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The Topological Index *Z* Before and After 1971

Haruo Hosoya

Ochanomizu University, Bunkyo–ku, Tokyo 112–8610, Japan

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The Topological Index *Z* Before and After 1971

Haruo Hosoya[#,*]

Ochanomizu University, Bunkyo–ku, Tokyo 112–8610, Japan

Abstract
The author's first paper on the topological index *Z* was published in *Bull. Chem. Soc. Jpn.* in 1971, where good correlation was found between the boiling points of alkane isomers and their *Z* values. This idea is based on the author's unpublished work performed in 1957, when the boiling points of octane isomers were predicted by scrutinizing the structural dependency of boiling points of alkanes up to heptane. Behind stories inside and outside of the country before and after the birth of *Z* index are introduced. Several academic encounters of the author and reactions of the contemporary chemists to the new idea are also described. In the end some aspects of QSAR problems for octane isomers are introduced.

Keywords. Graph theory; topological index; characteristic polynomial; alkane isomer; boiling point; mathematical chemistry.

1 INTRODUCTION

The first paper on my topological index *Z* was published in September of 1971 in the Bulletin of the Chemical Society of Japan (BCSJ) [1]. Since then nearly four hundred papers have cited it during three decades. Even when every detail of my memory on my favorite paper and its relevant events and rumors are beginning to fade out, I enjoy the observation that currently twenty to thirty papers per year are still citing my original work. Some of the authors [2] claim that the term "topological index" was first coined by myself followed by more than two hundred different topological indices proposed by the group of mathematical chemists scattered worldwide, and therefore the topological index has become the general name for the gigantically enlarged family of molecular graph descriptors.

Now I recall the birth pain which I experienced at each publication in the series of the *Z*–papers and also my awkward analysis of the structural dependency of the boiling point of alkane isomers, which was performed already in 1957. At that time I was an undergraduate third–year student.

[#] Emeritus professor at the Ochanomizu University.
[*] Correspondence author; fax: +81–48–267–9432; E–mail: hosoya@is.ocha.ac.jp.

In this short paper I would like to introduce how the idea of the *Z* index has evolved and also how conservative professors tried to repel new and strange ideas and intruders from their self–perceived closed territory. In the end an interesting byproduct on the QSAR study of octane isomers will be introduced, which was found out while I was writing this manuscript.

2 BIRTH OF Z INDEX

In April first, 1969, at the age of 32 I became associate professor of chemistry of Ochanomizu University in Tokyo, after returning from one year of postdoctoral experience in John Platt's laboratory, Ann Arbor, Michigan, where I was a biophysicist struggling with the eye balls of rats to measure electrical response to photochemical reactions in retina. Before visiting the U.S., I had obtained my PhD at Saburo Nagakura's laboratory, Institute for Solid State Physics, University of Tokyo with the title "Study on the Structure of Reactive Intermediates and Reaction Mechanism" mainly by measuring and calculating the electronic spectra of organic molecules with conjugated π–electronic systems. At that time only selected postdoctoral fellows could try to perform *ab initio* calculations in the Mulliken–Roothaan group, in Chicago. However, Nagakura's laboratory was one of the largest groups in the world performing semi–empirical calculations, such as PPP and "molecules in molecules."

Figure 1. My note (June 2, 1957) describing the prediction of the boiling point of octane isomers. One can read the sentence at the right bottom as "Agreement is good."

I was thinking and thinking what can be done for a lonely wolf in a poor university with only lady undergraduate and master course students. I did not either want to sharpen my awkward biophysical technique, nor to construct a laboratory of physical chemistry like a miniature of that of my former boss. Before long I recalled and found an old bundle of memos and diagrams, which were worked out by myself twelve years earlier (Figure 1).

2.1 My First QSAR Study

When I was a third–year student of chemistry in University of Tokyo, I happened to come across a table of the boiling points of alkanes up to heptanes and was fascinated by several interesting relations between the structure and boiling point (*bp*) of these hydrocarbon molecules. The *bp* values of a given series increase with the number of carbon atoms, while branching always lowers *bp*. Although the decrement depends on the size of molecules, one can trace its smooth variation with the size. The effect of lowering by 2,2–dimethyl substitution is much more larger than the double of 2–methyl substitution, and so on. Then by drawing a cross–diagram of *bp* values as in Figure 2 one can estimate all the decrements of *bp* of seventeen isomers relative to *n*–octane.
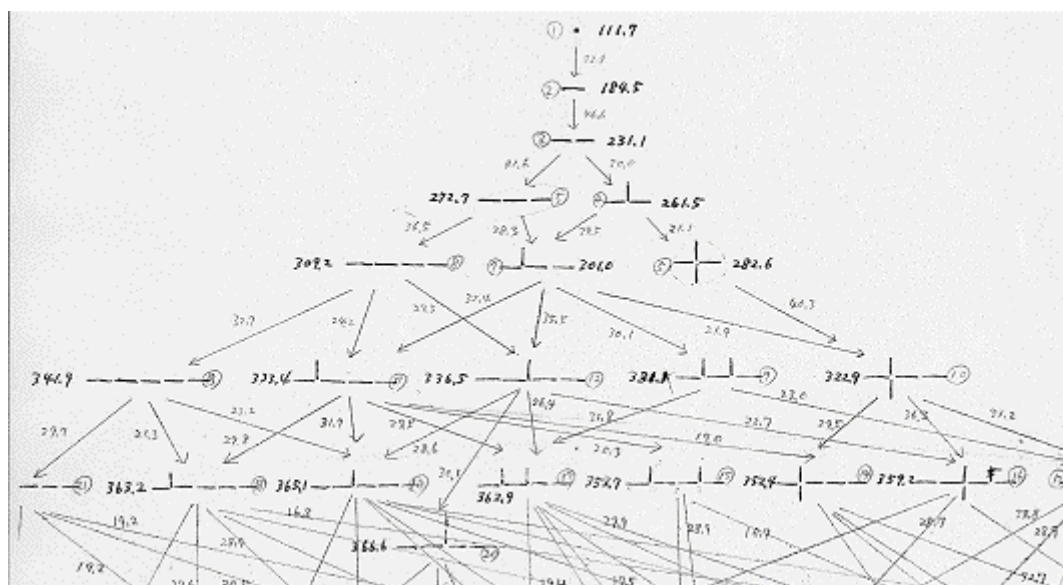

Figure 2. Cross–diagram showing the change of *bp* values of alkanes (not the original but reproduced later).

Many of the octane isomers have a few different ancestors. For example, 3–methylheptane may be deemed either as the next higher member of 3–methylhexane by tail elongation, 2–methylhexane by head elongation, or *n*–heptane by 3–methyl substitution. All the increments in *bp* from heptane to octane for these series were estimated from the cross–diagram of all the alkane isomers up to heptanes. Then these *bp* values obtained from different series were averaged to give the most plausible *bp* value of the isomer concerned.

After finishing up this study I found a table of the observed *bp* data in the Iwanami Dictionary of

Physics and Chemistry [3], whose page is copied in Figure 3, where melting point, liquid density, and refractive index are also tabulated. I was excited at the good agreement between the observed and estimated values (see Figure 4).

Figure 3. Copy of Iwanami Dictionary of Physics and Chemistry [3], "octane" and "octane number". There are three misprints. 1) *bp* of 2,2,3–trimethylpentane should be 110.3˚C. 2) *mp* of 2,2,3,3–tetramethylbutane should be + 101˚C instead of –101˚C. 3) liquid density of 4–methylheptane (0.7163) may be mistype of 0.7063.

Most of the estimated *bp*'s were lying within ±4˚C range of the observed ones. This is a rather good correlation for the whole group of octane isomers whose *bp*'s are scattered in the range of 20˚C, and the ρ value was 0.942. This was my first achievement in QSAR study, although I had no

idea about QSAR nor graph theory at that time, when even in the community of chemistry researchers QSAR and QSPR had not yet gained their current identity. It was in the midsummer of 1957, and my 21st birthday was approaching and as a mere student of chemistry I did not know what I should do next. Naturally I never thought of its publication in a chemistry journal but wrote a brief note with diagrams for myself and sealed it at a corner of my bookshelf as my personal and precious secret.
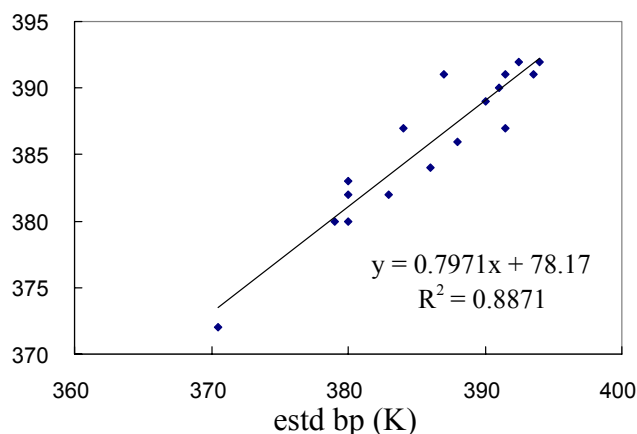
Figure 4. Observed and estimated *bp*'s of octane isomers (1957).

Very recently I learned that Harry Wiener found his *W* index at the age of 20 and wrote the pioneering paper in JACS in 1947 [4,5]. Moreover, he developed and strengthened his theory by applying it to many other thermodynamic properties, such as liquid density and refractive index, by combining with another index *p*, the polarity number. Now I am filled with special feelings and emotions by supposing what may have happened if I had continued to play with the other physico–chemical data in Figure 3, which actually contains three big misprints but they give big hints for further study. The story will be continued in this paper.

2.2 The Z Index and the Characteristic Polynomial

Twelve years have passed since my first discovery in QSAR study, and I had grown up as a kind of number crunching chemist trained by a huge pile of semi–empirical MO calculations. Then after finding out my own old memo on the alkane boiling points, my first trial was to apply the Hückel method to all the isomers of alkanes but not in an ordinary way. Namely, instead of solving the solution of the characteristic polynomial (CP) of the molecular graph representing the topological structure of the carbon atom skeleton of the alkane isomers, I become interested in the coefficients of the characteristic polynomial.

Namely, there seemed to be some hidden regularities between the set of the coefficients, $\{a_k\}$, of

CP and the structure of alkane isomers. It was soon found that each entry of $\{a_k\}$ of a given isomer never exceeded the corresponding value of the normal alkane, or the path graph. This inclination was just what had been observed twelve years ago in the correlation study of alkane *bp*. The *Z* index was thus rather naturally defined as the sum of the absolute values of the a_k's, namely,

$$Z = \sum_{k=0}^{N} |a_k|$$

and amazingly it showed beautiful correlation with *bp* among the set of isomers [1]. Many other chemical problems were found to be relevant to *Z*, but they will not be repeated here.

From this finding the direction to my interest was turned by 180 degree from number crunching calculation to discrete mathematics. By that time I had never read a book on graph theory, and I didn't even remember the name of the famous Fibonacci numbers. However, after I got involved in the application of the graph theory I am accustomed to telling my colleagues about God: "When I was doing semi–empirical MO calculations, I thought that God did not know mathematics, but now I am convinced that God really does know mathematics."

The *Z* index is formally defined in terms of the non–adjacent number, p(G.*k*), as the number of ways for choosing *k* disjoint edges from a given graph G. Further, I could find the following relation for a tree graph, or an acyclic hydrocarbon molecule with *N* carbon atoms [1],

$$P_G(x) = (-1)^N \det(\mathbf{A} - x\mathbf{E}) = \sum_{k=0}^{N} a_k x^{N-k} = \sum_{k=0}^{[N/2]} (-1)^k p(G,k) x^{N-2k} \tag{1}$$

where **A** and **E** are the adjacency matrix and unit matrix, respectively. Now without decomposing the secular determinant one can quite easily obtain the CP of a given tree graph.

Even Coulson had difficulty in his attempt to formulate the CP in terms of the ring contribution for non–tree graphs [6]. In France several people were trying to establish the "polygon method" for this problem, but the result was not complete [7,8]. Nagata and Fukui also studied this problem but did not obtain a publication [9]. Despite all these unsuccessful trials, Sachs succeeded in deriving a very neat expression for the coefficients of CP of any graph [10], and the Zagreb group was enthusiastically recommending his theory to theoretical chemists [11].

I was very lucky because in the beginning of this study I considered mainly tree graphs, or acyclic hydrocarbon molecules [12], and the relation (1) was confirmed. Then by the help of the two able masters course students, Keiko Kawasaki and Kimiko Mizutani, CP's, p(G,*k*) numbers, and the *Z* indices of small monocyclic and bicyclic graphs were extensively calculated [13] and the deviation from Eq. (1) was thoroughly checked out. For those simpler graphs the correction terms were found to be rather simple and tractable [12,13]. Then I could reach a general expression for the CP in terms of my p(G,*k*) numbers for the original and the set of its subgraphs [14]. This paper was published in Theoretica Chimica Acta (TCA) in 1972, which eventually triggered vigorous research

by the Zagreb group [11].

$$
\begin{aligned}
P_G(x) = &\sum_{k=0}^{m} (-1)^k p(G,k) x^{N-2k} \\
&- 2 \sum_{i}^{G} \sum_{k=0}^{m_i} (-1)^{k+n_i} p(G \ominus R_i, k) x^{N-n_i-2k} \\
&- 2^2 \sum_{i>j}^{G} \sum_{k=0}^{m_i} (-1)^{k+n_i+n_j} p(G \ominus R_i \ominus R_j, k) x^{N-n_i-n_j-2k} - \cdots
\end{aligned}
\tag{2}
$$

In this expression $G \ominus R_i$ stands for a subgraph of G obtained by deleting ring R_i together with all the edges incident to R_i, where the notation $\ominus$ has been proposed by myself [15].

2.3 Near–Miss at Ann Arbor

As has already been mentioned, I worked as a postdoctoral fellow in the laboratory of John Platt. He is famous in mathematical chemistry as the only person who immediately realized the importance of Wiener's pioneering work and wrote papers analyzing and interpreting the physical meaning of the W and p indices [16]. But in quantum chemistry he had already written many milestone papers and monographs on the free–electron model, classification and nomenclature of UV spectra of benzenoid hydrocarbons, and this was frequently deemed his significant work.

The reason why I chose Platt's laboratory for my postdoctoral work was that we had already met in Tokyo, where the International Conference on Molecular Spectra and Structure was held in 1962, and I was fascinated by his penetrative and attractive personality. At that time he was still working in Mulliken's laboratory with Ruedenberg and Roothaan, and later changed his field into biophysics. He was also one of the key members of the Club of Rome, which was warning against such many critical problems, such as population increase, food shortages, traffic, pollution, diseases, etc., that are threatening the future life of the mankind which is forced to live on the earth of a finite size with finite resources.

Besides his research interest and knowledge John Platt taught me many things which are instructive and profound not only for daily American life but also for future life planning. It is my great pity that at that time I knew nothing about graph theory and his paper on the Wiener indices. After returning back to Japan and changing the field of my work into graph theory I found his paper on the Wiener index [16]. I think I have made a good contribution to W by redefining it in terms of the distance matrix [1]. Very recently I found a physico–chemical interpretation of another index, the polarity number p [17]. Although I sent several of my graph–theoretical papers to him later, his interest seemed already to have been directed to more global problems.

I think this is a kind of near–miss or passing–by with John Platt in 1967–1968, but at the same time I might have experienced another near–miss with Frank Harary, who published his famous book "Graph Theory" in 1969 [18]. That is, at the University of Michigan union or at some street

corner in Ann Arbor I might have experienced a near–miss with Frank who must have been absorbed in writing and finishing up his book.

Actually in 1976 I did meet Frank Harary, when I visited Ann Arbor for other business. After having dinner I came back to my room in the Union and happened to find the telephone number of Frank Harary. I immediately dialed his home. He remembered my name because we had exchanged reprints a few times, and though late in the evening he drove to the Union and took me to his office. Very eagerly, he asked many questions about my work on molecular graphs. Discussion continued almost half an hour, and finally he took me to a bar near the campus. Since then we have met more than six times in many places. In December of last year he went to Manila to attend a symposium dedicated to his 80th birthday. After this meeting he flew to Japan and called me up to his hotel in Tokyo. Our relation is something like an uncle and cousin, and we have written a joint paper [19], thereby joining a group of mathematicians of "Erdös number" two [20].

2.4 Topological Index Tour in Europe, 1973

In July of 1973 after attending the ICQC (International Conference on Quantum Chemistry) at Menton, France I made a round trip in Europe. In Menton I already met Dennis Rouvray from Johanesburg and Roger Mallion from England. In Basel, Switzerland, I met Heilbronner in his office, and he told me that although he had rejected my paper submitted to Chemical Physics Letters (CPL) a few years ago, he was appreciating my work at the time of my visit. Then my memory suddenly went back to the autumn of 1970.

In September of that year there was held the annual Symposium on Molecular Structure at the University of Electro–Communications in Tokyo, organized by Yasumasa I'haya, who kindly gave me thirty minutes for my presentation at the end of one of the morning sessions. The chairman was Kimio Ohno of Hokkaido University, who declared that my paper was so novel and interesting that he did not mind to prolong the discussion time, where Kichisuke Nishimoto, who is the inventor of the Nishimoto–Mataga parametrization for the PPP model, gave an encouraging comment to me. The debut of the *Z* index ended in success.

Soon after this symposium I submitted a note on the proposed *Z* index and the discovery of its good correlation with the boiling points of alkane isomers. After three months of waiting it was rejected. The comments by the editor (G. J. Hojtink) and an anonymous referee (E. Heilbronner), which I still keep with me, were as follows: "I have a definite feeling that these relationships must be known, as they are rather obvious." "More work should be done and an attempt should be made to give more depth from a physical chemistry point of view." "At the moment it is just an interesting academic exercise."

Anyway I continued my trip to Zagreb, where Nenad Trinajstić, Ivan Gutman, and other members of the Zagreb group were waiting. I was like a determined warrior with a concealed

nominal weapon entering the enemy's headquarters to interview with the General and his officers for negotiating future actions. Just one year earlier I had received a challenging letter from them stressing that despite my paper having been published in TCA on the graph–theoretical derivation of the CP of a graph [14], Sachs has already solved this problem [10], and their paper using the Sachs theory would soon appear in the same journal [11].

However, in Zagreb they afforded me the warmest hospitality. Almost at the end of the discussion I answered Nenad's question about the future of graph–theoretical study by saying "I think I have at least two more years of study," then he became so glad that he went out to watch a soccer ball game. Ivan Gutman, the youngest among them and engaged in writing his doctoral thesis, offered to do a joint work with me. After returning back to Japan we exchanged several letters within a short period of time and wrote a joint paper which was also published in TCA [15], but at that time he was forced to serve in the army for a year and a half. Joint work with him has been continued up to today, and the newest joint paper was just published in the August issue of BCSJ this year [21].

The last visiting place of my pilgrimage was Bucharest where Balaban was actively writing a big series of papers on "Chemical Graphs" mainly in Revue Roumaine de Chimie. Having enjoyed comfortable drive in his graceful Mercedes Benz I happily returned to Tokyo in the summer of 1973. As I could not succeed in getting any grant money for this travel, I had to pay all the cost by myself. Nevertheless I was well rewarded and could enjoy the fruitful yield of a variety of European crops.

2.5 Dark Side of Graph–Theoretical Work

However, in Japan I was not so happy in my research life for several years after having jumped into the graph theoretical world. As mentioned above my first note on *Z* was rejected by CPL. Then by taking this experience into account I wrote a full paper and submitted it to BCSJ. Again I had to wait for several months to receive the answer from the editor, but this time the referee's comment was rather favorable, and finally my paper was published seven months after submission to BCSJ, one year after writing the note to CPL. Several years later I was told that at least two persons refused to referee my paper, which apparently was so curious as to make a correct judgment difficult. Anyway, except for a few papers, I had to fight for my graph–theoretical papers against invisible enemies, *i.e.*, ignorant and offensive referees and editors, inside and outside of the country.

Also several years later I was told by Shigeyuki Aono of Chiba University that he himself wrote the favorable comment to my paper and that my former boss had a suspicion if I might have become a little lunatic after beginning to work in Ochanomizu University. Dr. Aono said by smiling "Even at that time I didn't think you had become lunatic." My immediate protest was "Why didn't you tell your judgment to my boss at that time?"

I recall the comment of my boss, which was directed to me after I gave my *Z*–index talk in the seminar which his staff and students attended. "I think I've got your theory. I put two points on this blackboard, one for MO and the other for VB worlds. It is generally known that the truth is somewhere in between these two points, but your theory is located somewhere far off this segment." Several of my younger friends who attended that seminar still remember this event, which must have been impressive to them in whatever way. His comment was nothing else but the proof that he did not understand anything about my theory.

There were not only senior scientists but also young researchers and researchers–to–be who did not properly understand my topological index and my way of thinking. After the two bright students left Ochanomizu almost every year one or two master students came to my laboratory and worked hard for my project. I was very lucky to have had so many consciencious coworkers for thirty consecutive years and I am very grateful to them. However, occasionally I felt some invisible power of disturbance or perturbation that was overwhelming my students.

It was a rule for a master course student in my laboratory to perform at least one oral presentation in a symposium or conference of a certain academic level before writing her thesis. Once an able student made a good performance with her accomplishment, it seemed that often she suddenly froze and became rebellious to me. Same things happened more than once during the first ten years of my graph–theoretical study in Ochanomizu. Many years later the mystery was gradually solved by putting together various information from more than one source. Namely, after a debut of a young lady in a science community she would soon be acquainted with many young male researchers. There were actually a few reports to me that one or more among them must have told my students an unfair criticism of me and the *Z* index, and thereby displayed their ignorance, though often they were very influential to young lady students. One remark was: "The work which you and your boss have been doing is just what a retired professor is supposed to do." Ironically I am writing this paper after retiring from Ochanomizu University. Another comment was "You are doing similar things as our Emperor." The former Emperor of Japan was a taxonomist in biology and published a series of illustrated books of seaweeds and animals living in Sagami Bay near Tokyo. Of course, my students must have taken negative or ironical meaning of this comment.

Among my students Kikuko Hosoi (which is a surname irrelevant to Hosoya) was very bright especially in mathematics but did not want to follow me in every respect. One day when she wanted to choose a target for her master's thesis, she said to me "I would like to disprove your theory. What shall I do?" Then I hit upon a good idea. "Well, why don't you study the papers by Longuet–Higgins and Coulson dealing with the complex integral [22]? There might be a hint for you to disprove my theory." She must have studied very hard, and finally, contrary to her expectation, discovered that I was right. Her finding was a kind of a special solution which was expanded into the general solution which I had made. Then I could write one of my favorite papers, which was

published in JCP without any offensive comment by the referees [23].

A little more than thirty years have passed since I jumped into mathematical chemistry. The present atmosphere in the community of scientists has dramatically changed. If a young ambitious researcher proposes a quite revolutionary theory opposed to some conventional paradigm, he or she might be dispelled, disproved, or neglected, but nobody would say he or she had become lunatic. This is a global change of attitude of today's scientists toward the works outside their territory and new things within it. However, I think the chemists community as a whole is still far behind the average standard in this respect. A majority of the readers in this journal would agree with my opinion, when they are going to submit their paper on mathematical chemistry to some standard journal in chemistry. However, I also think that some repulsive factors from conventional chemists were caused by many of easy–going comrades who just play with such–and–such new topological indices, which is nothing else but the number crunching as I myself was doing more than thirty years ago.

2.6 Encouragement

Let us again turn the clock back to the mid 1970s. In Europe I could find so many friends and colleagues in this field. However, in my own country as the Japanese economy was so rapidly increasing, scientists in general were getting richer spending much money either for buying big machines or doing jumbo calculations. In this atmosphere and above prejudice I could continue to do my work with the help of a number of mathematical chemistry friends, in Europe, the US, and China.

Among chemists in Japan many people realized the importance of informatics or information chemistry, and they began to form research groups and to organize special meetings and conferences devoted to this new field in chemistry. Within this group not many but several people gradually got interested in the application of graphical and combinatorial theories to chemistry. Jun–ichi Aihara of Shizuoka University, who had long been interested in the resonance energy and aromaticity, proposed to define the reference polynomial [24] (the same as the acyclic [25] and matching polynomials [26]) by using my $p(G,k)$ numbers [1], and he has vigorously advocated his theory. Shinsaku Fujita of Fuji Photo Film Company has built up a new and big tower of group theory for enumerating the number of possible derivatives of different symmetries of complicated structures and for representing the possible reaction passes [27].

Since 1977 Dr. Hideyuki Narumi, who was teaching chemistry in a high school in Sapporo, has been collaborating with me on the correlation of Z with thermodynamic properties [28,29] and on the analytical solutions for perfect matchings on cubic lattices [30]. Although the number of people outside of Ochanomizu University working with me and also working in my favorite area is not so large, thanks to the help of these academic comrades I have continued to do research up to today. Of

course, the most helpful to me were my students who studied and worked in my laboratory at Ochanomizu, where I moved from the Department of Chemistry to the Department of Information Sciences in the same Faculty of Science in 1992. During the 33 years of working in Ochanomizu about 150 undergraduate and master course students launched into their new life from my laboratory. Among them more than one third got a master's degree and 17 students got a PhD, and still three candidates are preparing for their theses. In various universities ten of my former students hold positions, namely, one full professor, four associate professors, two full time lecturers, and three assistants. Besides these students so many other people are actively working also. I am most proud of the activity of my former students.

3 REVISITS TO OCTANE ISOMERS

Although in 1957 I used only the values for the boiling point of octane isomers from Figure 3, more interesting QSAR problems could have been addressed if I had scrutinized all the given data. Actually in our later analysis of the thermodynamic properties of alkane isomers, it was found that those thermodynamic properties can be classified into a few groups with respect to their different topological dependencies [29,31]. That is, boiling point, absolute entropy, heat of vaporization, *etc*. (type A) are largely dependent on *Z*, while the liquid density and refractive index, *etc*. (type–B) show large positive correlations with *p*. Specific dispersion, critical temperature, *etc*. (type–W) are dependent on both *Z* and *p*, and melting point (type–X) has really no correlation with either *Z* or *p*. Roughly speaking, type–A and B properties are, respectively, determined by dynamical motion and static packing of the alkane molecules.
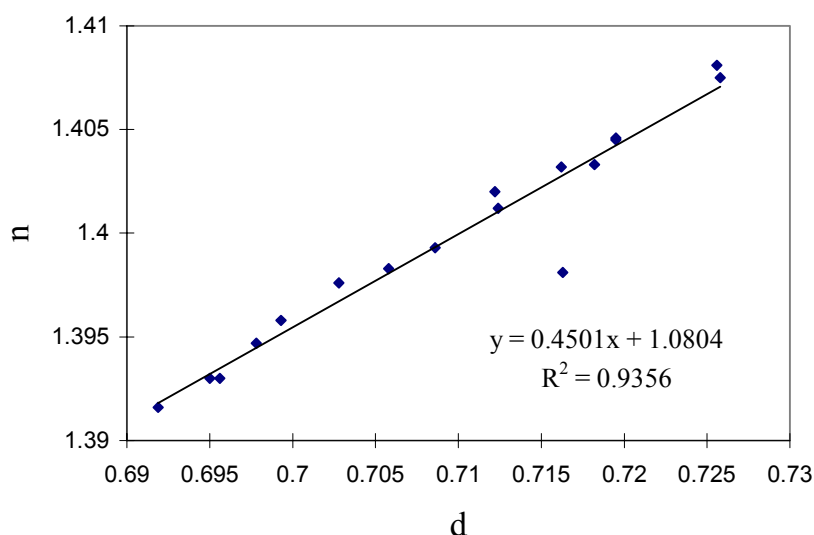
Figure 5. Plot of the refractive index (*n*) against liquid density (*d*) of octane isomers. The data were taken from Ref. [3]. The only point deviating from other points is suggested to be due to a mistype.

Among type–B properties, liquid density (*d*) and refractive index (*n*) are known to be highly correlated with each other. Then if we plot these data from Figure 3, an almost linear plot came out as in Figure 5 (ρ is as high as 0.967). However, the point for 4–methylheptane is found to deviate largely from the other points. Although each of the numerical values in Ref. [3] is a little different from the authentic value in the AIP Report [32], global trends of these two databases should be and actually are found to be the same. It is then suggested that the liquid density of 4–methylheptane (0.7163) given in Ref. [3] may possibly be the mistype of 0.7063 (corresponding to 0.70463 in [32]). Amazingly, if one corrects this value the correlation coefficient ρ is increased up to 0.9965.

Another mistype is found in the melting point of 2,2,3,3–tetramethylbutane. At first sight everybody may have little doubt about the printed value of $-101°$C in Figure 3, because it is not far from the other observed values of *mp*, and the difference between *mp* and *bp* also does not seem to be unnatural. However, the *mp* of 2,2,3,3–tetramethylbutane is $+101°$C, which means that the solid state or the crystal of this substance is so stable that the temperature range of its liquid state is only $6°$C under atmospheric pressure. This substance is called "plastic crystal" and has been much investigated in physical chemistry [33]. The abnormal values of this property for this substance is easily explained by the molecular conformation of this isomer, which forms a part of the stable diamond lattice.

In this way the thermodynamic data of alkane isomers, even with a few errors, contain interesting and thrilling secrets of the microscopic world, where molecules of a variety of characters express openly and consistently their identities. Very recently I wrote a paper on the chemical meaning of the octane number [34]. My conclusion therein was that, together with ample knowledge of experimental facts, careful scrutiny of the regression analysis by using a selected number of physico–chemically meaningful topological indices would give a novel chemical interpretation to the conventional concepts and empirical rules in chemistry. Number–crunching is nothing more than itself.

Acknowledgment

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Biographies

Haruo Hosoya is emeritus professor of chemistry at the Ochanomizu University, one of the two national universities only for women students in Japan, where he has been working for 33 years (1969–2002). He graduated from the University of Tokyo in 1959. After obtaining a Ph.D. degree in physical chemistry from the University of Tokyo in 1964, he became a researcher in the Institute of Physical and Chemical Research, Tokyo for five years, during which he undertook postdoctoral research with Professor John Platt at University of Michigan for one year (1967–68).

Besides the scientific activities described in the text he has served many important roles in the Chemical Society of Japan: vice president (1996–1998), president of the Council of Chemical Education (2001–), president of the Division of Chemical Information (1994–1996, 2002–), and editor of the journal "Chemistry and Education" (1992–1994). He has been president of the Society of Chemical Software (1996–2001), Society of Computer Chemistry, Japan (2002–) and CBI (1993–2000). He has served as a member of Board of Directors of International Society for Mathematical Chemistry from its beginning. He has been chairman of Quantum Chemistry Data Base Group (QCDBG) (1990–), which supplies the internationally known Quantum Chemistry Literature Data Base (QCLDB) for more than twenty years. Dr. Hosoya is called as godfather of the topological index, which was the name specially given to his *Z* index in 1971.