The Bright Side of Mathematical Chemistry

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The personal history of the present author's research career of almost forty-five years in the application of graph theory to chemistry is briefly described in an essay with particular reference to the author's "bright side of mathematical chemistry." The chosen topics are as follows: two seminal papers by the present author, more than 1500 citations of his topological index, \( Z \), Hosoya polynomial, Hosoya items, more than 200 papers carrying "Hosoya" in the title, Erdös number, etc.

Keywords: Topological index, Hosoya index, Hosoya polynomial, Hosoya items, Mathematical chemistry, Conjecture

1 Introduction

My research experience in mathematical chemistry has been continuing at least for 45 years, and now the atmosphere around me has rather changed but still not to my satisfaction. The biggest change is that nowadays nobody can mutter that I got mad as was suspected by my former boss, but only whisper they still don't fully understand my mathematics. It is because, in my opinion, chemists at large have lost their energy to strive to understand mathematical thinking, or they might have been caught in their own trap that they are unable to understand even elementary mathematics.

I think that my academic career of being a mathematical chemist was a precious gift to myself by which I could learn and realize the deep mathematical structure of chemistry and chemical thinking in the middle of natural science. In the global history of chemical and physical science many important findings obtained by us cannot be denied by the whole community of scientists including our hostile and ignorant enemies. All the stones aimed at and thrown at us have been crushed down or buried in the garbage.

On the other hand, one cannot forget our awkwardness in the averaged quality of the papers in mathematical chemistry. I dare hesitantly point out such a large number of various "topological indices," [1] which as a matter of fact are my headache rather than a kind of pride. I don't think that "the more the better" does not necessarily rule science.

In 2002 I wrote an essay "The topological index \( Z \), before and after 1971," [2] in which I wrote several incidents in the "dark side of graph-theoretical work." It is interesting to observe that this essay has been cited more than thirty times according to Google Scholar. In a recently published book by Randic [3] several examples of the hostility to the papers and/or authors of mathematical chemistry, specifically of chemical graph theory, are vividly documented and murmured. Those who are joining our club must have been involved in similar experiences more than once. However, here I will disclose quite opposite instances, so to speak, of the bright side of mathematical chemistry, mainly limited to my atmosphere, in order to encourage younger mathematical chemists.

2 Seminal papers

Happily I know that two of my papers are honored to be called seminal papers by several groups of people, one on the proposal of my \( Z \)-index, or Hosoya index [1], and the other on the Wiener polynomial, or Hosoya polynomial (vide infra) [4]. Later on let me call these items HI and HP, respectively.
3 Citations

I don't know the reason why, but according to Google Scholar my first HI paper was cited more than 1500 times up to the end of 2016, and this paper published 45 years ago is still being cited by the speed of about one hundred times per year. Although detailed analytical data are not available, nowadays so many mathematicians and information scientists outside of Japan seem to be citing my first HI paper.

The title of the HP paper is "On some counting polynomials in chemistry" [4] published in Discrete Applied Mathematics in 1988, which was cited around 280 times mainly by mathematicians.

4 H-paper

The reason why the main "citers" of HP paper are mathematicians is deduced from the following list which was recently prepared by myself, but, unfortunately, cannot be given here owing to its big size. It is the "List of papers carrying 'Hosoya' in the title." Here let us call such paper "H-paper." During 1980's my good friend Ivan Gutman wrote more than ten H-papers flourishing the opening part of this list, and above all he has kindly contributed in total more than 25 H-papers! Moreover he has written 14 joint papers with me since 1975. I don't know why but the publishing rate of H-paper rapidly began to increase from 2007 at the pace of 10 ~ 20/year, and at the end of 2016 the number of H-papers went up almost to 200, although the list is inevitably incomplete. As the journal base MATCH contributes 40 papers, J. Math. Chem. 13, Croat. Chem. Acta 9, Discrete Appld. Math. 8, followed by Z. Naturforsch., etc., and so many different kinds of mathematics journals and archives. Then in total almost half of H-papers are estimated to have been written by pure mathematicians, and the other half by mathematical chemists.

5 Hosoya items

All the 200 H-papers are found to carry at least one of the "Hosoya items," namely, Hosoya index (a little less than 2/3 of the list), Hosoya polynomial (~1/3), and Hosoya something (~10%), which includes, triangle, matrix, conjecture, operator, cube, point, theorem, descriptor, entropy, and mystery! The interested readers can easily follow these items through Internet. Out of these Hosoya items it is not necessary to explain Hosoya index any more, and here only polynomial and entropy are selected and will be explained.

6 Hosoya polynomial

In the list of H-papers "Hosoya Polynomial" appeared first in 1999 by the joint work of four authors including Gutman [5], who proposed to call my Wiener polynomial the Hosoya polynomial. He is a good propagandist not only for my HP but also for all kinds of my graph-theoretical work, and I deeply acknowledge him. In 1999 he wrote three more HP papers consecutively, which might have triggered pure mathematicians and mathematical chemists in many countries including Iraq, Iran, and China. Up to now nearly 70 H-papers carry HP in the title.

7 Theses and Books

While I was preparing this list of H-paper I happened to know that in 2011 Iraqi mathematicians wrote two books on Hosoya polynomial [6,7], and further, in Iraq two people wrote their Ph.D. theses, one on Wiener and one on Hosoya polynomials (essentially the same thing), and at least three other people wrote their M.Sc. theses on Wiener polynomial. Now it is evident that my HP is one of the big targets among the graph theoretical mathematicians in Iraq. However, curiously enough until today I haven't received any correspondence from them.

8 Invitation

On the contrary, Iranian mathematicians are very kind to have invited me (by entirely covering) to attend The First Iranian Conference on Chemical Graph Theory (FICCGT 2010) [8] held in Tehran with the late Graovac, together with other two Croatian chemists and one Chinese mathematician. There we could enjoy exotic experiences in Persia, and learned that almost eighty per cent of Iranian university students are women. Moreover, in this year they asked me to write a paper for a special issue of Journal of Mathematical NanoScience to be dedicated to me, and I have just sent my MS to them. Also very recently in Japan I was invited to give a lecture on my Z-index by the departments of mathematics of universities.
in Kyoto, Hiroshima, and Fukuoka, and also by several small meetings of mathematicians, as they got interested in my book, "Topological Index—New Mathematics Bridging from Fibonacci Numbers to Pythagorean Triangle—", published by Nihon Hyoronsha, Tokyo (2012) but in Nihongo (native language in Japan) [9]. I wanted to let the mathematicians in Japan know my Z-index, as I already had some confidence in the abroad popularity of my theory. Then by excluding almost all chemical discussions I tried to write a mathematics monograph on my Z-index, and I think I have done a good job. In what follows, I would like to introduce several examples of the internationally good reputation obtained for my work in various areas.

9 Intel contest

The world famous Intel, a leading electronic technology company, is annually holding a programming contest, Intel Threading Challenge. The theme chosen in 2010 was: Parallel computation of Hosoya index [10]. As I am not deeply involved in programming, I cannot give any technical comment on its results, but this actually happened, meaning that my Z-index and also its computational difficulty has already been known to mathematicians and computer scientists. Actually the fact that my Z-index is NP-complete to compute has already been introduced in the columns of "topological index" in Wikipedia and MathWorld.

10 Erdős number

Among certain kinds of mathematicians especially involved in number and graph theories the Erdős number is a kind of honor indicative of his or her academic distance to famous wandering mathematician Paul Erdős. I can confidently declare that my Erdős number is 2 through the two great mediators, Ronald Graham and Frank Harary. Namely, I have written joint papers with them in 1977 [11] and 1993 [12], respectively. Actually I hauled up the two big fishes by myself. As early as 1973 I wrote a paper in a domestic journal, Natural Science Report of Ochanomizu University, to propose the distance polynomial (DP) just by substituting the distance matrix for adjacency matrix in the characteristic polynomial [13], luckily which was soon after abstracted in Mathematical Review. Although we found many theorems on this new polynomial, the most interesting one had to be left as a conjecture which had been assured by a heap volume of calculated results. Quite independently Graham read a paper on the same definition of DP in a meeting of AMS, but was told by an audience that it had already been abstracted in MR. Soon after this he came to Japan and visited my laboratory and discussed very eagerly with me.

The result was that the team of able and experienced mathematicians could give a proof of my conjecture and submitted our joint paper [11] to the first issue of J. Graph Theory in 1977, founded by Harary.

What a coincidence it is. One year before I visited Ann Arbor, Michigan, and got acquainted with him. The joint paper with him [12] was published more than a decade after that, but he had given me a hint to apply the matching polynomial and Z-index to some unexplored kinds of graphs. This means that Harary, the authority of graph theory, realized the essence of my work in mathematical chemistry.

11 Hosoya entropy

Mowshowitz is a renowned professor of computer science in City College of New York and has written several books related to the concept of entropy. In 2015 he wrote a paper, "The Hosoya entropy of a graph" with Dehmer, a German professor of biomedical information [14]. They got a hint from my HP and defined the partial Hosoya polynomial and further Hosoya entropy for discussing quantitative measure of graph complexity. Details of his paper are not introduced here, but the readers can see full Hosoya items in this paper, for example, Hosoya-equivalent, Hosoya profile, and Hosoya graph decomposition. The journal "Entropy" carrying this paper is an international and interdisciplinary journal of entropy and information studies. I myself have not yet fully understood the essence of their paper, but found so many mathematical chemists in the references, e.g., Bonchev, Todeschini, Balasubramanian, Wiener, Doslic, Gutman, etc. Let us toast the efforts and achievements accomplished by we mathematical chemists.

While I was surfing over Internet to learn more about Mowshowitz, a destined but virtual encounter with him was found. He received his Ph.D. in computer science from University of Michigan in 1967, possibly in Autumn, just when I was staying in Ann Arbor as a postdoc for John Platt, who was the only researcher appreciating the pioneering work of Harold Wiener.
However, at that time Platt and I were doing vision research as biophysicists, and I was a pre-graph theorist. On the other hand, in 2013 Aurues (an amateur scientist in Japan, pronounced as o-ryuh) wrote a very interesting paper "The Fibonacci sequences in nature implies thermodynamic maximum entropy," [15] in which he writes that my $Z$-index might provide the maximum entropy values of molecular surface electrons. Actually I already knew that in QSAR study very good correlation was found between my $Z$-index of tree graphs and not only the boiling point but also the entropy of saturated hydrocarbons [16].

12 Kekulé, Hückel, Hosoya

This is not a Hosoya item, but the most astonishing powerpoint Figure I ever saw is a lecture note of Makowsky, a computer scientist in Israel but giving lectures for EMCL (Engineering Mathematics and Computing Lab) in Heidelberg. In one of his lectures, [17] "Some applications of graph polynomials in chemistry," he introduces three "pioneers of structural chemistry," August Kekulé (1829–1896), Erich Hückel (1896–1980), and Haruo Hosoya (1936–), with their photographs but with no other explanation.

With all these instances I honestly admit that the mathematical structure of my HP and HI originated from a mathematical chemist is well admitted by and rooted in the world of mathematics and computer sciences (See also [18]).

For other Hosoya items the interested readers can easily get access to them through Internet.

13 How to fight and how to win

In concluding this essay I would like to point out three big elements for fighting and winning the war against your enemy no matter what hostility to you it has.

1) Good conjectures with
2) Firm mathematical structure durable for whatever logical attack, and
3) Good friends to become your propagandists like Gutman and Balaban for me.

At least with the first two weapons in your hands, walk into the center of your enemy or opponent. In my case in 1973 I walked into the headquarters of Boskovic Institute in Zagreb headed by Nenad Trinajstic, and I could get acquainted with Ivan Gutman who was about to write his Ph.D. thesis.

Finally I must add one sad thing about Shinsaku Fujita, who is Fighting against the conventional structural organic chemistry from the definition of chirality including its naming system to the enumeration algorithm invented by Polyá, and finally he could almost construct "Fujita’s world," [19] by publishing a series of monographs on this matter [20,21]. At present there cannot be found either of any competing enemies or comrades to polish up his work, not only in organic chemists, of course, but also in mathematicians. Able young mathematical chemists, please, help this lonely king.

References