeritus* at UWA and passes on his knowledge and abundant enthusiasm for chemistry. His passion for science remains undiminished, maintaining his keen interest in lepidopterology and ensuring the last synthetic work from his PhD studies was published in this issue of the *Australian Journal of Chemistry*,<sup>¶</sup> complemented by modern *ab initio* calculations – a circle completed.

<sup>§</sup>The YouTube video can be viewed here: <https://goo.gl/C6wUca>.

<sup>¶</sup>G. S. Chandler, W. H. F. Sasse, Bromination of Acridine, *Aust. J. Chem.* **2018**, *71*, 285.