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IN MEMORIAM

Reminiscing about Ron Gillespie

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Abstract
The interactions between Ronald J. Gillespie (1924–2021), the initiator of the VSEPR model of molecular geometry, and the author started in the early 1970s and culminated in a joint book about the model in 1991, republished in 2012. In 1998, they recorded a conversation about Gillespie's life and career, which he augmented by his thoughts about the similarities between his demeanor as a scientist and that of Charles Darwin.

Keywords Ronald J. Gillespie · Christopher Ingold · VSEPR · Ligand–ligand repulsions · McMaster University · George A. Olah · Charles Darwin

I first contacted Ronald J. Gillespie (1924–2019; Fig. 1) in the early 1970s when I was writing an article about the VSEPR model for a popular Hungarian science magazine [1]. I wanted to use the simplest AX_4, AX_3E, AX_2E_2 series of molecules to demonstrate the predictions of the geometrical changes by the model, and it did not work. I was a fledgling research chemist, and he was a big name professor, but he responded and took my problem seriously. He cautioned me not to rush to any quick conclusion that would induce doubts about the broad applicability of the model. It took years and a good deal of quantum chemical computation in cooperation with Peter Pulay, the brilliant Hungarian-American quantum chemist, before I could interpret the apparent discrepancies and thereby expand the applicability of the model. This is how it happened that a crucial diagram about geometrical variations in series of simple molecules appeared first in a Hungarian popular science magazine and later in a most prestigious American chemistry journal [2].

A good on and off interaction developed between Ron and I, which eventually culminated in co-authoring a book on the VSEPR model [3]. The production of the book was not invariably an enjoyable experience, but it was instructive. I was working in Budapest, and he was sailing most of the time along the intracoastal waterway of the Atlantic Seaboard as he was beginning his retirement. This was no easy arrangement in pre-Internet time and I had to follow his stops at the marinas. I had to re-write and sometimes re-write again various chapters until Ron was satisfied with them. Even in the most minor and trivial details, it was not easy to convince him, like that the correct writing is Le Bel and van 't Hoff (rather than le Bel and van't Hoff). In any case, our working together was a great lesson for me whose essence was that every page must be sound and clear and *didactic*. Nothing could be left opaque and nothing could be left that would not be easy to perceive and would not stand the test of a freshman chemistry lecture. I have carried that lesson with me ever since.

One of the difficulties in our joint work on the book was that at the time, Ron tended to ignore ligand–ligand repulsions in shaping molecular geometry. He appeared very protective of the model and not at all eager to expose its limitations. The significance of ligand–ligand repulsion in molecular geometry was first pronounced by Larry Bartell in the early 1960s. Later, Magdolna Hargittai and I presented case studies demonstrating their importance. Considering them expanded the possibilities of structure determination by using well-established non-bonded distances as constraints in the analysis. In time, Ron learned to appreciate ligand–ligand repulsion and even became its dedicated researcher. His interest in these interactions appeared at times even overtaking his appreciation of the VSEPR model. He became a strong advocate of what he called the ligand close packing (LCP) model. Nonetheless, the LCP model never took the place of the VSEPR model in pedagogy, let alone in research.

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Fig. 1 Ronald J. Gillespie (photograph by I. Hargittai)

In his account of the 50-year-old VSEPR model [4], Ron remembered his reluctance of taking ligand–ligand repulsions into account in discussing molecular geometry: "And I continued to do so after later further suggestions by Istvan and Magdolna Hargittai (here, [5] and [6]) that, at least in some molecules, they appeared to be important." ([4], actual quote, p. 1319) Then, as if the above note had not sufficed, he graciously added in the acknowledgments: "Istvan Hargittai for the exchange of ideas on molecular geometry over many years, and for his collaboration on the book we wrote together (here, [3]). I also apologize to him not at first taking his strong convictions that ligand repulsion plays an important role in determining molecular geometry too seriously." ([4], actual quote, pp. 1326–1327).

Notwithstanding the difficulties in producing our joint book, I have cherished our interactions [7]. Over the years, Ron and I visited each other in Budapest and in Hamilton. During my brief visits with him, I observed how efficient he was even in managing tasks that could be labeled secretarial, when time was scarce, for example, in changing a flight reservation. Then, on the occasion of one of the molecular structure meetings in Austin, Texas, in March 1998, we recorded a conversation for my magazine, *The Chemical Intelligencer* [8].

Ron was born and grew up in London, and at the age of 11, he was awarded a scholarship to the local grammar school. He enjoyed school, but his performance was only average because of his sports activities. During the last 2 years, they specialized in preparation for university. He chose chemistry, physics, and maths. Physics was dull because the teacher simply read the textbook. The chemistry teacher, George Cast, made the lessons exciting and gave the students interesting lab work. He inspired Ron and his classmate, William Moffitt, to go into chemistry. Moffitt went to Oxford, became Charles Coulson's student, and was a professor at Harvard. He had the promise of becoming an international leader in theoretical chemistry, but died tragically young. Ron did well in the finals, amid the raging war, and was awarded a scholarship to continue at University College London (UCL).

During 2 years of his undergraduate studies, the school was evacuated to the University of Wales in Aberystwyth. Toward the end of his undergraduate studies, Christopher Ingold (1893–1970), the head of the department, told him to stay on. He helped Ron in his initial steps in research, and he started an investigation of the ionization of solutes in sulfuric acid. He accumulated a good amount of experimental results, and Ingold published seven papers on Ron's work in the *Journal of the Chemical Society* in 1950, all written up by Ingold with several of them carrying Ron's name only. Ingold each time asked Ron to review the draft manuscript, but Ron would not dare to suggest change. Ron got his Ph.D. in 1949, and Ingold continued charting his career. It appears that Ingold cared for the young people at the department, regardless whether they were in inorganic or organic chemistry, although his research interest was in physical organic chemistry.

Ron was doing well at UCL and enjoyed his research and teaching in inorganic chemistry. When a new professor, Ronald Nyholm (1917–1971), from Australia joined the department, their mutual interest in science and, in particular, inorganic structures, invigorated the already attractive conditions of Ron's situation. In 1957, the two co-authored a review on inorganic structural chemistry with Ron covering the main groups and the other Ron the transition metals. This was the cradle of the VSEPR model of molecular geometry.

When Ron started traveling, a new world opened up for him because until then, he had not considered leaving UCL. In time, however, the care by Ingold was gradually becoming a burden. Ron could not do anything on his own; he had no funds of his own and was totally dependent on Ingold, as were his colleagues. When in 1958 Ron received an offer from McMaster University in Hamilton, Ontario, which would double his salary, and would provide a Raman spectrometer and a state-of-the-art NMR machine, Ron decided to move to Canada. It was a good time for doing so as the National Research Council of Canada supported research with large grants

and Ron excelled in devising and executing important projects.

For some time, Ron's involvement with the VSEPR model was hardly more than being its propagandist. In a few years' time, the VSEPR model had become part of the curriculum worldwide. In research, Ron made great strides in super acid research. In this, there was considerable overlap with the future Nobel laureate George Olah (1927–2017) [9]. Olah was a refugee scientist from Hungary at the end of 1956, following the ruthless suppression of the anti-Soviet revolution. On his way to North America, Olah spent some time in London, and they met. When Olah could not find a job in academia, he worked at an industrial laboratory in Canada. There, he continued his own research after the official work hours. Olah solved the famous controversy between the two great American organic chemists, Herbert Brown and Saul Winstein, concerning the structure of the reaction-intermediate norbornyl ion. Olah did not have an NMR spectrometer, and Gillespie welcomed Olah's samples although he did not like them as they looked contaminated. However, as Ron told me, Olah found the carbonium ion in those samples, which he stabilized with superacids and decided the Brown–Winstein debate. This gave him unprecedented fame, which facilitated the recognition of his new chemistry and his Nobel Prize in 1994. Olah always recognized Gillespie's pioneering research in superacid chemistry. In the preface to one of his books, he expressed his admiration for Gillespie's seminal work on superacids. He told me that if the superacid discoveries had been awarded a Nobel Prize, Gillespie would have become a laureate. Actually, there have been nominations of Gillespie for the Nobel Prize. In 1983, I was also asked to prepare supportive material for such a nomination, which I did with great enthusiasm.

In our conversation, Ron mused about the differences between his and Olah's research philosophy. I got to know Olah quite well during the last 25 years of his life, from 1993, that is, from the time when he was not yet distinguished by Nobel fame. He was a genuinely generous and caring human being, generous toward his associates and generous in his research demeanor. I think that this generous approach helped him recognize the carbocation in the samples that Ron judged to be of dubious purity. Apparently, Ron continued musing about our exchange long after we had turned off our recorder in our 1998 conversation. In preparation for its publication, he added some afterthoughts. It was about the similarity of his thoughts and circumstances with those of Charles Darwin. Ron found that he shared many of the attributes that Darwin singled out as important for his success and inserted a long Darwin quote at the end of our conversation. The last paragraph of this quote is reproduced here, which conveys its essence: "Therefore, my success, as a man of science, whatever this may have amounted to, has been determined, as far as I can judge, by complex and diversified mental qualities and conditions. Of these the most important have been – the love of science – unbounded patience in long reflecting over any subject – … and a fair share of invention as well as of common sense. With such moderate abilities as I possess it is truly surprising that I should have influenced … the beliefs of scientific men on some important points." (see [8], p. 10 in the magazine and p. 56 in the book, referring to the Appendix of the book *Darwin: A Life in Science* [10]).

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