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An Autobiographical Account of Chemical Graph Theory in the Years Surrounding the Launch of *MATCH*: An Oxford Participant's Highly Personal and Parochial Reminiscence about the Period 1969–1976

by

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1. Introduction: Department of Chemistry, University College, Swansea, University of Wales, 1969

"What's your Graph Theory like?" This was a question smilingly thrown at me in somewhat jocular fashion one day in spring 1969 by Mr. C. W. Haigh, my erstwhile mentor and Ph.D. supervisor in the University of Wales, as we amiably perused a reprint of Balaban and Harary's *Proposed Nomenclature for Benzenoid Hydrocarbons*[1,2] that had just arrived in the morning post. Claude Haigh — an old member of Winchester College, an *alumnus* of King's College, Cambridge and of New College, Oxford, and a Master of Arts of both those ancient universities — is one of that fast-disappearing breed of culturally well-rounded English scientists from a gentler age who firmly believe that an 'educated gentleman' just naturally knows Mathematics (as he would also, of course, know Latin and Greek) as a result of his general background schooling; consequently, as my research supervisor, 'C. W. H.' frequently paid me the sometimes uncomfortable courtesy of assuming that I knew more Mathematics than, in those days, I actually did. At that time I have to confess that, to me, a 'graph' was simply a plot of y against x — and that was an end of the matter!

My Ph.D. Thesis[3] was entitled *Nuclear Magnetic Resonance: a Theoretical and Experimental Study of the Spectra of Condensed, Benzenoid Hydrocarbons.* The primary aim of this work was to compare predictions[4] of the Pople[5] and McWeeny[6] theories of so-called 'ring currents'[7] in conjugated molecules with a consistent set of experimental[8,9] ^{1}H-NMR chemical-shifts that were all measured under uniform conditions of solvent and concentration.[8,9] At that time, the nomenclature of the condensed, benzenoid hydrocarbons was disconcertingly variable[1]: for example, the molecule of main interest to us, the notorious carcinogen 3,4 benzopyrene,[8] was variously known under that name and also as 1,2 benzopyrene, benzo[*a*]pyrene and even benzo[*def*]chrysene.[10] As already alluded to at the beginning of this account, it was just at the time when I was writing my Thesis[3] that Balaban and Harary published[1,2] their own graph-theoretical nomenclature for certain classes of the condensed, benzenoid hydrocarbons, based on their idea of the 'characteristic graph'[a] associated with such molecules. I was intrigued by the Balaban–Harary approach and initially thought that I might use the names that they were proposing for the hydrocarbons that were dealt with in the Thesis[3] then in preparation; (this idea — in retrospect, perhaps wisely — was not, in the end, finally taken up). Although one of Professor Harary's affiliations on the Balaban–Harary paper[1] was given as 'University College, London', he was, even then, well established at Ann Arbor, Michigan, U.S.A. In the meantime, I had gleaned from an address-footnote in a subsequent paper[2] on the same topic by Professor Balaban (alone) that he — a Roumanian citizen who, though an organic chemist, was based at the Institute of Atomic Physics in Bucharest — had somehow got himself from President Ceauşescu's Roumania[b] to a three-year sabbatical stint at the International Atomic Energy Agency in Vienna. Because postal rates to Austria were cheaper than those to the United States — remarkable as it may seem now, this fact was a material consideration to me then — it was to Vienna that I had written for a reprint and, as a raw, 24-year-old research student, I was delighted and most flattered to get, in reply, a prompt, detailed and wonderfully courteous[c] letter from such a distinguished scholar in the field as Professor Balaban.

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[a] In fact, though, this is something of a misnomer; the so-called 'characteristic graph' is not actually a graph *per se* for its depiction involves geometry, as well as connectivity. This observation has been made elsewhere[11] and it is immediately evident from even a cursory examination of Balaban and Harary's proposals in ref. [1].

[b] However, since the fall of the Ceauşescu *régime* in 1989, Professor Balaban has recorded[12,13] (both publicly, in *MATCH*,[12] as well as privately[13]) that because his only sister and one of the two brothers of his wife both illegally fled from Roumania with their families in 1971, his own travel outside the country was subsequently restricted by the Roumanian authorities.

[c] I eventually grew to realise, as I was privileged (much later) to get to know Professor Balaban considerably better, that such courtesy was characteristic of the man.

2. Mathematical Institute, University of Oxford, and Jesus College, Oxford, 1969–1971

That, therefore, in the spring of 1969, was my first explicitly conscious encounter with Graph Theory. I was to begin a more gradual and more extended exposure to it — and to start to realise that I had in fact been using graph-theoretical techniques, albeit unknowingly, throughout my Ph.D. period (1966–1969) — later that same year, by which time I had moved to the University of Oxford. The Swansea Ph.D. Thesis was written up — just about on time — and, subsequently, on November 24th, 1969, it was duly examined, at the Royal Institution, London, and passed fit by Claude Haigh and my external examiner, Professor J. N. Murrell, F.R.S., of the University of Sussex. I was admitted to the degree at a Congregation of the University of Wales held at University College, Bangor (in North Wales), on December 20th, 1969 — an event to which I was valiantly driven, through ice and snow, by my then recently widowered father, the seemingly vast distance from our home in Cardiff (South Wales). There then arose the question of what to do next and, with Claude Haigh's help, I decided to follow in his own footsteps and 'sit at the feet' of Professor C. A. Coulson, F.R.S., then currently the Rouse Ball Professor of Mathematics at the University of Oxford, and Fellow of Wadham College.[d] 'C. A. C.' was, by common agreement, the 'father figure' of British (and, one might even claim, European) Theoretical Chemistry at that time and he was also highly respected in the United States, which was then home to quantum-mechanical giants of the ilk of Linus Pauling and Robert Mullikan. Accordingly, in October, 1969, I considered myself privileged to join his Wave Mechanics and Quantum Theory Group at the Mathematical Institute, University of Oxford, as a Science Research Council Post-Doctoral Fellow. During my tenure of this post (1969–1971), I was associated with Jesus College as a Supernumerary Member of their Graduate Common Room; as will very soon be recounted, this College aspect of my initial life at Oxford also had its own particular graph-theoretical resonances.

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[d] Charles Alfred Coulson, F.R.S. (December 13th, 1910 – January 7th, 1974).[14–16] During an academic career of exceptional international distinction, C. A. Coulson was Professor of Theoretical Physics at King's College, University of London (1947–1951), Rouse Ball Professor of Mathematics in the University of Oxford (1951–1972) and he finally founded, and was the first occupant of, the Chair of Theoretical Chemistry at Oxford University (1972–1974). This Chair was initially personal to Professor Coulson and, during his short occupancy of it, he continued his Fellowship at Wadham (where the Rouse Ball Chair is held), by agreement with the Governing Body of that College. After his demise, however, when the post became known as the Coulson Chair of Theoretical Chemistry, it was based at University College. In addition to all of this, 'C. A. C.' was well-known for his writings on the relationship between religion and science.[15] As Professor Roy McWeeny, Professor Brian O'Leary, and I have observed in a tribute elsewhere,[16] C.A. Coulson was ". . . perhaps one of the last of science's 'renaissance men' who, in a single lifetime, could hold chairs of Mathematics, Physics and Chemistry in such prestigious universities as those of London and Oxford."

At the Mathematical Institute, I found myself sharing an office with Robin Wilson, sometime undergraduate of Balliol College, who, in October, 1969, having completed his Ph.D. at the University of Pennsylvania the year before, and having spent the intervening twelve months in the University of Cambridge, had returned to Oxford as a Lecturer of Jesus College — the very institution with which I had myself only recently become associated. As a College Lecturer, Robin was, by right, a Member of the Jesus College *Senior* Common Room (the 'S.C.R.'): *I* was merely a Member of the *Graduate* Common Room (the 'G.C.R.') at Jesus though, in the vacations, I and my fellow G.C.R. Members were accorded the privilege of *lunching* in the S.C.R. Recalling my correspondence with Professor Balaban some months earlier, I was intrigued by the fact that Robin Wilson's current area of mathematical interest was Graph Theory. Of parallel, though unrelated, interest at that time was the fact that Robin was also the elder son of the man who was then currently my Prime Minister, Mr. Wilson.[e] Robin Wilson had in fact written his Ph.D. on Number Theory, but had become fascinated by Graph Theory through occasionally going to M.I.T. during his time at 'Penn' and attending the lectures of Professor G.-C. Rota. During his time in Cambridge (England) (1968–1969), Robin Wilson further compounded this influence by attending the lectures of Dr. Hallard Croft of Peterhouse, to the extent that, by the time he came to Oxford, he had turned his attention, full-time, to Combinatorial Theory. Furthermore, in the absence of Dr. Dominic Welsh (of Merton College) on sabbatical leave, Robin contributed to the University's programme of lectures on Combinatorial Theory, famously wearing a garish and wildly clashing combination of bright colours, *via* shirts and ties of doubtful taste, whenever he was lecturing on the Four Colour Conjecture.[f] It was during the time when I was sharing this Mathematical-Institute office with Robin Wilson that he began to write his classic book *Introduction to Graph Theory*[18] — now, 35 years later, still in print, and into its fourth edition, having been published in eight languages. A feature of this book was the (fairly) humorous quotations that head each of the chapters in it. Much fun was had in finding and researching these, and I used to joke with Robin that he seemed to have spent almost as long meticulously sifting and anguishing over the selection of suitable quotations, as he had on actually writing the book itself.

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[e] The Right Hon. J. Harold Wilson, M.A., F.R.S., (March 11th, 1916 – May 24th, 1995), three times British Prime Minister in the 1960s and 1970s: 1964–1966 (first Administration), 1966–1970 (second Administration), and finally, 1974–1976 (third Administration). Later (1976) Sir Harold Wilson and then (1983) Lord Wilson of Rievaulx, Mr. Wilson, a sometime Fellow of University College, was himself an *alumnus* of Jesus College — where Robin Wilson and I were stationed in 1969 — having been an undergraduate there in the period 1934–1937; to this day, the late Lord Wilson's portrait hangs in the Hall of Jesus College.

[f] As it was then; now properly called 'the Four Colour *Theorem*'[17] about which, 30 years later, Robin Wilson wrote what is already becoming a celebrated work: *Four Colours Suffice*.[17]

It was as a result of conversations with Robin Wilson in the Autumn of 1969 that I began to realise that all the theoretical work[4] that I had done in Swansea during the preceding three years on the Pople–McWeeny[5,6] theory of 'ring-currents' in conjugated hydrocarbons[3–7] — based on the London theory of diamagnetism[19,5,6] that was itself founded on the molecular-orbital theory of Erich Hückel[20–29] — was, in essence, *an unconscious and unknowing application of Graph Theory.* The Hückel Hamiltonian-matrix[20–29] was isomorphic with the vertex-adjacency matrix[18,30,31] of the corresponding molecular graph, in which the carbon atoms denoted the vertices[18,30,31] and the carbon-carbon bonds in the conjugation network represented the edges[18,30,31] of that graph. It gradually began to become apparent to me, on further being acquainted with the literature, that these isomorphisms, which had dawned on *me* independently through my discussions with Robin Wilson, had in fact explicitly been pointed out on several occasions in the preceding 20 years — by authors such as (among others) Samuel,[32] Frost and Musulin,[33] Gordon and Davison,[34] Heilbronner,[35] Gouarné,[36] Günthard and Primas,[37] Spialter,[38] Schmidtke,[39] and especially by Ruedenberg,[40] in a particularly extensive (and much neglected) series of papers published in the *Journal of Chemical Physics* many years after the work was done, starting in 1954 and continuing into the early 1960s (*e. g.* refs. [40]). Furthermore, it was also immediately evident — from what I had learned by talking with my office companion, Robin Wilson — that the 'open chains' of carbon atoms that featured in McWeeny's formulation[6,7,3,4] of the 'ring-current' effect in conjugated molecules were nothing other than spanning trees[18,31] that constituted semi-Hamiltonian paths[18,31] within the graph representing the carbon-atom framework of the particular conjugated hydrocarbon under study.

It was early on in my time at the Mathematical Institute that Dr. D. H. Rouvray, an *alumnus* of Imperial College, London, came to Professor Coulson's group on a sabbatical leave from the University of the Witwatersrand in Johannesburg. He, too, had been thinking independently about the connection between Hückel Theory and Graph Theory. Furthermore, Dennis Rouvray was a great collector of the literature in this field, and it was through him that I discovered several of the references to the pioneering work on this subject, just mentioned;[32–40] he also led me to some of the early-to-mid 20th-century theorems on matrices (such as those of Perron,[41] Frobenius[42,43] and Wielandt[44,g]) that were relevant to our interests.

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[g] I wish that I had known then that, although his name was on a theorem[41] of 1907, Oskar Perron (May 7th, 1880 – February 22nd, 1975) was, at that time, still alive. So, also, was Erich Hückel (August 9th, 1896 – February 16th, 1980) still living[45] but, regrettably, that fact was likewise not then known to me. Furthermore, it was only during the course of preparing this Reminiscence that I learned Helmut Wielandt's dates,[46] which showed that he even lived about six weeks into this 21st century: December 19th, 1910 – February 14th, 2001. The opportunity to meet these distinguished and celebrated pioneers thus sadly slipped away through ignorance.

Through Robin Wilson, I learned of two substantial and influential mathematical works on graph spectra, by Collatz and Sinogowitz[h,47] and by Cvetković.[48] These historical aspects began increasingly to fascinate me, and I was very gratified that by browsing the initial volumes of *The American Journal of Mathematics* — then to be found on open shelves[i] in the Mathematical Institute's Whitehead Library — I was able to discover a seminal article[50] by the founder of that *Journal*, the distinguished 19th century British Mathematician J. J. Sylvester, F.R.S. (later Savilian Professor of Geometry in the University of Oxford and Fellow of New College, Oxford). This was a delightfully entertaining exposition somewhat cumbersomely entitled: *On an Application of the New Atomic Theory to the Graphical Representation of the Invariants and Covariants of Binary Quantics, — with Three Appendices*. This paper brought to me, for the first time, the comforting realisation that the word 'graph' used in this sense by Mathematicians had been introduced (by Sylvester, in that paper) in the context of so-called 'graphical' formulae in Chemistry. Further discovering that another British 19th century mathematical giant,[51] W. K. Clifford, F.R.S., had connected[49,52] Graph Theory with Chemistry, and following this finding with a detailed study of the classic 'memoir' on the theory of matrices[53] by A. Cayley, F.R.S. — generally agreed to be the greatest British Mathematician of the 19th century — all contrived to re-enforce my growing view that, because I was an Englishman in Oxford in the second half of the 20th century, this subject — in some mysterious and ill-defined way — was somehow part of my natural 'cultural heritage'; accordingly, the further I delved into it, the more I began to warm to it.

The aforementioned new member of the Coulson group, Dennis Rouvray, was instrumental in the early 'popularisation' of Chemical Graph Theory in the first half of the 1970s, introducing it to a wider circle by means of a large number of highly regarded reviews; the half-dozen listed in refs. [54] will adequately serve as representative examples. The two of us did some collaborative work on the connections between Graph Theory and Hückel Theory — emphasising the graph-theoretical aspects of the latter in chemical contexts[55–57] and suggesting that certain physical quantities[58] accessible *via* Hückel Theory, in association with the *Aufbauprinzip*,[55,59] could be adapted and carried over into pure Graph Theory.[58] To

[h] It should be noted that, despite its 1957 publication date, some of the work reported in this paper[47] was in fact done before the mid-1940s because, sadly, it is recorded in a footnote on the title page that one of the co-authors, Ulrich Sinogowitz, was killed in an air-raid on Darmstadt on September12th, 1944.

[i] It was emphasised to me what 'prehistoric' times I am reminiscing about in this article when, on February 17th, 2004, I returned to the Whitehead Library in the course of researching this account, with the intention of securing a further copy of ref. [49], my original 1969 xerox of it having been lost in the intervening 35 years. Instead of being ushered to the open shelves as I expected — and as would have happened in 1969 — I was astonished when the Librarian went straight to her computer and, there and then, ran me off a pristine facsimile of Sylvester's 1878 note,[49] from the 'JSTOR' ® electronic archive.

this end, we demonstrated that the *Aufbau* process may itself be regarded as a purely graph-theoretical 'recipe',[55,59] and we suggested[58] that charge densities in non-alternant hydrocarbons could be thought of as entirely abstract, graph-theoretical quantities that may be carried over into pure Graph Theory and considered to characterise the vertices of certain non-bipartite graphs[58] — provided that the (frequently hypothetical) 'hydrocarbons' that (for convenience) these non-bipartite graphs were imagined to represent were possessed of a π-electronic structure uniquely defined by the *Aufbau* process.[55,58,59] The fruits of some of my collaborations with Dennis Rouvray were not published until a very long time (*ca.* 20 years) after the work itself was actually done; for example, our homage[56] to the Coulson–Rushbrooke 'Pairing' Theorem[60] of 1940, though largely settled in the early 1970s — and, in the meantime, partly incorporated by each of us into various other works, *e.g.*, refs. [26] and [61]–[63] — did not in fact appear[56] until 1990, by which time it conveniently served as a 50th anniversary tribute to the original Coulson–Rushbrooke Theorem;[60] (and it was itself, in its turn, almost immediately extended to Möbius molecules by the two of us in collaboration with the present Editor of *MATCH*, Professor Ivan Gutman[57]). Meanwhile, in the intervening period, Dennis Rouvray and I pursued these matters independently, complementing and, on one occasion, answering, each other's contributions[64,65] to the literature and (perhaps unusually for Englishmen) immersing ourselves in the French language[64,65] to do so.

During all this work with Dennis Rouvray, I continued to talk, both in the office at the Mathematical Institute and at Jesus College, with Robin Wilson and it was he who, one day, brought to my attention the wonderfully elegant and aesthetic Matrix Tree Theorem[66,31,11] for determining the number of spanning trees in a graph. As mentioned earlier, I had already realised that the entities known to graph theorists as 'semi-Hamiltonian spanning-trees'[18,31] were fundamentally material to McWeeny's theory[6] of π-electron 'ring currents' in conjugated molecules and, at just this very time, a unitary transformation that is more general than that proposed by McWeeny[6] — one that, unlike McWeeny's,[6] is applicable even to *non*-semi-Hamiltonian spanning-trees — had recently been devised by Gayoso and Boucekkine.[67] As soon as I became aware of the Matrix Tree Theorem I was immediately beguiled by its manifest beauty and simplicity and, there and then — 35 years ago — I began what looks like being a life-long 'love-affair' with that theorem, as it is for me a passion that continues even to the present day (*e.g.*, ref. [68]).

At the turn of the decade I also started a short connection/collaboration — right at the end of his long and distinguished career in the synthesis and study of benzenoid hydrocarbons — with the veteran and venerable Professor Erich Clar[j] of

[j] 1902–1987. I had the privilege of personally meeting Professor Clar when he lectured in Oxford.

Glasgow University. By this time, Professor Clar's highly graphical and diagrammatic ideas concerning 'the aromatic sextet'[69] were, regrettably, beginning to be openly ridiculed by orthodox and mainstream theoretical chemists[k]; sadly, it was really only around the time of his demise[l] nearly two decades later (1987) that he (posthumously), his theories, and the concepts that he was arguing for[69] were, in a sense, rehabilitated by means of a proper theoretical justification — and, it has to be said, through the agent of Chemical Graph Theory, even then (being due, in no small measure, to the admirable efforts of the current Editor,[71] Professor Ivan Gutman, and the present honorand, the late Professor Oskar Polansky.[71]) Professor Clar very kindly supplied me with ^{1}H-NMR spectra of some rare benzenoid hydrocarbons that he himself had synthesised, and I, in turn, used the McWeeny[6] method to calculate the 'ring-current' intensities extant in their several rings.[6] On New Year's Eve, 1970, Professor Clar wrote,[72,73,m] with some evident delight:

> "I was interested to learn that your calculation leads to the same results as the strict application of the aromatic sextet."

All this was carried out in collaboration with my former supervisor, Claude Haigh, who presented a paper concerning it on April 1st, 1971 at a session (chaired by the late Professor H. C. Longuet-Higgins, F.R.S.) of a conference[n] held at the Mathematical Institute, Oxford, and at Brasenose College, Oxford, to commemorate Professor Coulson's 60th birthday. In the event, however, this work remained unpublished for nearly 20 years.[73]

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[k] To many in the field, Clar's theoretical ideas[69] about 'bond fixation' and the 'aromatic sextet' seemed to be overly simplistic in the extreme and, to some, they appeared almost to verge on the eccentric; even C. A. C. himself, who was normally so generous and charitable about the work of others, was not entirely immune from this somewhat disparaging view. On June 11th, 1970, Professor Coulson wrote to me[70]: ". . . I enclose three reprints from Erich Clar in Glasgow. He is a wonderful synthetic organic chemist, but an awful interpreter of his own work! What is the real interpretation of the nmr effects in . . . these papers? Can you let me have this stuff back . . .(but no hurry at all!) since one day I shall have to write to Clar about the ideas that he discusses." Six days later, after a further letter from Clar, Coulson bemoaned to me[70]: "I must reply, one day, to his earlier letter, and now to this one, also." It was unusual for C. A. C. — who, even in those pre-word-processing days, routinely turned around *ca.* 30 letters per day — to procrastinate in a correspondence.

[l] According to the Web-Site of the International Society for Polycyclic Aromatic Compounds, even when, at its 1987 gathering at the National Institute of Standards and Technology in Gaithersburg, Maryland, U.S.A., the 11th International Symposium on Polynuclear Hydrocarbons resolved to initiate a Lifetime Award in the field and to invite Professor Clar to be its first recipient, news of the honour arrived just days after his death at Clar's household in Southern Spain, to which he had retired after leaving Glasgow; the Award was eventually collected by his widow.

[m] I very much regret that when this remark was quoted in part (*d*) of ref. [7] the (important) words ". . . the strict application of . . ." were inadvertently (but inexcusably) omitted.

[n] It was at this conference that I first met the honorand of this issue of *MATCH*, Professor Polansky (March 28th, 1919 – January 15th, 1989), who was then based in Vienna. He gave a talk on April 2nd entitled: *Character Orders — a Generalization of Bond Orders*.

3. Christ Church, Oxford, 1971–1972

On September 30th, 1971, my Science Research Council Post-Doctoral Fellowship determined and, the next day, I took up my new post as a Research Lecturer of Christ Church, Oxford, to which I had been elected four months earlier by the Dean, Canons and Students of that august Foundation. This was a five-year appointment (though, by Statute, it was not extendable beyond that) which carried a very small 'stipend' (£950 [*ca.* €1400] per year was the initial 'emolument') but (more importantly) it gave the rights to rooms in College and the privilege of Dining Rights at the High Table of Christ Church — all "...free of rent, rates and taxes...", as the Christ Church Bye-Laws quaintly put it. Membership of the Christ Church Senior Common Room was an additional agreeable aspect of the appointment. The sole and entire duties of this Office were to carry out my own personal research, although I was also allowed (for extra payment) to give tutorials to undergraduates for up to six hours per week. When he heard the good news of this Election, Professor Coulson called me in and compared my current situation with his own when, precisely 37 years earlier, he had been elected to a four-year Prize Fellowship at Trinity College, Cambridge.[o] He made this comparison with the memorable words: "Well, Roger, *you* are now an *independent gentleman*!" The disadvantage of this new arrangement, however, was that Christ Church, unlike the Science Research Council, made no payments to the Mathematical Institute for affording me facilities like an office, xeroxing privileges, postage rights, typing services *etc.* and so I had to move out of the Mathematical Institute and become entirely college based. It was for this reason that — unusually for a scientist — I had a *college* address, rather than a departmental one, on the three papers[74] (not, however, on graph-theoretical topics) that were written and submitted during my first year at Christ Church.

It was during this year that I began to be aware of increasingly intense current and independent activity in Chemical Graph Theory in 'the outside world'— notably in Zagreb,[75,76] Tokyo,[77] and El Paso.[78] The paper that changed everything and gave a verve and momentum to the subject unlike any other was undoubtedly *Graph Theory and Molecular Orbitals — Application of Sachs Theorem*, by A. Graovac, I. Gutman, N. Trinajstić and T. Živković, that emanated from the Rudjer Bošković Institute,

[o] As it happens, Trinity College, Cambridge and Christ Church, Oxford are 'sister' colleges, as they were co-founded, in 1546, by King Henry VIII (reigned 1509 – 1547). In 1541, the same English monarch also *re*-founded The King's School, Canterbury — originally founded by St. Augustine in 597 — of which I have been privileged to be a Member for the last 28 years.

Zagreb, and appeared in the 1972 *Theoretica Chimica Acta*.[75] This paper, which introduced the chemical world to Sachs' method[79,29,80,81] for constructing characteristic polynomials, essentially launched the modern era of Chemical Graph Theory single-handedly. At about the same time, I also began to become familiar with the work of Professor Haruo Hosoya[77] and Professor William Herndon.[78]

At this point, it might be of some historical interest to collect together in one place, and thus to put on record, exact quotations of all the observations by means of which C. A. Coulson expressed to me a view on the uses and relevance of Graph Theory in Chemistry — for I have previously published only one of his written remarks on this matter (and that nearly a quarter of a century ago[82]). Although a great devotee of the exploitation of *Group* Theory in molecular-orbital work, Coulson was always rather sceptical about the use of *Graph* Theory in this context because he feared that in dealing only with the *connectivity* of the atoms in a molecule Graph Theory 'lost' what he regarded as one of a molecule's most important attributes — namely, its *geometry*.[p] In a letter dated September 1st, 1972, Charles Coulson wrote to me[82,83] (concerning Graph Theory):

"It's not a field that I know at all, other than as someone who has occasionally had to invent something that I needed for my quantum theory."

On November 4th, 1972, after reading a copy of ref. [75] that I had sent him, Professor Coulson wrote:[83]

"It bears a considerable likeness in parts to a little note that I published in the Cambridge Philosophical Society Proceedings in 1949 [*sic*[q]]. There is, I believe, a limit to the usefulness of approaches of this kind. But they are very far from being negligible."

Professor Nenad Trinajstić also independently sent Coulson a copy of his own ref. [75] and, on December 2nd, 1972, Professor Coulson replied to him,[85] saying:

"You are right that the use of Sachs' theorem gives similar results to those obtained by me when expanding the secular determinants. In fact, I knew nothing of Sachs' theorem until I read your paper; but I had obtained it — and used it — in my own work as a further way of expanding secular determinants."

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[p] I cannot now recall who the lecturer was but, on one occasion during my early time in Oxford, a visiting speaker gave a talk on Chemical Graph Theory and started by drawing out of a bag a 'ball-and-stick' model of a molecule, with 'bonds' made of rigid wire; he then pulled out of another bag a second model of the same molecule but, this time, the rigid bonds were replaced by string; whereupon, he held up this second 'molecule', dangling it like a bunch of grapes, and triumphantly announced: "*That*'s what Graph Theory does to a molecule!" It was this 'geometrical loss' — which an application of Graph Theory ostensibly brings about — that Professor Coulson did not like.

[q] *Sic*: this should have been '1950';[84] the reader is directed to the detailed and comprehensive papers by Gutman[80,81] for a complete history of 'sub-graph' techniques for determining characteristic polynomials.

In a covering letter[83] of May 25th, 1973, when forwarding to me some reprints that he had received from a well-known Chemical Graph Theorist, Charles Coulson wrote:[83]

"A lot of it seems to me to be rather remote from what I call chemistry; but maybe that's not fair to him."

On November 14th, 1973, commenting on some graph-theoretical papers on 'local aromaticity' that he was sending onto me, Professor Coulson wrote:[83]

"I think you may find them interesting, though whether the concept of local aromaticity is of much value I cannot say. I am a bit frightened of things of this sort which aren't susceptible of any very easy experimental assessment."

4. Theoretical Chemistry Department and Christ Church, Oxford, 1972–1976

By the early 1970s, Charles Coulson had been the Rouse Ball Professor of Mathematics for some 20 years. In October, 1972, he finally achieved his goal of founding a Department of Theoretical Chemistry at Oxford, and personally occupying its Chair. Accordingly, his Group at the Mathematical Institute duly moved with him to the large Victorian pile at 1, South Parks Road that constituted the Department. Now that he was in overall charge — and not merely temporary 'Curator', as the (rotating) head of the Mathematical Institute was (and is still) called — C. A. C. generously made available to me an office and full secretarial facilities in the new Department. As a result, I partially emerged from my former seclusion in the 'ivory tower' of Christ Church and the next 15 months — until Professor Coulson's demise on January 7th, 1974 — were amongst the most productive and invigorating ones of my entire time in Oxford. With my access to Christ Church High Table I had the privilege of entertaining my former supervisor Mr. C. W. Haigh as well as already legendary scholars such as Professor Roy McWeeny (an especially revered figure for me, in the context of my work on 'ring currents'[6]) and the veteran pioneering Chemical Graph Theorist Professor Manfred Gordon.[34] Through colloquia, I met a host of distinguished speakers such as Nobel Laureate Robert Mullikan and Professor H. N. V. Temperley, F.R.S., who memorably gave an Applied Mathematician's insight into applications of Graph Theory by a lecture (on November 2nd, 1972) entitled: *Graph Theory as a Basic Method of Applied Mathematics*.

As a Research Lecturer of Christ Church I was entitled to Membership of the Faculty of Physical Sciences, for which the Degree of M. A. was a prerequisite. Consequently, on May 8th, 1972, I was accorded the status of Master of Arts for the duration of my Lecturership. However, despite this, in Michaelmas Term, 1972, Professor Coulson reminded me that the total time for which I would have been in

Oxford by the end of the Christ Church Research Lecturership was comparable with the period spent in my original University (Wales). In order, therefore, to maintain a permanent link with Oxford similar to that which I already had with the University of Wales, Professor Coulson agreed that I should do what *he* had done under similar circumstances when lecturing at the University of St. Andrews — that is, to submit some current research for a degree of the University. The idea of preparing a D. Phil.[r] Thesis (Oxford's name for a Ph.D.) was thus conceived, and Professor Coulson very kindly agreed *de jure* to be the Supervisor; (after C. A. C.'s death some 15 months later, Professor Mark Child, F.R.S., formally acted in that capacity). Accordingly, in Michaelmas Term, 1972, I began 'putting in Terms of Residence' for this purpose.[s]

In 1972, José A. N. Ferreira Gomes arrived in Oxford on leave from his lectureship at the University of Porto to read for a D. Phil. In Oxford, he was a member of Linacre College. He was interested in the magnetic properties of molecules and C. A. C. asked me to supervise him, day-to-day. (Professor Coulson was the official Supervisor: under the rules of the University, despite being a Member of the Faculty, I could not take on that rôle, as I was myself a candidate for that same degree!) We did indeed carry on a successful collaboration, and the results — though (with one exception[87]) not actually graph-theoretical — were published[88] over the succeeding years, some (posthumously[t]) with Professor Coulson as the co-author. In his Thesis entitled *Some Magnetic Effects in Molecules*[89] (the wo.k for which, after Professor Coulson's death, was supervised by Dr. P. W. Atkins), José Ferreira Gomes arrived at the idea of 'conjugated circuits' independently of Randić,[90] who is invariably universally credited with devising this concept. We in fact called[87,91] these 'conjugation circuits' which, we felt, was a somewhat more apt and evocative term emphasising, as it does, that these are indeed circuits *of* conjugation. We published the 'ring-current' applications of this in José Ferreira Gomes' national chemical journal.[87] In the meantime, I got on with my own graph-theoretical work, publishing, in the *Proceedings of the Royal Society of London*,[92] an exposition of the topological ideas that underlie the concept of 'ring currents' in conjugated molecules,[3-7] and starting[93] my long-term interest[68] in the number of spanning trees in a molecular graph.[93]

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[r] I have to confess that another (and rather less noble) motivation for doing this D. Phil. was that holding that degree would entitle me to life-long 'dining rights' at Christ Church!

[s] The Thesis was eventually submitted in Trinity Term, 1979,[86] and was subsequently examined in the Physical Chemistry Laboratory, Oxford, on June 21st, 1979, by Professor G. G. Hall (University of Nottingham, external examiner) and Dr. P. W. Atkins (Lincoln College, internal examiner); the degree was awarded at a Congregation held on December 1st, 1979.

[t] Correspondence between R. B. M. and Professor Coulson concerning these posthumous publications is deposited in Files No. B. 42. 11 and No. B. 42. 12 (part of MS. Coulson 62) in the Coulson Papers to be found in the Department of Special Collections and Western Manuscripts of the Bodleian Library, University of Oxford, England, United Kingdom. I thank Mr. Steven Tomlinson for the shelf numbers.

With the exception of the years 1970 and 1972, Professor Coulson had given, in each year since 1967, a course of eight lectures to third-year Chemistry undergraduates entitled *Hückel Theory for Organic Chemists*. He started delivering this course during his final illness in Michaelmas Term, 1973, but it had to be discontinued (after only two lectures) when his health broke down, and I was privileged to be asked by C. A. C. to complete it. This lecture series, though quite extensive in its content and by no means superficial in its treatment, was tailor-made for its undergraduate recipients, the only mathematics assumed (mainly a rudimentary knowledge of the theory of matrices and linear equations) being taught in the first-year *Mathematics for Chemists* course at Oxford.[26] With his typical thoroughness, Professor Coulson sent me his notes for the course and wrote, on November 3rd, 1973, in characteristically modest tones, as follows:[83]

"Thank you so much for agreeing to take on the rest of my Hückel theory course — 3rd year — Fridays 10.10 – 11.00 a.m. — I.C.L. [= *Inorganic Chemistry Laboratory*]. I am very grateful.

Here are my notes — too many, since bits get added from time to time — also not so clear to someone else as to me! But you know all about this stuff and should be able to compensate for my deficiencies. . . [*There then follows a list of topics*] . . .

Do let me know how it goes, and call on me for any further help."

C. A. C. was also predictably reassuring when I subsequently reported to him complaining of a somewhat exponential fall-off in my undergraduate audience. On December 7th, he wrote[83] back, giving the following consolation and 'fatherly' advice:

"Thank you very much for returning my notes, and for letting me know about the lecture course. I am not surprised that not many people turned up on the last Friday of Term! Don't feel too depressed about the drop in audience — it is inclined to happen a bit as the term wears on, and it has been a great comfort to me to know that the lectures were being offered when I could not do them myself. I expect that you too will have learned something from giving them. I well remember starting off this sort of thing and one can never stop trying to improve it. I always try to see from their faces how much is going in and adjust what I say accordingly."

Now, with C. A. C.'s permission, his 1971 series of lectures in this course had been tape-recorded by Dr. Brian O'Leary, also (since 1970) a post-doctoral member of Professor Coulson's Groups at the Mathematical Institute and at the Theoretical Chemistry Department and (from 1974) Professor of Chemistry at the University of Alabama in Birmingham, U.S.A. Complete notes of all diagrams and equations drawn on the blackboard were taken at the time that the lectures were delivered in 1971 and, after the Professor's death, the above-mentioned notes that I had borrowed for the purpose of completing the 1973 lecture series were again generously loaned to us from the Coulson Archives by C. A. C.'s widow, Mrs Eileen Coulson. Armed with this exceptionally complete documentation of the 1971 lectures, Brian O'Leary and I, with Mrs. Coulson's blessing, wrote up the lectures to form a book with the same title as the lecture series: *Hückel Theory for Organic Chemists*.[26] We published this[26] largely because we wanted to have a record of Hückel Theory as taught by the man

who virtually created it in its [then] modern form; financially, the proceeds went to the Coulson Memorial Fund, set up with the object of supporting necessitous students to study or research Theoretical Chemistry in Oxford. We did not miss the opportunity to crusade a little on behalf of Graph Theory in ref. [26], though, in deference to C. A. C.'s known views,[83] we did make unambiguously clear in the Preface that ". . . some Graph Theory is . . . used in the text, but the major part of it is banished to Appendices . . . which are entirely due to R. B. M. and B. O'L."[26]

Except for widespread and major consternation at the manifestly deteriorating health of C. A. C., the year 1974 looked set, graph theoretically, to be a good one. On June 14th, 1973, Professor Coulson wrote[85] to Professor Nenad Trinajstić of the Rudjer Bošković Institute, Zagreb inviting him to consider a three-month visit to Oxford *via* a ". . . possible interchange arrangement between English and Yugoslav scientists. . ." under the auspices of the Royal Society of London. He went on:

"You may be interested to know that during this next academic year October 1973/1974 July there will be a large number of graph theorists here in Oxford, though in fact they will chiefly be at the Mathematical Institute about four minutes walk from here. They include:

Professor F. Harary (University of Michigan)
Professor E. M. Palmer (Michigan State University)
Dr. A. J. Schwenk (University of Michigan)
Professor L. W. Beineke (Purdue)

Also of course Dr. Roger Mallion is here in this department, and Dr. R. J. Wilson of the Open University is still living in Oxford and attending graph theory seminars etc. So it would be a good time to come."

Events proceeded apace, and Nenad Trinajstić's visit was duly arranged to start on January 7th, 1974. Members of the Department were therefore stunned to receive, on January 5th, the following duplicated letter[83] from C. A. C.:

"You probably know that a recent operation revealed an inoperable cancer. There is effectively no chance of my returning to the Department, and I am resigning my Chair. Arrangements will be made for the supervision of all students: please do not worry. . .

May I say thank you to you all for what you have done to make the new department so successful so quickly. I am sure that with your help this will continue. I send you my best wishes."

I myself later received one last personal letter (January 4th)[83] showing what incredible thought for others and attention to detail C. A. C. had even in his dying days:

"I shall have to ask you if you would be kind enough to look after Trinajstić when he comes. Rosemary [*Schwerdt, C. A. C.'s Personal Assistant*] will know all about the arrangements for his finance from the Royal Society, and she has fixed him up with a flat with some friends of ours [*name and address given*]. . . I gather that he will come alone on January 8th, and that his wife will join him later on. We have put him down to speak on Tuesday 12 February on Topological properties of conjugated systems. You may like to get together with Mark [*Child*] and decide whether you or he would introduce Trinajstić at the PCL [*Physical Chemistry Laboratory*]. Perhaps you can also spread the word a little in the Mathematical Institute since some of the folk there may be interested to hear him. I should also be grateful if you could take him over there for tea one day and introduce him to some of the visitors, and perhaps Robin Wilson if he is about. I am sorry that I cannot deal with all this myself.

Yours, as ever,
C. A. C. "

Less than three days after writing the above, Charles Coulson was gone (at 2.30 a.m. on Monday, January 7th, 1974), and, later that very day, Nenad Trinajstić arrived to a Department plunged inexorably into an immense gloom.[u]

Despite this inauspicious start brought about by the highly unfortunate timing of his arrival, Nenad Trinajstić (later joined by his wife, Judita) settled quickly into the Department (by then headed by Dr. Mark Child as *Inter-Regnum* Professor) and immersed himself with vigour and enthusiasm into collaborations both with me and with some of our American visitors (Drs. Harary, Palmer, Beineke and Schwenk) over at the Mathematical Institute. It was during his three months with us that I experienced at first hand why Nenad Trinajstić is such a prolific author. He worked himself (and his co-workers) extremely hard and, by a mixture of cajolery and sheer charm, he persuaded his otherwise-busy collaborators[v] to give priority to his own projects and he invariably inveigled the departmental secretary into typing up the resulting manuscripts absolutely instantly. The upshot was that, during Nenad's brief visit, we published three papers[94-96] in collaboration with Dr. Allen Schwenk. All were concerned with extending and applying Sachs' Theorem[79-81] to the so-called 'rooted' molecular graphs that were considered to represent heterocylic conjugated systems: the first[94] offered a formalism that provided the 'global' characteristic polynomials of a limited class (see later) of such graphs in their entirety; the second[95] enabled the coefficients of individual powers in such characteristic polynomials to be separately evaluated; the third[96] dealt with the mathematical details.

During the academic year 1973–1974 I was also privileged to collaborate with the most celebrated of our American visitors, Professor Frank Harary. Frank (as he was universally known) was ensconced in a large house in Museum Road, just around the corner from the Mathematical Institute, and was a Visiting Fellow of Wolfson College, then only recently founded and having solely post-graduates as its Junior Members. My collaboration with Frank Harary was focused on finding an elementary necessary condition for a graph to be Hamiltonian,[18,31] a problem that tied in nicely with my 'ring-current' work[92] and with my other graph-theoretical interests centred on spanning trees.[93] This venture was carried on throughout the course of the Lent

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[u] Rosemary Schwerdt told me that when Nenad Trinajstić arrived she telephoned the bank to finalise arrangements for his Royal Society funds; she was astounded to be told that they knew all about the matter as Professor Coulson had himself been into the bank only a few days before to sort out the financial business of Nenad Trinajstić's visit. C. A. C. had therefore apparently arisen from his sick bed at that late stage in order to ensure personally that his guest would have no difficulties with his finance. This, in my observation, is absolutely typical of Charles Coulson's unselfish dedication and his remarkable sense of propriety, duty and obligation.

[v] I recall, on one occasion, sitting up in bed at 2.00 a.m. in my rooms in the Meadow Buildings of Christ Church drafting a section of a joint paper being co-authored with Nenad that I had been rash enough to promise him for the following morning, and suddenly thinking to myself: "Why I am doing this?"

Term, 1974, and our results were largely achieved by means of fortnightly meetings which alternately consisted of Dinner at Christ Church[w] (after which we would retire to the S.C.R. for port and dessert) and lunch at Wolfson (after which Frank would usually play table-football with some post-graduate students, while I looked on having coffee). I had a really sociable time with Frank Harary. For example, I was Senior Member[x] of the University Jazz Club (1972–1976) and, each fortnight, the Club used to forgather in an up-stairs private room at *The Roebuck* Inn to listen to a local traditional-jazz *ensemble*. Frank was a regular attender at this. As for our joint work, as with any attempt at such a notoriously intractable problem as the Hamiltonian-Graph Question, all we succeeded in doing was casting the necessary conditions for a graph to be Hamiltonian in an alternative form. The work was published[97] in a somewhat obscure[y] (and, I believe, now defunct) journal run by the Lee Kong Chian Institute of Mathematics at Nanyang University in Singapore, with the Latin title of *Nanta Mathematica*. Frank had twice been Visiting Professor at that Institute, working there with Professor H. H. Teh, and from time to time he used to submit papers to their journal. Ours was one of them.

When I first met him, in Lent Term, 1975, Michael Rigby was a third-year Chemistry undergraduate at Oriel College. Although reading Chemistry, Michael had always regretted that he had not chosen Mathematics as his degree subject; (in the event, his subsequent career was in the Church). When it came, therefore, to choosing his Part II topic,[z] he resolved that it should be as mathematical as possible. Having heard the reaction from Oriel Chemistry undergraduates one year above him to my Hückel Theory lectures (*vice* C. A. C.) in Michaelmas Term, 1973 — namely, that they were exceedingly mathematical and hence, to most Chemistry undergraduates,

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[w] As a Visiting Fellow of Wolfson College, Frank had also been accorded M. A. Status in the University for the duration of his tenure of that post. Now Christ Church (unlike Wolfson) is very formal and traditional, and, *de rigueur*, academic gowns are to be worn at Dinner. Frank thus always relished the opportunity to sport his M. A. gown whenever he dined with me at Christ Church.

[x] Any club run by Junior Members of the University (*i.e.*, undergraduates and/or postgraduates) that wanted to call itself 'The Oxford University [X] Club' had to be registered with the Proctors (the University Authorities) and had to have a Senior Member (*i.e.*, a Member of the University's Congregation, which I was by virtue of being a Member of the Faculty of Physical Sciences) to take responsibility for it and to ensure that the 'good name' of the University was not 'brought into disrepute.'

[y] Obscure the journal may be, but I always note with amusement that *this* is the publication[97] that, since 1974, has allowed me to make the proud claim of having an 'Erdös Number' of 2 — for Frank Harary has an Erdös Number of 1, having himself (twice) been a direct co-author of the late Paul Erdös.

[z] The Oxford system for undergraduate Chemists that operated at that time required candidates to take the 'Part I' examinations at the end of the third year; these were conventional timed, written examinations that largely determined the class of the degree finally awarded. In order to gain an honours degree, however, candidates had to undertake a fourth year that was entirely devoted to research, at the end of which a Part II Thesis had to be presented for assessment.

utterly incomprehensible — Michael decided there and then (as he subsequently divulged to me) that, regarding his possible choice of Part II Supervisor, ". . . that's the man for me!" Accordingly, Michael sought me out and asked if I would supervise him for his Chemistry 'Part II'. Although very pleased to be asked, I had some hesitation, for the academic year in question, 1975–1976, was to be the last of my Christ Church Lecturership. I was at the time applying for all and any of the (very few) permanent academic posts that, in those sparse times of the mid 1970s, were becoming available and I was therefore reluctant to agree to take on Michael for that academic year when there was a realistic possibility (albeit probably a small one) that I myself might have left Oxford by then. However, I was aware of Dr. A. C. Day, of University College; although Tutor in Organic Chemistry at 'Univ.' and a permanent Member of the Faculty, being based in the Dyson Perrins Laboratory, Colin Day had extensive 'amateur' (as he would put it) mathematical interests, and, indeed, he had done some very elegant (but unpublished) work involving a neat application of the eigenvalues of skew-circulant matrices to the Hückel energy levels of Möbius annulenes. I therefore approached Colin Day and asked him if he would jointly supervise Michael Rigby with me for his 'Part II'. This he readily agreed to do and there thus began a one-year tripartite collaboration that culminated in Michael Rigby's Part II Thesis[98] in Summer Term, 1976, entitled *Graph-Theoretical Aspects of Some Chemical Problems*. This Part II Thesis gave rise to more published papers than do most Ph.D. theses; there were eventually five[99–103] that *I* know of (all of which dealt with 'applications'); I also encouraged that there should be one purely mathematical paper with Michael Rigby as the sole author — as he had largely, by his own efforts, devised the underlying mathematical ideas in his Part II Thesis[98] — but, sadly, I do not think that such a paper, though drafted, ever, in the end, got submitted.

The first paper with Michael Rigby[99] reported a complete generalisation of the earlier formalisms[94–96] for obtaining the characteristic polynomials of 'rooted' graphs — mentioned before and devised in collaboration with Schwenk and Trinajstić[94–96] — which had been applicable only to a very restricted family of hetero-conjugated systems containing just one kind of hetero-atom *and* having all their resonance integrals set at a common value (usually that appropriate for the carbon-carbon bond in benzene). Ref. [99] commented (critically) on an alternative extension (likewise a complete generalisation of refs. [94–96]) that Nenad Trinajstić himself (and his collaborators, one of whom was Professor Polansky)[104] had independently made to the same 'Oxford' work[94–96] of 1974 on his subsequent return to Zagreb. Both these new approaches,[99,104] unlike the earlier ones,[94–96] could cope with the characteristic polynomials of *general* molecular graphs in which any number of vertices representing arbitrarily diverse hetero-atoms, as well as any number of edges representing bonds with arbitrarily diverse resonance-integrals, could be

accommodated. (It is an interesting observation on the 'simultaneity' of scientific research that, meanwhile, Aihara,[105] in Hokkeido University, Japan, was *also* engaged, at the same time, on the identical quest, entirely independently of the machinations going on in both Zagreb[104] and Oxford[99]). The thrust of our own paper[99] was that a claim that the expressions of ref. [104] allow calculation of the coefficient of any individual power in the characteristic polynomial, without the necessity to evaluate the entire polynomial, appeared to be unfounded: the generalisation we presented in ref. [99] *does*, however, enable individual powers to be separately calculated on their own (as also, incidentally, does the formalism independently devised by Aihara.[105]) Another topic of especial interest to Michael Rigby and Colin Day was Möbius molecules, this work being written up considerably later.[102,103] In the meantime, I independently investigated two other areas with Michael Rigby: one was an extension of the Coulson-Rushbrooke Theorem[56,57,60,26] to bipartite *heterogeneous* graphs (as — in the mathematical literature, where we published this work[101] — we called the graphs representing alternant hetero-conjugated systems); the other was showing by means of a counter-example[100] that the union of the spectrum and the 'regular spectrum'[93] of an arbitrary, simple finite graph does not constitute a complete set of invariants that characterises it up to isomorphism. This second project was in collaboration with the distinguished Mathematical Graph-Theorist, the late Dr. D. A. Waller. Derek Waller was on the Faculty in the Department of Pure Mathematics at my *alma mater*, University College, Swansea, and I had got to know him in the mid 1970s through my former Swansea supervisor Claude Haigh (who, by this time, had followed a similar 'Road to Damascus' to mine and had himself become fascinated by Graph Theory and used frequently to discuss graph-theoretical matters with his mathematical colleague.) Derek Waller's major contribution to the theory of graph spectra was his concept of the 'row-regularised' graph.[106] The addition of loops to the vertices of a graph produces another graph with the same number of spanning trees;[93] it is possible to add loops to a graph in such a way that the modified graph is regular (*i.e.*, each of its vertices is of the same degree). As a result of this clever device, these modified graphs, thus 'row-regularised', then enjoy some of the pleasant algebra associated with graphs that genuinely *are* regular. This is the essence of Waller's procedure of 'row-regularisation';[106,93,107] the eigenvalue spectrum of such a graph is said to be the 'regular spectrum' of the original (in general, non-regular) graph, and the associated eigenvectors are its corresponding 'regular eigenvectors'. Although Derek Waller was a genuinely Mathematical Graph-Theorist he was very much 'on a mission' — sadly to be abruptly curtailed, as will be seen — to collaborate with Scientists and generally to spread the application of Graph Theory outside the confines of Pure Mathematics. Indeed, at his instigation, he and I advertised the perceived advantages of this 'row-regularisation' approach[106,93,107] for counting

spanning trees in one of the very early issues of *MATCH* (No. 2, 1976).[108, aa] Appeal to the regular spectrum of a graph was invoked when providing, in ref. [100], our counter-example (involving two isospectral, non-isomorphic, regular graphs on 12 vertices) to the suggestion that that the union of the spectrum and the regular spectrum[93] of an arbitrary, simple finite graph does constitute a complete set of invariants that characterises it up to isomorphism.[bb]

5. Conferences, 1970–1975

To finish this account, I just add a short section reviewing some of the conferences and symposia that I attended during this period (in France, England, Scotland and Germany), culminating in the 'Micro-Symposium' held in Mülhiem under Professor Polansky's auspices (May 26th–May 28th, 1975) that conceived the idea of *MATCH*. I have already mentioned the conference (organised By Dr. S. L Altmann) held in Oxford (March 31st–April 3rd, 1971) to commemorate Professor Coulson's 60th Birthday. The previous summer (1970) I and my Australian colleague Dr. R. G. A. R. Maclagan (who was the third member of the Mathematical Institute office shared with Robin Wilson) represented Professor Coulson at a quantum chemistry conference held at the *C.N.R.S.* in Paris, under the chairmanship of Dr. C. M. Moser, a collaborator of Charles Coulson's from the mid 1950s. No graph theorists were there, but I did at one stage briefly find myself *à deux* with Professor Bernard Pullman during a social event for members of the conference at the Pullmans' apartment; having plucked up sufficient courage, I risked asking him whether he had anything more to add to the theory (well accepted by 1953[109] but subsequently widely doubted) that he and Mme Pullman had proposed about the so-called '*K*-region' in carcinogenic hydrocarbons (such as 'my'[8] 3,4 benzopyrene) that had so fascinated me during the previous five years.[110] He answered with a resounding and definitive '*Non*!' — and that was the end of the conversation.

[aa] Initially, *MATCH* took on the nature of a private newsletter, rather than a journal as such, and so Professor Polansky decreed that citation of its articles was strictly forbidden without the expressed permission of the author (and, even then, such citations had to be in the form of a 'personal communication.') Consequently, although ref. [108] is now nearly 30 years old, this is the first time that I have ever made reference to it in print; the reason is that because of this 'newsletter'status that *MATCH* then had, I did not at the time include this joint note with Derek Waller in my list of publications. Indeed, until my recent researches for this Reminiscence, I have to admit that I had in fact quite forgotten all about ref. [108], and I was actually somewhat surprised to re-discover it.

[bb] It is sad to record that, even though ref. [100] was sent to the fast-publication journal *Chemical Physics Letters*, between the original reception date of March 31st, 1978 and the receipt (after the refereeing process) of the revised version of the manuscript on July 26th, Derek Waller had died suddenly (from a leukaemia), on June 23rd, 1978 (a fact recorded in a footnote to that paper[100]). Accordingly, ref. [100] was, for Derek Waller, posthumous, when — less than eight months after its original submission — it was eventually published, on November 15th that same year.

The year 1973 saw the 50th anniversary of Louis de Broglie's proposal of the electron wave–particle duality and a conference to commemorate this (organised by Professor Raymond Daudel) was held (once again, appropriately, in France) on the *Côte d'Azur* at Menton, near Monte Carlo (July 4th–July 10th, 1973). C. A. C. was too ill to attend and deputed some of us from the Theoretical Chemistry Department (I, and fellow 'post-doctorals' Drs. Jim Eilers and Brian O'Leary) to go in his stead and to report back to him on it. It was rumoured that Monsieur de Broglie himself would be attending but, unfortunately, for health reasons, he did not. Instead, we all listened attentively to a sound recording of his inaugural message, played over loud-speakers in the Municipal Hall at Menton during the opening ceremony, whilst — projected onto a large screen — slides of photographs of him were shown, in his Academician's uniform (complete, I recall, with *épaulettes*). I thus did not see de Broglie then but, on another occasion, when making a 'fraternal' Oxford visit to the offices of the *Académie des Sciences* on *Quai Conti*, opposite the Louvre, I did very briefly set eyes on Louis de Broglie, from afar, as he fleetingly passed across a corridor in *La Coupole*. That was the nearest I ever got to meeting this legendary figure.[cc]

Almost immediately after Professor Coulson's death in January, 1974, I was both touched and delighted to receive an unexpected letter from the distinguished Applied-Mathematical Graph Theorist Professor H. N. V. Temperley, F.R.S.,[dd] whom I have already mentioned as having heard lecturing in Oxford in 1972. This letter is, unfortunately, temporarily lost, but I well recall that it began in the splendidly old-fashioned 'academic vocative' ("Dear Mallion") and opened with the somewhat stark, direct and unnerving sentence: "I don't know you." Professor Temperley did, though, go on to invite me, in Professor Coulson's stead and at his dying request, to a high-level *Rencontre* (as it was called) sponsored by the Science Research Council and being held in Aberdeen, Scotland, in July, 1975. The object of this *Rencontre* was to bring together Mathematical Graph Theorists and Scientists who had an interest in

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[cc] I do, though, have — somewhere in my archives (temporarily lost) — a personally signed letter from Monsieur de Broglie dating from 1973, written in his capacity as one of the *Secrétaires Perpétuels* of the *Académie*. It was in fact a 'rejection letter' to ref. [65], which was eventually published in *Bulletin de la Société Chimique de France* but which was originally designed for the *Comptes Rendus* because the manuscript was intended to be a reply to the paper by Dennis Rouvray in that journal, detailed in ref. [64]. This letter was co-signed by fellow *Secrétaire Perpétuel* Monsieur Robert Courrier. Out of curiosity, I looked them both up in the publication *Who's Who in France*: Monsieur de Broglie was born in 1892 and Monsieur Courrier was born in 1894. I recall at the time making some considerable humorous capital during Dinner at Christ Church High Table out of the fact that this was the first time that I had ever received a letter jointly signed by *two* people who were *both* born in the 19th century. It made one have especial belief in the description of them as *Secrétaires Perpétuels*!

[dd] Professor Temperley was also well known to me — from a distance — in a 'former existence', as-it-were, in the early 1960s when I was an undergraduate at University College, Swansea, and he was Professor of Applied Mathematics. By his rather 'other-worldly' and somewhat 'preoccupied' demeanour, Professor Temperley was every 1960s undergraduate's rather fanciful, but affectionate, idea of 'a brilliant, absent-minded Professor'!

applying and adopting Graph Theory in their respective fields. I take up the story by quoting from my letter of condolence[83] to Mrs. Eileen Coulson of January 19th, 1974:

> ". . . I was most touched to receive the other day a letter from Professor H. N. V. Temperley of my old College in the University of Wales, concerning an S. R. C. *Rencontre* in Combinatorics, to take place in Scotland in July next year. Apparently, one of the last acts of Professor Coulson was to ask if his invitation to this very exclusive small gathering be passed on to me. I shall indeed be most honoured to step unworthily into the Professor's shoes for this *Rencontre* — although it is too much to hope that I shall do the occasion anything like justice; I shall, however, do my best to justify the confidence which the Professor was kind enough to express in me by making this suggestion to Professor Temperley."

In her reply, received on January 24th, 1974, Mrs. Coulson wrote:[83]

> "I hope you enjoy the Rencontre too . . . how like my husband to arrange that for you!"

The *Rencontre* itself (July 6th–July 12th, 1975) was one of those very *gemütlich* conferences in which one meets a good proportion of the participants on the aeroplane travelling there, and I recall finding myself sharing a taxi from the airport with Professor J. S. Rowlinson, Professor of Physical Chemistry at Oxford. At the *Rencontre* proper, I renewed my acquaintances with Frank Harary and with Robin Wilson. For me, though, the main *pièce de résistance* of this gathering was the privilege of at last meeting the celebrated Professor Dr. Horst Sachs, of 'Sachs' Theorem'[79] fame. I was amazed and gratified to find that someone who — by his repute as the author of the *Koeffizientensatz*[79] — was, in a sense, my mathematical 'hero', turned out, in reality, to be such a charming, self-effacing and modest man. This meeting was a rare opportunity; it has to be recalled that these were the days of the *D.D.R.* — that country was then only just over five-eighths of the way through its 40-year existence — and Horst Sachs was indeed making his first visit to these islands for almost 30 years. My own contribution to the proceedings was a talk on the work that I had done the year before with Schwenk and Trinajstić.[94-96] Following the convention established by Graovac *et al.* in their classic paper,[75] I referred to Sachs' *Grundfiguren*[79] that feature in, and are material to, his *Koeffizientensatz*,[79] as 'Sachs Graphs'. In the discussion that followed my presentation, Professor Sachs said: "I am rather embarrassed to have my name associated with these graphs — especially when they are such *trivial* graphs!" Frank Harary was also present at my talk and he confided to me later that he likewise was not very keen on the 'Sachs' Graph' *appellation*, for he pointed out that he himself had also independently devised[111,112] what Chemists, in this context — ever since the publication of ref. [75] — had called

'Sachs Graphs'.[ee] This delicate matter is all gone into in some considerable detail in two compelling (though diverse) articles by Gutman.[80,81,ff,gg]

There are many entertaining stories that I could relate about this conference, but I limit myself to just two; the first concerns the illustrious name of Dirac. One of those invited to the *Rencontre* was the late Professor Gabriel Dirac, Mathematical Graph Theorist from Aarhus University (and sometime member of the Mathematics Faculty at University College, Swansea). As is usual at conferences, several participants brought 'accompanying persons' with them to take part in the social events connected with the affair. Gabriel Dirac's 'accompanying person' was an elderly man who was very quiet and reserved at meals; nobody took much notice of him until the rumour began to circulate that Gabriel Dirac's 'accompanying person' was none other than his step-father, the celebrated veteran Nobel Laureate P. A. M. Dirac. Wanting to be able to claim that I had met the great man, I espied and shamelessly seized my opportunity at an especially bibulous reception towards the end of the *Rencontre*. Encouraged and fortified after imbibing a certain amount of 'Scottish wine' — something that I never normally partake of — I intercepted (unforgivably, I now feel) P. A. M. Dirac just as he was on the point of leaving. He was very gracious and tolerant about having this young stranger foisted on him when he was just going, but, nevertheless, he did not linger very long. . .

Taking place immediately after the Aberdeen *Rencontre* was the Fifth British Combinatorial Conference (July 14th–July 18th, 1975), also at the University of Aberdeen. There was naturally a certain amount of overlap and interchange of personnel between this and the *Rencontre*; for example, I recall that Frank Harary received an honorary degree from the University of Aberdeen during the

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[ee] Because of these difficulties, in the work that I did with Schwenk and Trinajstić[94–96] we followed the practice of Allen Schwenk's Ph.D. Thesis[113] in referring to what Graovac *et al.*[75] called 'Sachs Graphs' as 'mutation graphs'. When the method needed to be extended to graphs representing heterocyclic conjugated molecules, the definition of what constituted a 'mutation graph' had, accordingly, to be widened.[94–96,98,99]

[ff] In view of the [then] recently published ref. [80], I had extensive and lengthy discussions with Professor Sachs[114] — during the Conference on C_{60} held at Spandau, Berlin in December, 1994 — on the matter of who had priority of the 'Sachs Theorem' for calculating characteristic polynomials of graphs. As a result of these conversations, it is now unambiguously clear to *me* (at least) that the two virtually simultaneous publications that constitute refs. [79] and [112] *were* genuinely independent — *both*, though, unknowingly building on the (likewise independent) foundations of Samuel,[32] and of Coulson,[84] some 12 or 13 years before.

[gg] Professor Sachs is in any case of the opinion[115] that the *Koeffizientensatz*[79,112] ". . . is not really a theorem; it is nothing but the translation of Leibnitz's definition of the determinant, extended to the concept of the characteristic polynomial, into the language of graph theory." In ref. [115], Professor Sachs also went on to say that ". . . in *Spectra of Graphs*[28] (page 36), Dragos Cvetković and I tried to give a report as factual as possible. I do wonder why L. Spialter[38] (whom I do not know) who formulated the proposition in a chemical context has (it seems to me) been forgotten."

Combinatorial Conference.[hh] Especially fortunate for me was the fact that my former supervisor Claude Haigh was attending an N.M.R. meeting in nearby St. Andrew's, also taking place at about the same time as the *Rencontre* and the British Combinatorial Conference, and he, too, made occasional sorties from St. Andrew's to the events at Aberdeen. Now, my return journey home to Oxford consisted of stopping off in Edinburgh to do some sightseeing, and then continuing by flying on down south from there. Frank Harary had at one stage asked me how I was going to get to Edinburgh; he suggested that I might fly, with him, and I provisionally agreed to this. Later, though, I learned that Claude Haigh, that same day, was returning to South Wales by train — of course, travelling *via* Edinburgh. At that time, we had some work to do on a joint manuscript that we then had in preparation;[73] in order, therefore, to take advantage of the opportunity presented to advance this project with C. W. H., I changed my plan and, instead of flying with Frank Harary, I decided to travel from Aberdeen to Edinburgh by train with Claude Haigh. In the event, because of a fire at Stonehaven, the line was blocked and, in the end, our train ('The Aberdonian'[ii]) was re-routed all the way north to Inverness and we finally limped southwards back down to Edinburgh by an alternative route (crossing, in the final stages, my favourite railway land-mark, the Forth Rail Bridge) some nine hours after leaving Aberdeen for our supposedly three-hour journey to Edinburgh. The up-shot of all these events was that Claude Haigh and I got an unexpectedly large amount of work done on our joint manuscript.[ii]

A mere six weeks before the start of that Aberdeen *Rencontre*, I found myself steaming away from 'the White Cliffs of Dover' *en route* for the Continent and Professor Oskar Polansky's 'Micro-Symposium' on "Graph Theory in Chemistry", held at the *Institut für Strahlenchemie im Max-Planck-Institut für Kohlenforschung*, Mülheim (May 26th–May 28th, 1975). Unlike the Scottish *Rencontre*, this was essentially an 'all-European' affair; 29 participants came from Germany or German-speaking Switzerland, with only seven delegates from elsewhere: Drs. Trinajstić and Graovac (Yugoslavia), Drs. Bonchev, Fratev and Tyutyulkov (Bulgaria), Dr. Rouvray (who could properly have been designated as 'U.K.' but was still, at that time, affiliated to South Africa), and the present author (U.K.). Professor Balaban

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[hh] I learned later that Paul Erdös was present at the British Combinatorial Conference (though I did not meet him or see him). Therefore, in that July week in Aberdeen in 1975, two legendary 'giants'—Dirac and Erdös — were both 'in town' virtually simultaneously. . .

[ii] As may be imagined, 'The Aberdonian', being a classic railway train that runs between Edinburgh and Aberdeen and is prominently labelled as such, was given many a 'double-take' by passengers waiting on platforms at railway stations in the vicinity of Inverness!

[ii] Which, nevertheless, was still not in fact actually published for another 14 years[73]. . .

(Roumania) was advertised as attending but, of course, he had his usual difficulties — see footnote *b* in §1 — and, regrettably, did not, in the end, materialise.

Despite the fact that, as already noted, some 80% of the participants were germanophone, Professor Polanksy insisted that because, as he put it, ". . .English is the international language of Science . . .", all the proceedings were to be conducted in that medium[kk] — which, of course, admirably suited the 6% of us (namely, me and Dennis Rouvray) who were native English speakers! Professor Polansky himself spoke English with a very strong Viennese accent — which, to a British ear, is a delightfully attractive sound. The main embarrassment for me, though, was that, time and again, when Professor Polansky was speaking publicly in English and he suddenly had a doubt about a particular phrase, he would invariably turn to me (as the only participant registered from a British address — and an *Oxford* one, at that) and smilingly ask, in his charming but thick Viennese brogue: "Is this correct Oxford English, Doctor Mallion?" It was at these times when I felt that I just wanted to sink through the floor in embarrassment at suddenly having to be the centre of attention, with all eyes on me as a designated 'oracle' on the English language. My own contribution to the scientific part of the proceedings was a talk on spanning trees and Hamiltonian circuits and my only recollections of it, now, are (a) that much good-natured fun was derived by Professor Polansky, at my expense, from my pronunciation and recitation (in full) of the complex German title of Kirchhoff's 1847 paper,[66] and (b) that he joked that the frequent mention of my sole publication with Frank Harary[97] was making the journal *Nanta Mathematica* ". . . famous . . ."!

The lasting consequence of this colloquium was, however, the decision — reached after discussion and deliberation at a special session of the Micro-Symposium devoted to it — to found *MATCH*, under Professor Polansky's auspices, with its publication centred on the Max-Planck Institute, Mülheim. It is, of course, this event that the current issue of *MATCH* is commemorating, and the 1975 Mülheim Micro-Symposium is specifically the subject of a special article by the Editor, elsewhere in this *Festschrift*.

[kk] I am prepared to concede that English *is* genuinely the international language of *written* Science. Whether it is in practice always an effective means of international communication when *spoken* (especially when it is spoken — as, on occasions, it is — ungrammatically and/or with a strong accent), I rather dispute. . .

6. *Postscript*: The King's School, Canterbury, 1976–2005

The above period is, by definition, outside the remit specified by my title. I do, though, mention it in order to connect this Reminiscence with the present. I did not manage to secure a university post on the determination of my Christ Church Research Lecturership on September 30th, 1976: instead, on September 1st that year, I joined the Mathematics Department of The King's School, Canterbury (see footnote *o* — §3). Because the School is a residential one, this has been a 24-hour-per-day, seven-day-per-week job during the term times. However, the position has had the distinct advantage that it has afforded the agreeable benefit of long periods when the School is not in session and, during these times, I have been able to pursue my own individual interests in Mathematical Chemistry, virtually as a 'hobby'. Being what one colleague once facetiously described as "a 19th century 'gentleman' scientist" has meant that, during the last 30 years, I have had the luxury and privilege of being able freely to choose my co-workers and, as a result, I have effectively collaborated only with my *friends*. A sizeable number have already been introduced to the reader by my descriptions of them in this account. Others who came later included my colleague and mentor here at King's, Mr. Paul Pollak (Canterbury), long-standing family friend Dr. Edward Kirby (Pitlochry), *MATCH* Editor Professor Dr. Ivan Gutman (Kragujevac), Dr. Peter John (Ilmenau), Professor Douglas Klein (Galveston) and even one of my pupils at King's, Mr. (now Dr.) Toby Brown (later of St. John's College, Oxford), who collaborated with me whilst he was still at School.[107,117]

Europe is a very different place now from what it was 35 years ago, the point at which I started this Reminiscence.[ll] Then, as a British subject, I could travel at will, and on a whim, to anywhere in Yugoslavia, including Zagreb, Dubrovnik and Kragujevac — the triennial Dubrovnik conferences organised by Nenad Trinajstić from the late 1970s till the mid 1980s were the high spot of those halcyon days — but to go to Ilmenau involved some formidable forward planning, as well as a diplomatic dance about visas in order to prevail over the Teutonic thoroughness and invariably hostile attitude of the *D.D.R.* authorities. Since 1990, Ilmenau has been in a fellow state of the European Union and I can go there — and even, if I wished, *work* in the *ehemalige D.D.R.* — by *right*; (indeed, for the past five years my own nephew has done just that). It would, though, these days, need some preparation to visit Kragujevac — a city that, in the dying years of the 20th century, even had to bear the brunt of hostile action on the part of my own air force. (This was the first occasion in my life-time on which my own country — albeit as part of a N.A.T.O. campaign — was militarily targeting a population containing people known personally to me).

[ll] As it so happens, I originally drafted that sentence on April 30th, 2004. At midnight that day, Europe changed yet more, with enlargement of the European Union from 15 to 25 member states.

Furthermore, over the years, one has sadly had to get used to losing co-authors — *e.g.*, of those mentioned here, Charles Coulson, Derek Waller and Colin Day are now deceased — but, in the course of the last two decades, I have had the novel and unnerving experience of publishing a paper (in 1988)[116] with two co-authors (Nenad Trinajstić [Yugoslavia] and Pavel Křivka [Czechoslovakia]) whose very *countries* subsequently disappeared! Meanwhile, now freed from the dead-hand of the Ceaușescus, Alexandru Balaban (with whom I began this story — §1) is at last able to attend any conference that he wishes, and indeed he is even, these days, a U. S. and Roumanian citizen. As my former Prime Minister Lady Thatcher once famously observed (in quite another context): "It's a funny old world!"

Nevertheless, any perceptible constancy in our field that has somehow managed to pervade all this European upheaval and political change has very largely been due to the personalities of, and the enduring friendships between, those involved in the small but close world of Mathematical Chemistry. Long may it continue! I for one deem it a real privilege to have been a minute part of all this, over the last 35 years, and it is in this sense of international friendship and goodwill that I offer this highly autobiographical Reminiscence as a small personal tribute to the first 30 years of *MATCH*.

Acknowledgements

Finally, of all the friends and colleagues referred to in the text of this Reminiscence, I should like to make especial mention of four people: Mr. C. W. Haigh, Mr. P. Pollak, the late Professor C. A. Coulson and the late Mrs. E. F. Coulson. I am greatly indebted to Claude Haigh for his valued friendship and stimulating academic support over a period of some 40 years, and to Paul Pollak for similar invaluable kindness for almost 30 years. As I have previously stated elsewhere,[7,26] to have been a member of Charles Coulson's group at the Oxford University Mathematical Institute and to have moved with him to his Theoretical Chemistry Department represents the rarest of privileges — speak to any 'Coulson Chemist' and the same response will be evoked. For over 20 years after C. A. C.'s death, until her own demise, his widow, Mrs Eileen Coulson (1914–1997), was a source of continuous and warm encouragement in all my scientific endeavours, but especially concerning those that in any way involved her late husband. To all these, and to the others whom I have reminisced about here, I am immensely grateful.

R. B. **MALLION**, *The King's School, Canterbury,* **May 29th, 2004**

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[pp] This letter was quoted in ref. [73] and *mis*quoted in part (*d*) of ref. [7]; (please see footnote *m* — §2 — for details). My own personal archives contain an extensive correspondence with the late Professor Clar, carried on during the early 1970s.

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Index of Names

These columns list the pages on which mention is made of those discussed in the text or referred to in the footnotes: persons cited only in the literature References are excluded.