ELSEVIER

Coordination Chemistry Reviews
197 (2000) 21–35

COORDINATION
CHEMISTRY
REVIEWS

www.elsevier.com/locate/ccr

Echoes of our VSEPRing

István Hargittai *

Institute of General and Analytical Chemistry of the Budapest Technical University and Structural Chemistry Research Group of the Hungarian Academy of Sciences at Eötvös University, H-1521 Budapest, Hungary

Received 26 February 1999; accepted 30 April 1999

Contents

Abstract 21
1. Pre-VSEPR times. 22
2. Enter Gillespie 23
3. The book 25
4. Ron's beginnings 26
5. Ingold's impact 27
6. The birth of VSEPR 29
7. Maturity of a model 30
8. Converging and diverging careers 31
9. In Darwin's footsteps 33
Acknowledgements 35
References 35

Abstract

The author's interest in understanding molecular structures brought him into very active interaction with Ronald Gillespie. This interaction culminated in a joint book in 1991, *The VSEPR Model of Molecular Geometry*. Segments of a recent interview by the author with Ronald Gillespie in *The Chemical Intelligencer* (1999, July) are presented along with the author's comments. It is suggested that comparison with two contemporaries, L.S. Bartell and G.A. Olah may be instructive in understanding Gillespie, whereas Gillespie himself reaches back to Charles Darwin for an intriguing parallel. © 2000 Elsevier Science S.A. All rights reserved.

Keywords: Science history; VSEPR model; Molecular structure; Contributions of R.J. Gillespie

---

* Tel.: +36-1-463-4051; fax: +36-1-463-4052.
E-mail address: hargittai.aak@chem.bme.hu (I. Hargittai)

PII: S0010-8545(99)00151-4

1. Pre-VSEPR times

I initiated our gas-phase electron diffraction molecular structure research in Budapest in 1965 when the technique was barely 35 years old. The literature was still full of structural information from the visual technique of gas-phase electron diffraction. My first two objects were sulfuryl chloride and thionyl chloride [1] to test our apparatus under construction and to possibly improve on the literature data on these two fundamental molecules. Had I been acquainted with the VSEPR model by then I would have jumped into the reinvestigation of the thionyl chloride structure even with more zest. A report from 1938 [2] gave 106 and 114 degrees for the bond angles O=S–Cl and Cl–S–Cl in clear violation of VSEPR predictions. The author of the original communication could not have been aware of the VSEPR rules in 1938, and, although I could have in 1965, alas, I was not.

In January 1969 I was headed from Budapest to Austin, Texas to join Otto Bastiansen who had started a Visiting Professorship there from the University of Oslo, at the Physics Department of the University of Texas. Almost at the last minute I got an invitation from Russel Bonham to make a stopover in Bloomington, Indiana and present a seminar there. Only later did I find out that the sponsor of my visit was the United States Air Force. At the time of writing this contribution, in 1999, Hungary is about to join NATO, so this is not so strange as it was back in 1969. I presented my first ever seminar in the United States at the Department of Chemistry of Indiana University. I talked about the structures of simple sulfur compounds and about their variations. There was some discussion and Russ suggested applying the VSEPR model to my systems. He gave me some literature and I spent half a night reading it and writing a long report about it to my wife and first graduate student, not only long-hand but illustrated with colored loops for the various electron pairs. I was a latecomer to the VSEPR model but it was a revelation for me.

Of course, the ideal first exposure to VSEPR is in introductory chemistry. However, we did not have it in freshman chemistry in 1959/60 at the Budapest University. Then, when I was preparing my Master's thesis at Moscow State University, the model would have come in handy, in hindsight. However, it was missing from the curriculum there too and was not even mentioned in our everyday discussions in the laboratory. The model makes much use of the concept of electronegativity, a largely qualitative but very useful concept. At that time (1964/65), however, electronegativity was very much in disfavor in official Soviet chemistry although not to the extent of the resonance controversy of the early fifties [3]. It was in sufficient disfavor though to make the VSEPR model nonexistent for us in the lab, in spite of the otherwise vigilant effort, on everybody's part, to keep abreast of the literature. Later the situation changed, and Russian editions of the two subsequent VSEPR books have appeared.

When having gotten acquainted with the VSEPR model it was obvious that my re-determination of the thionyl chloride structure was in complete agreement with the model and at variance with the previous determination, which, however, kept its place for many years to come in the literature. The reason was, obviously, that the early, 1938, paper appeared in the *Journal of the American Chemical Society* [2] and my report thirty years later in *Acta Chimica Hungarica* [1].

A four-walnut cluster representing a tetrahedral shape in the spirit of the VSEPR model (photo by I. Hargittai).

By the early 1970s I decided to write a popularizing article [4] about the model which had proved itself so useful to me. I collected the simplest possible examples, which should be the best for a popularizing article. To my amazement, exactly for some of these simplest examples, the model was failing. A simple improvement in some of its subrules, however, has put it back on its track, and eventually a detailed quantum chemical computational study confirmed my reasoning [5]. There has been a lively interaction back and forth between the VSEPR model and observations. The careful delineation of the scope of applicability of the VSEPR model helps keeping the model alive.

2. Enter Gillespie

Back in 1972, during the preparation of the popularizing Hungarian article, I started an interaction with the famous Ronald Gillespie. It was gratifying to me that he responded to my letter, took my worries seriously, and suggested to take it

Ronald J. Gillespie in 1998 (photo by I. Hargittai).

slowly, trying to figure out why the model broke down for apparently such a simple set of molecules. What was the problem? We expected that going from CF_4 to NF_3 and to OF_2, there would be a gradual decrease of the bond angles just as there is such a decrease in the set CH_4, NH_3, OH_2. However, this did not happen. The AX_4 to BX_3 change is unambiguous, going from four bonding pairs to three bonding pairs and one lone pair. The BX_3 to CX_2 change, however, is complicated. In CX_2 there are three different kinds of interaction, viz., bond/bond, bond/lone pair, and lone pair/lone pair, and the direction of the change of the bond angle as compared with BX_3 is not really predicted by the VSEPR model.

Although our correspondence did not resolve the discrepancy at that time, it brought me an invitation from Ron to present a seminar at McMaster University. This visit took place in 1974. Our next meeting then did not happen until after the publication of our co-authored book in 1991. Our second meeting was when Ron came to Budapest to join us in celebrating the 25th anniversary of our first gas-phase electron diffraction experiment.

3. The book

Writing the book, *The VSEPR Model of Molecular Geometry* [6], together with Ron was a unique experience for me. This was not my first book, but for the first time since many years I found myself in a junior position. I was pretty much used to work on my own, I did not even have a supervisor for my Ph.D. project. However, I still had a lot to learn and I can hardly imagine a gentler educator than Ron. All this was by mail, fax, and eventually by e-mail. It took us almost five years to complete the book. Ron was very democratic in that he was willing to listen to me and was never tired to explain me again and again something. His patience should not be mistaken for being stubborn but he was not one to give in easily. From him I learned that, especially for a textbook, every word, let alone a whole page or a section, is of great importance.

R.J. Gillespie and I. Hargittai in Austin, Texas in 1994 (by unknown photographer).

Also, during the joint writing of this book I came to understand how much Ron considers the VSEPR model his own child. Listing the limitations of applicability or sneaking in a section on the importance of non-bonded ligand–ligand interactions à 'la Larry Bartell would become a tour de force. No wonder then that when I am reading Ron's current papers on his recent conversion to the ideas of ligand–ligand interactions I can hardly believe my eyes. But I find this also to be the most beautiful example of the pragmatism of a great scientist. I am only afraid that in his new enthusiasm Ron's deep love toward VSEPR may diminish. I very much hope that this will not happen. There has been a longstanding concern by Ron that many may take the simplicity of the VSEPR model as a proof for it being unsophisticated. I have myself heard on many an occasion disparaging comments by theorists purists to this effect. Yet, to me the VSEPR model continues to be the most wonderful teaching aid and also a powerful research tool. Among the best examples I think of the distorted rather than regular octahedral geometry of XeF_6, the $OClF_3$ structure of C_s symmetry versus the OPF_3 structure of C_{3v} symmetry, and the PCl_2F_3 structure having C_{2v} symmetry rather than D_{3h} symmetry.

4. Ron's beginnings

Ron and I have met a few more times recently while both attending the Austin Symposia on Gas-Phase Molecular Structures, every other year. At the latest meeting I recorded a conversation with him that appeared in the July 1999 issue of the magazine, *The Chemical Intelligencer* [7], on the occasion of Ron's 75th anniversary. I appreciate the permission by the copyright holder Springer-Verlag New York to reproduce excerpts from this article. I also appreciate Ron's consent to use again this material in this form. I first asked Ron about his background.

> "I was born in 1924 in London. When I was eleven I was awarded a scholarship to the local grammar school. Although my parents did not have to pay fees, they did have to pay for school uniforms, sports clothing and train fares, which was difficult for them. I enjoyed school and did fairly well. During the term my performance was only average because I spent a lot of time playing sports, but I did well on the final exams, particularly in science. During the final two years we had to specialize in preparation for University. I chose to study chemistry, physics, pure math and applied math. I was never good at math, but by working hard I managed to do reasonably well. I did much better in both physics and chemistry, but the physics class was deadly boring because the teacher simply read the textbook. The chemistry teacher used the lessons to make chemistry much more exciting than the textbook and gave us a lot of interesting lab work. It was the chemistry teacher, George Cast, who inspired me to go into chemistry. He also inspired a classmate, William Moffit, who was really brilliant at math in school to also go into chemistry. He went to Oxford, worked with Coulson, and eventually became a professor of theoretical chemistry at Harvard but tragically died at an early age.
>
> "We were well into the war in 1942 when I passed the final examination at school and did well enough to be awarded a bursary to do a special two year war time degree in chemistry at University College London. We were evacuated to the University of Wales in Aberystwyth and that was where I spent my

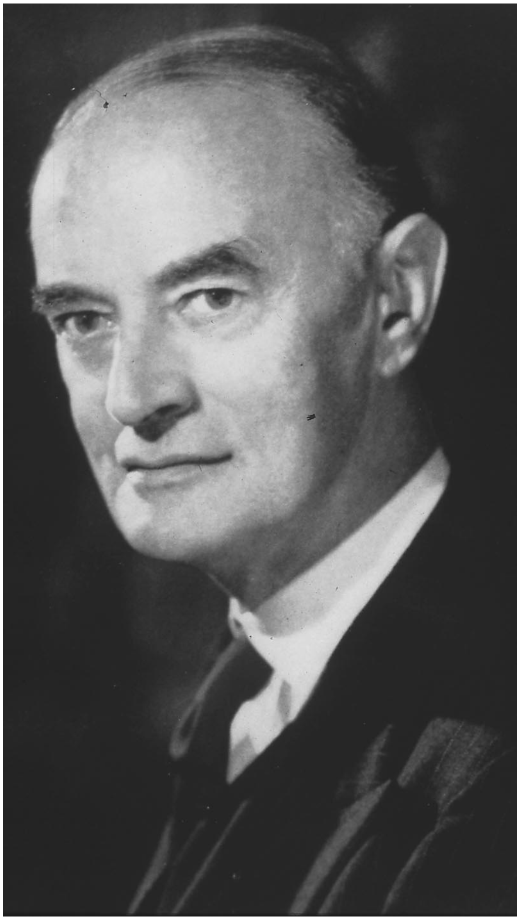
two undergraduate years. Towards the end of the second year, Ingold, the head of the department, said to me “You are going to stay and do research, aren’t you”. That summer (1944) the department moved back to London; it seemed that the war was coming to an end. Ingold had a team working on aromatic nitration. He put me on cryoscopy of nitric acid in sulfuric acid to look for the nitronium ion. Someone else (Jim Millen) was working on the Raman spectra of these solutions, and another student (Dan Goddard) was attempting to prepare stable salts of the nitronium ion, and there were others working on the kinetics of aromatic nitration. That’s how I got started on acids. After the nitronium ion I got intrigued with what else you could do in sulfuric acid.”

5. Ingold’s impact

Ingold’s name sounds very powerful to me. At least on one occasion, as editor of *The Chemical Intelligencer*, I received stern protests when another author had written disparaging remarks about him. He seems to have generated some controversy and must have had followers as well as he must have alienated others. I thought that being so close to him, Ron must be able to give us a close-up of Ingold. So it was only natural that I asked him about Ingold.

“I never really got to know him. Although he could be friendly in a formal way, he was a very remote person. For several years I was in awe of him. He would come around the lab about once a month, usually with Ted Hughes, for a short chat about what you were doing. That was almost the only time that you saw him except at the department research colloquia. He always had a good knowledge of what you were doing or should have been doing. We never talked about anything outside my research project. After I found the cryoscopic evidence for the nitronium, I made suggestions about other things that I might do. He always said, “OK, go ahead”. He let me do more or less what I wanted. I began to study the ionization of other solutes in sulfuric acid. That was the beginning of my studies of sulfuric acid and later of other superacids.

“Ingold published seven papers on my work in the *Journal of the Chemical Society* in 1950. All were written up by Ingold, but several of them carried my name only. He wrote the papers, gave the final version to me to read, but I didn’t dare to suggest any changes. He didn’t consider my area of research to be his main interest, which was in kinetics and reaction mechanisms. I suspect that if I had been working in that area I might have had less freedom. But, Ingold nevertheless had very wide interests. He was an organic chemist, a physical chemist and knew some inorganic chemistry.



C.K. Ingold (courtesy of William B. Jensen from the Oesper Collection in the History of Chemistry, University of Cincinnati).

> "I got my Ph.D in 1949, but before that, and it was typical Ingold, he came to me one day and said "I'd like you to give a few lectures. We need a course on molecular properties". That was it. A few weeks later I got a letter from the University saying that I had been appointed an Assistant Lecturer. I received no suggestions about the content of the course, but prepared a series of lectures on molecular geometry, dipole moments, the parachor, magnetism, etc. Thus I was already on the faculty before I got my Ph.D. I knew almost nothing of what was going on outside University College. I never considered any other university.
>
> "I continued with my research on sulfuric acid, now quite independently from Ingold. From time to time he sent a student to me. Ingold chose his students and allocated others to the faculty. I started to branch out, looking at the conductivity of solutions of other substances in sulfuric acid and measuring acidities. That's how I got interested in superacids.

> “In 1953 I got a Commonwealth Fund Fellowship to work in the US. I had the idea that sulfuric acid had a very high dielectric constant because the solutions seemed to behave in an almost ideal way. There was an expert (Robert Cole) in dielectric constants at Brown University, so I went there for a year. It was a difficult measurement because 100% sulfuric acid is very highly conducting because of its extensive self-dissociation. However, everything went well, though the dielectric constant wasn’t quite as high as I had thought, turning out to be 120.
>
> “The Commonwealth Fund Fellowship gave me sufficient money to buy a second hand car to tour the US and then write up my impressions of the States. My wife had stayed behind in Britain, but she came over for the summer and we toured and camped all around the U. S. and into Canada. It was then that I began to think that it might be a good idea to move to North America.
>
> “When I returned to University College I tried to further expand my research, but it was not easy. I wanted to use Raman spectroscopy, for example, but that was Jim Millen’s field. It was frustrating because everything had to be obtained through Ingold. I had no research money. If I wanted anything, I always had to go and ask him.”

6. The birth of VSEPR

It was at University College London, initiated by his teaching inorganic chemistry and his encounter with Ronald Nyholm that led to Ron’s pioneering work what eventually became the VSEPR model. This is what he told me about this.

> “Eventually I was fully into research and teaching in inorganic chemistry. Ron Nyholm, a newly appointed faculty member from Australia, also taught inorganic chemistry. I got to know him well and had many discussions with him. When I was teaching bonding I was never satisfied with the textbook explanations of bonding in terms of sp^3 hybrid orbitals. It seemed to me to be a circular argument. Then I came across a paper by Sidgwick and Powell who showed that geometry could be related to the number of electron pairs. I also found another paper by Lennard-Jones on the importance of the Pauli principle in determining geometry. By then I was also teaching quantum mechanics. I talked to Nyholm quite a lot and we decided to write a review on inorganic stereochemistry. I would do the main groups and he would do the transition metals. Writing this review I formulated the rules that later became the VSEPR model. Even in that article I pointed out that it was not just an electrostatic model but is based on the Pauli principle. But people did not think much about that; they just took the rules and used them widely, although it took fifteen years to get VSEPR into the US textbooks.”

Then came the move to Canada.

> “Soon after I decided it was time to move. There were a lot of us at University College who was quite dissatisfied at the time. People were moving. I was interested in Australia but my wife thought that it was too far away. I was also

> interested in Canada, possibly Vancouver or McMaster. Nyholm and I had decided that we needed an NMR, and we built a machine. It was tiny and not very useful so we decided to try to buy one. Nyholm was trying to get some money while I went to the States to talk to Varian. On the way back I visited McMaster. I knew Art Bourns, who was the Dean of Graduate Studies, from a period he had spent at UC. I knew rather little about McMaster, except that it was growing rapidly from a small Baptist college under Harry Thode, who envisioned it as a major research university. I soon had an offer from McMaster, which doubled my salary, and we decided to move. I went on the condition that I got a Raman spectrometer and an NMR. I went to Canada at a very good time. The National Research Council of Canada was awarding what seemed to me to be large grants. This was the first time I had my own research money. Peter Robinson came over with me as a post doc to help get research going.”

7. Maturity of a model

Since I thought that my bias for the VSEPR model may make me ignore other areas of Ron’s research, I decided to double check this point. Hence my question: Is it superacids and VSEPR that are your most important areas of research?

> “My research has been mainly in superacids, sulfuric acid, fluorosulfuric and hydrogen fluoride, which led me naturally into fluorine chemistry. I didn’t do a lot more on VSEPR except for trying to promote it. I was excited by the discovery of the noble gas compounds and it was an obvious opportunity to show that it was easy to use VSEPR to predict their structures. At one of the early conferences on noble gas chemistry Larry Bartell asked me to predict the structure of XeF_6. I believe he had already determined the structure by electron diffraction but not yet published it. I told him that it could not be octahedral, which the MO theorists believed they had proved, but was probably a distorted monocapped octahedron which turned out to be correct. Since then he has been a great fan of VSEPR and has done much to promote it as a useful theory.”

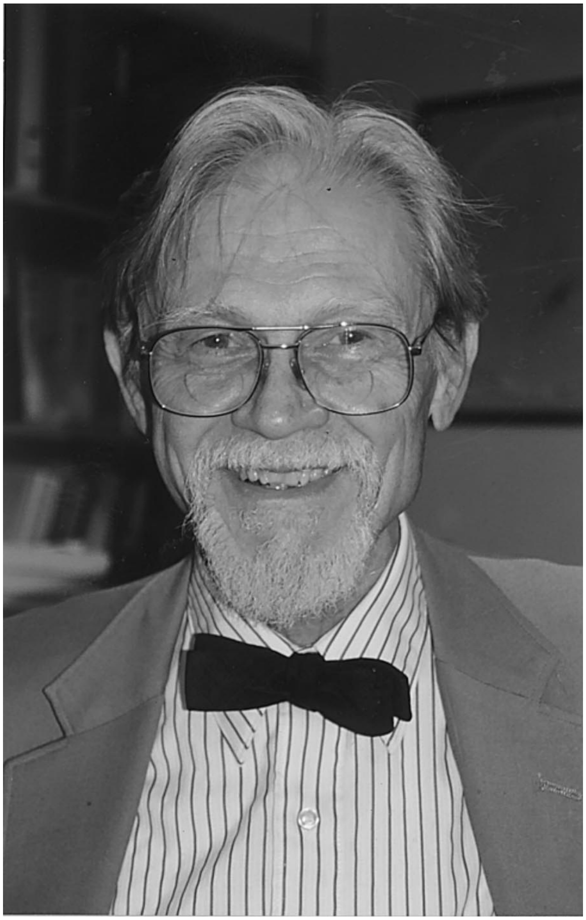
Remembering Ron’s continuous search for a quantum mechanical justification for the VSEPR model, I posed the following, somewhat provocative question to him: Is it true that you almost have been embarrassed by the simplicity of the VSEPR model?

> “I would not say that I was embarrassed by its simplicity but I was trying to improve it mainly to try to account for the exceptions which have always challenged me. One of my colleagues, Richard Bader, originally did not believe in the VSEPR model because he had shown that electrons are not as localized as the model claims. It was not until he began to study the Laplacian of the electron density in the mid 1980’s that he was converted to VSEPR. He had a student, Preston MacDougall, who found that the Laplacian of the electron density provides strong support for the model. This is how I got interested in Bader’s work. About this time in 1989 I officially retired. I planned to continue my

research but my funding from NSERC (the Natural Sciences and Engineering Research Council) for my experimental program stopped. However, I had already decided that I wanted a change so this was the opportunity to finally do some real research on VSEPR. In collaboration with Richard Bader and Peter Robinson, I began to look at the apparent exceptions and more deeply at the physical basis of the model. Now I have a small grant from NSERC to work on transition metal molecules.''

8. Converging and diverging careers

The total time of my personal encounters with Ron is very little, less than a total of two weeks. Sometimes I think of Ron as if I knew him very well, other times he is an enigma to me. Thus, somehow I find comparing Ron with other two great scientists helpful.



Lawrence S. Bartell in 1998 (photo courtesy of Magdolna Hargittai).

Ron Gillespie and Larry Bartell have an almost anti-symmetric relationship in their interests and careers. Both have been interested in molecular structure. Larry dispersed his magnificent ideas around, sometimes appearing more interested in satisfying his own curiosity than converting his colleagues and creating a large number of followers. At least in the field of molecular structure, Ron had stuck to the VSEPR model for a long time and had played a most effective role in popularizing the model. Larry initiated the considerations for non-bonded interactions and introduced the intramolecular van der Waals radii, wrote a citation classic paper on them for the *Journal of Chemical Education* [8], but expressed hardly any interest in other people applying his ideas. He did not seem to mind when they did not and he seemed not to care either when they did. Ron, on the contrary, did not miss an opportunity to popularize his model and his was a most effective way of doing so. The anti-symmetric relationship between Ron and Larry has been enriched with yet another aspect. Curiously, lately, Ron and Larry seem to be changing roles in that Larry is forcefully singing the praise of VSEPR considerations whereas Ron advocates the importance of ligand–ligand interactions as if VSEPR considerations had hardly existed. Of course, I know I am oversimplifying all this in my eagerness to get my point through, but I find this comparison interesting.

There is then the possibility of another comparison, between Ron Gillespie and George Olah. There are some similarities, however far-fetched, between their careers. Both started in good schools, Gillespie at University College London under Christopher Ingold and Olah at Budapest Technical University under Geza Zemplen. At some point both converged in Canada. By then George had made an independent career in Budapest rising to a leading position in a research institute of the Hungarian Academy of Sciences in addition to his university post. In contrast, before leaving for Canada, Ron had still been under Ingold with very little say even in his own affairs. George arrived in Canada as a refugee, starting everything anew, and not even in academia, whereas Ron got a coveted position to which he was lured away from London. It was Canada and the research area of superacids where their careers did cross directly. Ron had an early advantage in superacids compared with George, but somehow it seems to have melted when compared with the fruits of George's bold initiatives. It is most telling what Ron told me after I posed the following rather provocative question to him in the interview: "I remember George Olah writing in a Preface to one of his books, expressing his admiration to your seminal and fundamental work on superacids. Eventually he got the Nobel Prize but you didn't."

> "I can understand why. He exploited superacids in organic chemistry to an enormous extent. I was never very interested in organic chemistry and I stuck to inorganic chemistry. But going back in history, I should tell you that I first met George when he spent a very short time at UCL after he left Hungary as a refugee. Then I moved to Canada and he did also work at Dow in Sarnia. At that time I had the only NMR spectrometer in Canada and George sent his technician from Sarnia to obtain spectra of his samples on our machine. I must

say that these samples often looked like black gunk. If my students got anything that sort of color I sent them back to the bench.. In those black solutions George found the trimethyl carbonium ion. I was too insistent on purity and perhaps I shouldn't have been. One could say I missed an opportunity, but I always had in the back of my mind similar looking solutions in sulfuric acid that we had prepared which did not give any useful results. Although I did most of the first experiments showing how to make superacids and measuring their acidity, George thoroughly exploited superacids in organic chemistry."

George A. Olah in 1995 (photo by I. Hargittai).

9. In Darwin's footsteps

As is customary with my interviews for *The Chemical Intelligencer*, I usually have a follow-up interaction with the interviewee even when I do not have the kind of close relationship with him (or her) as I have with Ron. It is not only that the interviewees are given the opportunity to check and correct what they had said but they may also want to augment the conversation. This is also what happened in Ron's case. Hence these "Afterthoughts" by Ron Gillespie:

> "Giving this interview got me reflecting on what I had contributed to chemistry and how it was that I had done reasonably well. At the time I had just finished reading "Darwin, A Life in Science" by John Gribbin and Michael White. At the end of this book there is an Appendix which quotes what Darwin wrote about himself in his autobiography. I was struck by the fact that much of what he wrote I could have written about myself although not in the same elegant, if rather ponderous, Victorian English. It seemed to be of interest therefore to quote some of what Darwin wrote about himself even if comparing oneself to Darwin might appear somewhat pretentious. The attributes that contribute to success are many and varied but I was quite surprised to find that I shared many of these attributes with Darwin as I am sure many other scientists do. This is not to say, of course, that quite different qualities might not be important for others, but it seems that for a certain type of researcher, the qualities that Darwin possessed are important for success. Darwin wrote:
>
>> 'I have no great quickness of apprehension or wit which is so evident in some clever men,… I am therefore a poor critic: a paper or book when first read excites my admiration, and it is only after considerable reflection that I perceive the weak points. My power to follow a long and purely abstract train of thought is limited: I should moreover never have succeeded with … mathematics. My memory is extensive yet hazy: it suffices to make me cautious by vaguely telling me that I have observed or read something opposed to the conclusion which I am drawing, or on the other hand is in favor of it; and after a time I can generally recollect where to search for my authority. So poor, in one sense, is my memory, that I have never been able to remember for more than few days a single date or a line of poetry (or a humorous story RG).
>>
>> '… my love of natural science has been steady and ardent. This pure love however, has been much aided by the ambition to be esteemed by my fellow naturalists (chemists RG). From my early youth I have had the strongest desire to understand or explain whatever I observed, that is, to group all facts under some general laws. These causes combined have given me the patience to reflect or ponder for any number years over any unexplained problems. As far as I can judge I am not apt to follow blindly the lead of other men. I have steadily endeavored to keep my mind free, so as to give up any hypothesis, however much beloved, as soon as facts are shown to be opposed to it. On the other hand I am not very sceptical, – a frame of mind which I believe to be injurious to the progress of science.
>>
>> '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 posses it is truly surprising that I should have influenced … the beliefs of scientific men on some important points.'
>
> "Darwin also noted that he had 'had ample leisure from not having to earn my own bread.' By this I think he meant he had plenty of time to pursue what interested him, because for Darwin, as for many other scientists, it is often difficult to distinguish work from leisure. The 'gentleman scientist' of the Victorian era has disappeared today but as a privileged academic, and even before as a graduate student, I have been lucky enough almost my whole life to have been able to do, very largely, just what interests me – clearly another important factor in contributing to success in science as Darwin recognized."

Acknowledgements

I am grateful to Ron Gillespie for having created the VSEPR model and having made it known in broad circles so that it reached me in time to fully appreciate its benefits. I am also grateful to him for being accessible and frank in our interactions. And I am grateful to him for his exemplary love of and dedication to structural chemistry. I also appreciate Barry Lever's urging me to prepare this rather unorthodox contribution and Magdi Hargittai's constructive criticism. Our research is being supported by the Hungarian Ministry of Education (FKFP 0364/1999) and by the Hungarian National Scientific Research Foundation (OTKA 030053).

References

[1] I. Hargittai, Acta Chim. Hung. 60 (1969) 231.
[2] K.J. Palmer, J. Am. Chem. Soc. 60 (1938) 2360.
[3] I. Hargittai, Chem. Intell. 1 (1) (1995) 34.
[4] I. Hargittai, Természet Világa 104 (1973) 78.
[5] A. Schmiedekamp, D.W.J. Cruickshank, S. Skaarup, P. Pulay, I. Hargittai, J.E. Boggs, J. Am. Chem. Soc. 101 (1979) 2002.
[6] R.J. Gillespie, I. Hargittai, The VSEPR Model of Molecular Geometry, Allyn and Bacon, Boston, 1991; Russian translation, Mir: Moscow, 1992; Italian translation, Zanichelli: Bologna, 1994.
[7] I. Hargittai, Chem. Intell. 5 (3) (1999) 6.
[8] L.S. Bartell, J. Chem. Educ. 45 (1968) 754.