

## *In Memoriam: Edward Cameron Kirby* (1934 – 2019)

**E**DWARD CAMERON KIRBY (August 25<sup>th</sup> 1934–January 19<sup>th</sup> 2019) was a Scottish scientist, a Fellow of the (British) Royal Society of Chemistry and a member of the International Academy of Mathematical Chemistry, who made contributions to a unique combination of areas: problem solving in practical Chemistry, editorial work in Nutrition and Health, Chemical Graph Theory, and the use of small personal computers in Computational Chemistry, of which he was an early pioneer. For a period of some forty years, he was a keen and dependable supporter of Mathematical Chemistry in Croatia, even in the dark days of 1991–1995 and the post-war years 1996–2000. This solidarity was much appreciated by Croatian colleagues who habitually attended the annual MATH/CHEM/COMP conferences in Dubrovnik and elsewhere; this steadfast, unequivocal and unconditional backing on Ed's part was recognised by the allocation, on the occasion of his 70<sup>th</sup> birthday, of a special session at the 2005 MATH/CHEM/COMP, the preface to which was written by the late Ante Graovac in *Croat. Chem. Acta* **2005**, 78 (2) XXIII–XXIV.

Edward was an *alumnus* of Scotland's most ancient university, having taken his BSc and his PhD (supervised by D. H. Reid) at St. Andrews. Ed's doctorate was on Azulenes, which remained a life-long fascination for him — even impinging on my own work with him, some thirty or forty years later. After postdoctoral work at the University Chemical Laboratory at Cambridge (with F. G. Mann), Ed spent approximately seven years in industry before becoming a free-lance consultant on technological innovations and industrial research management. (Please see the above account by Ante Graovac for further details of Edward's activities during this period.)

As a free-lance worker, Edward joined the Resource Use Institute (RUI), founded in Pitlochry precisely 50 years ago by the late Robert Robertson and presided over by the

late Iain Murray, the 10<sup>th</sup> Duke of Atholl, in nearby Blair Castle, Perthshire. The Resource Use Institute is a limited liability company with a strong ethical base, its philosophy being the wise use of resources — a subject that has, of course, recently become immensely topical, world-wide. Again, Ante Graovac's account, cited above, may be consulted for very full details of Ed's activities at RUI. One of Edward's other, and completely different, technical interests was nutrition and he was for many years the editor of *Nutrition and Health*.

From 1982 onwards, Edward developed his Mathematical Chemistry project, and it was at this stage that his interests and my own began to overlap. Ed's major contributions at that time revolved around the fact that he was one of the first innovators in the application of personal computers to Mathematical Chemistry — having one as early as the 1970s — and he specialised in devising, and making widely available, quantum-mechanical programs for use on such a computer.

Edward made his living out of his RUI consultations, as well as, with his wife Jean, running a small hotel in Pitlochry. The RUI work involved conventional practical chemistry (largely carried out at home!) In his 'spare' time, however, Ed devoted himself to his real passion which was the new (and entirely theoretical) area of Mathematical Chemistry, then only recently beginning to be established, in the late 1960s/early 1970s. The first major paper in the field was in 1972 and it was from the Ruđer Bošković Institute, Zagreb — I. Gutman, A. Graovac, N. Trinajstić, T. Živković, Graph theory and molecular orbitals. Application of Sachs's theorem, *Theoret. Chim. Acta* **1972**, 26, 67–78 — hence the prominence of Croatia, and several other countries of former Yugoslavia, in this new and emerging field. After a seven-year stint at the University of Oxford that ended in the mid-1970s I also simultaneously

gravitated towards this novel area of Mathematical Chemistry, which became a kind of ‘hobby’ (because I was subsequently in a post in which there was no requirement for me to do research). When we met at the Dubrovnik MATH/CHEM/COMP conference of 1982, therefore, Edward and I were immediately linked as kindred spirits as ‘independent gentleman scientists’ — and, fortuitously, we were in the same field.

Although my own employment subsequently prevented my participation for some twenty years (until my retirement), Edward continued to support the regular annual Dubrovnik conferences from 1987 and he carried on relentlessly attending, even during the difficult years of the 1990s — when, sometimes, the conference was exiled to then more-peaceful places like Bled, in Slovenia, and hardly anybody from outside Yugoslavia was brave enough to come. This stoicism and loyalty on Ed’s part was much appreciated by the Yugoslavian/Croatian hosts. So much so that, as previously alluded to, a section of the 2005 conference was devoted to commemorating Edward’s 70<sup>th</sup> birthday; and, of course, this memorial session at ‘MCC 31’, in June 2019, was held in order to honour the whole of Ed’s scientific life.

In addition to publishing more than twenty papers on which he was the sole author, Ed collaborated widely with many people — including several of the major international figures in the field of Chemical Graph Theory such as (in alphabetical order): G. Brinkmann, B. N. & S. J. Cyvin, M. V. Diudea, P. W. Fowler, A. Graovac, I. Gutman, P. E. John, D. J. Klein, T. Pisanski, D. Plavšić, H. Sachs, and others. For a ‘gentleman scientist’ for whom his work in this field was virtually a hobby — and, furthermore, a hobby that was run in parallel with another career — this is indeed impressive, by any standards.

By the time of his 70<sup>th</sup> birthday tribute he had published more than sixty papers and patents. It was not until ten years after we first met, however, that Ed and I (together with my colleague Mr. Paul Pollak) had our first joint publication, which was subsequently widely cited: E. C. Kirby, R. B. Mallion, P. Pollak, Toroidal polyhexes, *J. Chem. Soc. Faraday Trans.* **1993**, *89*, 1945–1953. Over the succeeding 25 years, we gently published some half-a-dozen papers together (three of them in the *Croatia Chemica Acta*), the last one being in 2017; these are listed as Refs. [1–7] of my own contribution (with Dr. Timothy Dickens) to the accompanying the Kirby *Festschrift*. Much of our work was centred on spanning trees of graphs (especially molecular graphs) and, primarily, their enumeration (e.g. E. C. Kirby, D. J. Klein, R. B. Mallion, P. Pollak, H. Sachs,



Edward Cameron Kirby

A theorem for counting spanning trees in general chemical graphs and its particular application to toroidal fullerenes, *Croat. Chem. Acta* **2004**, *77*, 263–278.)

One of the advantages of being ‘gentleman scientists’ that Ed and I shared was that, as such, we both had the luxury of collaborating only with our *friends*. And one of the great joys of working with, and visiting, Ed was the warm and agreeable household that his guests were enveloped in. He and Jean were always so welcoming and Ed was never happier than when entertaining at home, folding his legs and having a ‘good yarn’ with his guest, who was invariably kept well supplied with gin-and-tonic. Hogmanays (the Scottish celebration of New Year) with Ed & Jean were a sheer delight.

I conclude with a charming image (from MATH/CHEM/COMP 2008 in Verbania, Italy) of Ed standing on a ‘crazy-paving’ path and tracing out pairs of neighbouring stones that constituted an adjacent pentagon and heptagon sharing a single edge — which would, thereby, with enough imagination, recall the carbon-carbon skeleton of his beloved Azulene.

Roger Mallion,  
Canterbury CT2 7RX, England, United Kingdom  
[mallionr29b@aol.com](mailto:mallionr29b@aol.com)