

Autobiographical Notes

Milan Randić

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If you know where you are going nobody can stop you

Let me start with a quote of Roberto Todeschini [1]:

“A good scientist should have imagination of a child, the determination of a boy, the rationality of a man, and the experience of an old man. The difficulty is to have all these qualities at the same time.”

I have passed all the stages indicated above and as I am approaching the end of the road I will briefly reflect on these various stages of our life from my perspective, if I may say so, of a scientist who has been over the time not understood by many outside Mathematical Chemistry and Chemical Graph Theory community, but, what counts more, understood by few that matter, few who appreciated my contributions to theoretical chemistry. So let me name them here at the beginning: E. Bright Wilson of Harvard, R. G. Parr of Johns Hopkins and Chapel Hill; Professor R. S. Hansen of Ames Laboratory, Roald Hoffmann of Cornell University, and Per Olov Löwdin of University of Florida in Gainesville and Uppsala, Sweden, and A. R. Katritzky also of University of Florida in Gainesville. My reflection on understanding and misunderstanding of much of my work by many quantum chemists and physical chemists I summarized in a quote of my own:

“A support of a single scientist who understands what one is doing is more important to have than 100 criticisms of those who do not understand what one is doing.”

And I was fortunate to have and continue to have understanding and support from more than one outstanding scientists of our time. As I ponder over my past I will point at the turning point when I knew the road that I have taken is the right road and that nobody will stop me on my journey. The sign on the road was “Mathematical Chemistry.”

I was born on October 1, 1930 in Belgrade, Serbia (then Yugoslavia), where my father was at that time working in state administration. It was only recently that I realized that I

should celebrate not only the first of October but also the first of January, which is in fact the beginning of my life. My family happens to be in 1930 in Belgrade but we are originally from a small village at the northern part of the Croatian Adriatic coast, which was exceptional in that most men were sea captains. The village earned this monopoly on education of sea captains by a local priest who was educating people for navigation in the time when there were not yet nautical schools (over 150 years ago). In the time of Austria-Hungary this village of 800 inhabitants owned some 60 trans-Atlantic sail ships (this was the time when captain owned sail ship), which was sizable part of the commercial fleet of Austria-Hungary. Both my grandparents were captains (and owned sail ship), but ended working on steam ship of one of larger ship company when after 1905 steam ship practically eliminate sail ship as competition.

My father was trained also to be captain, and had one trip from Rijeka to Barcelona, but World War I sent him to Russian front, where he surrendered (which is different from being captured), and was for five years a “free” citizen of Russia. He returned in 1919, but Austria-Hungary collapsed and there were no ships so my father went into custom office administration. After finishing the first year of elementary school in Belgrade in 1938 my father was advised to leave Belgrade, so I continued my elementary education in my native village, and later in 1939 in Split, till late in 1941, after Yugoslavia collapsed and Split was occupied by Italian army and we were forced to leave Split. After two days travel by train (what now takes five hours) we arrived in Zagreb, where I continued with education. The locomotive had ahead of it two wagons of sand, so if it hits a mine, the locomotive would be spared.

During World War II there were often, actually since the collapse of Italy and Allied Forces controlling the southern part of Italy, there were daily US airplanes crossing over Zagreb on their route to bombing Germany, while we often had to sit for hours in cellar as a precaution. To kill the time my father passed to me and my brother a sizable mathematical book on Algebra (in Italian) from which he learned mathematics as part of nautical education. Myself and my brother were thus busy for hours and competing in solving various equation and other problems and not only that we have no problem with mathematics in high school but we loved the subject. So were it not for WWI I would probably end as sea captain and were it not for WWII I might have miss my love for mathematics!

I studied Theoretical Physics at the Faculty of Natural Sciences and Mathematics of the University of Zagreb, Croatia, during 1949-53. In my last year I was given the book of Linus Pauling “*The Nature of Chemical Bond*” by my professor of Theoretical Physics (Ivan Supek,

a student of Werner Heisenberg) with request to write diploma work (an essay on some 20-30 pages) about application of quantum mechanics to molecules. In my diploma work I considered calculation of Hückel molecular orbitals (HMO) for a selection of substituted benzene derivatives. This was the year 1953 in which Stalin died. I was often working during school breaks in the university lecture rooms (which were spacious and empty) and through window I saw a colleague of mine, a classmate, shouting and smiling "Stalin is dead." He saw the announcement on the building across the street, which belonged to Yugoslav News Company. I tried to calm him as I was worried even though Tito has broken with Stalin in 1948, and pictures of Stalin were removed from offices for quite a time, that dislike of Stalin may for those who were not communist, interpreted as dislike of communism (which would be correct interpretation) and that this may lead to unpleasant event. In those times of fascism and communism the best policy was not to be noticed, and by laughing at Stalin death one is being noticed!

Professor Supek arranged for me to study for Ph.D. at the University of Cambridge, England, where I was from late 1954 to early 1958. This was a time when one could not travel outside Yugoslavia, unless one is highly privileged by the regime. When WWII started Supek was in Germany as one of students in Heisenberg's group. However, after Germany attacked USSR, another student of Heisenberg, his roommate, leftist, German, took a small plane and flew toward Russia to escape from Germany. His plane was shot, while Supek was arrested and was in one of camps for political prisoners waiting for interrogation. During his few months in prison camp he witnessed brutality of Nazi interrogations, but was fortunate that mother of Heisenberg knew personally Mrs. Goering, and she was successful in arranging that Supek gets invitation to join Heisenberg in Berlin. The situation was complicated when the Commander of the prison camp got a letter to let Supek, who witnessed atrocities of Nazi agents, to go, and to compensate asked if Supek has some wishes as traveling to Berlin. He asked if it would be possible for him to first go to Zagreb and see his mother on a route to Berlin. This was agreed (he got necessary papers) but when crossing from Austria to Slovenia Supek instead of going to Zagreb to see his mother went to Partisans. Thus he was among not so many who joint resistance to occupation already in 1941. It was therefore possible for Supek to arrange my scholarship in Cambridge, England. He sent already several of his students to other leading institutions in Europe and USA.

In Cambridge University I was working, on high resolution infrared spectroscopy (IR) under supervision of Dr. Norman Sheppard, one of the leading authorities in IR. During my stay in Cambridge I took advantage of the strong group of theoretical chemistry there, lead by

Professor H. C. Longuet-Higgins, which included John Pople, George Hall, Leslie Orgel, S. F. Boys, and among Ph. D. students David Buckingham and John Murrell. I also took advantage of the privilege to be in Cambridge and attended several lectures on quantum theory by P. A. M. Dirac and a course on quantum chemistry by S. F. Boys, who mentioned his *ab initio* calculations of H₂O using Gaussian orbitals. Finally I also attended two summer schools on quantum chemistry of C. A. Coulson in Oxford. After returning to Zagreb I was assistant research scientist at the Institute Rudjer Bošković, where I founded the Group for Theoretical Chemistry (1959-64).

As a postdoctoral student I spent a year (1964-65) with Professor John N. Murrell at the University of Sheffield, England getting familiar with Pariser-Parr-Pople (PPP) calculations, calculating spectra of anthracene, and a year (1965-66) with Professor David Bishop at the University of Ottawa, Canada who introduced me to the "Single Center Method" of Professor R. G. Parr, where we calculated not only very accurate wavefunction of H₂O but also (probably being the first) the *ab initio* vibrational frequencies of H₂O.

Between 1966-71, while continuing my residence at the Institute Rudjer Bošković, I was appointed first as Associate and then Full Professor at the Chemistry Department of the University of Zagreb, Croatia. The groups of Theoretical Chemistry at IRB, which started as "one-person-show" in few years grow to respectable size when the group was joined by younger graduate students: Z. B. Maksić, N. Trinajstić, Z. Meić, T. Živković, A. Graovac, S. Bosanac, T. Cvitaš and V. Bonačić.

Early in 1971 I left for a visit to USA by visiting for six months Professors R. G. Parr at the Johns Hopkins University in Baltimore, MD, where I worked on differential equations that could generate potential curves – work which was never completed and submitted for publication. After Baltimore I spent a year with Frank E. Harris (1972-73) at the University of Utah in Salt Lake City, where among other things I compiled an atlas of maximum overlap calculations on strained cyclic compounds, which is still on my shelf unpublished. We left Salt Lake City for Boston, MA, as my wife got a position at the Tufts Medical School in Boston. I spent my first three months in Boston area with Robert Silby (1974) at MIT, to join in 1974-75 group of Professor E. Bright Wilson at the Harvard University, Cambridge, MA. While at Harvard I attended a seminar of Professor Alexandru T. Balaban on Chemical Graph Theory, in which he mentioned several unsolved problems in chemical graph theory. At that time all the literature on chemical graph theory Balaban carried in his bag, and next morning made copies available to me. I was intrigued by some of the problems mentioned by Balaban in his lecture and continued to work on them. While still at Harvard I published my first

paper on graph isomorphism problem for molecular graphs [2], and re-directed my research towards application of Discrete Mathematics to Chemistry, what includes Chemical Graph Theory. This was the moment when I knew that I am on a road of no return.

The next two years I was unemployed but I worked as unpaid guest in the Chemistry Department of Tufts University, where I published very significant contributions to chemical graph theory: my paper on molecular branching in which was introduced the connectivity index, published in *J. Am. Chem. Soc.* [3]; and my papers on conjugated circuits and expressions for resonance energies (*Chem. Phys. Lett.* [4], *Tetrahedron* [5]), on aromaticity and extending Hückel $4n+2$ and $4n$ Rule to polycyclic compounds (*J. Am. Chem. Soc.* [6, 7]). These papers, just as the first paper [1], that on use of canonical labels to solve graph isomorphism, were well received. The paper on isomorphism was reviewed in *Nature*, while the paper on connectivity index was among 125 most cited papers published in *J. Am. Chem. Soc.* during its 125 years of existence [8], and among 30 most cited papers in *J. Am. Chem. Soc.* for a period of 30 years (1975-2005) [9]. It's a "classic," because it passed the citation 1000-mark, having by the end of the year 2009 over 1750 citations. The papers on connectivity index and aromaticity are probably among the cheapest scientific papers published in chemical literature, as there was no direct (grant) or indirect (salary) cost to taxpayers.

I spent a year at the Chemistry Department of SUNY at Buffalo, NY, where I met in the Department of Biophysics Professor Robert Rein and would one day a week be in his company. When he was editing a two volume book on Molecular Cancer Research he invited my contribution, and I obliged by sending a paper in which atomic descriptors were outlined in search for optimal anti-tumor compound within a family of compounds studied [10]. During that visit he invited me as an outside member of a Ph. D. thesis, the other person invited was Professor L. B. Kier, who was at that time in School of Pharmacy in Boston. At that meeting I told Monty Kier that every other weekend I am in Boston, where my wife was faculty at Tufts Medical School, and he invited me to give seminar at his institutions. I presented my work on the branching index (the paper was in press at that time), which later Kier re-named as the connectivity index, which was a better name, as index and be calculate for cyclic and linear molecules without branches! I should mention also that L. Hall, who was on sabbatical visit at Kier's laboratory, was in the audience of my seminar and was active in collaboration on connectivity index that followed. Kier not only renamed the index, but during a follow-up meeting we expanded the connectivity index by introducing the higher order connectivity indices [11]. After a additional single paper on application of the

connectivity index to QSAR with Kier and Hall [12] I was leaving Boston area, while Kier and Hall took the initiative in applying the connectivity indices to structure-property and structure-activity studies and generalizing the connectivity indices to valence connectivity indices, in order to accommodate presence of hetero atoms in molecules [13].

Soon we left for Iowa, where again for a while I was working without pay, though I had moral support from the vice-President of Research at Iowa State University Professor Zaffarano (physicist) and limited financial support of Director of Ames Laboratory, Professor R. S. Hansen (physical chemist), from his discretion funds. It is significant that this financial support continued for over 10 years, despite that in 1980 I got a position in the Department of Mathematics and Computer Science at Drake University in Des Moines, about 35 miles south of Ames, where there was Iowa State University, which offered my wife tenure and full professorship in the Veterinary Medicine School. The annual stipend of \$ 3,000 - \$ 4,000 made it possible for me to attend regularly annual Sanibel meetings, organized by Professor Per Olov Löwdin, which I attended for the next 20 years. After Professor Hansen retired his successor stopped the support and informed me that this support was illegal!

During (1978-79) I was visitor in Chemistry department of the University of Nebraska at Lincoln, NE collaborated with Professor C. L. Wilkins, and we had a very productive year focusing mostly on the use of paths as molecular descriptors. Finally in 1980 I got a position of Associate Professor in the Department of Mathematics and Computer Science, Drake University, Des Moines, IA, about 40 miles south of Ames. For next 20 years, till my retirement in the year 2000 (at the age of 70), four times a week I would drive from Ames to Des Moines and back, which took little bit less than an hour. Thus I had time for thinking (while driving), but by teaching three courses each semester I have not much time for work. Nevertheless, I was active and published several papers that opened novel directions in application of Discrete Mathematics to Chemistry, which included development orthogonal molecular descriptors [14], which finally resolved the “nightmare of QSAR” in variability of coefficients of regression equations when additional descriptors are introduced in multivariate analysis in stepwise regressions; a paper on retro-regression [15], which outlines construction of structure-property space and stable regression equations for general regression analysis; and construction of variable connectivity index [16], which has shown limitations of the concept of valence-tailored molecular descriptors for heteroatoms.

During 20 years at Drake University I published about 230 papers, which covered variety of topics, besides those listed above including: use of graph theoretical descriptors for search for pharmacophore [17]; graphical matrices, that is, non-numerical matrices whose elements

are subgraphs [18]; orthosimilarity, similarity based on orthogonal descriptors [19]; D/D matrices, defined for structures of fixed geometry, the elements of which are given as quotients of the Euclidean and graph theoretical distance between each pair of vertices and the leading eigenvalue of which is interpreted as a measure of the degree of folding or bending of chain structures [20]; generalization of the Wiener number to hyper-Wiener number which considers contributions of non-adjacent vertices [21]; a dozen papers on symmetry of graphs, including symmetry properties of the graph for rearrangement of P_7^3 , which has $7!/3$ vertices [22]; use of the sum of ^{13}C atomic chemical shift in a molecule as novel molecular property [23]; and use of linear combinations of paths as molecular descriptors [24]. Many of the topics mentioned have been done in collaboration with other leading researchers in chemical graph theory, including N. Trinajstić, A. T. Balaban, D. J. Klein (particularly work on the innate degree of freedom [25] and the resistance distance [26]), H. Hosoya, and D. Plavšić.

My work at Drake University was appreciated by the faculty, with whom I had very successive collaboration including Wayne Woodworth, A. F. Kleiner, K. Kopecky, B. Baker, T. Oxley, H. Krishnapriyan, D. Oakland, L. Naylor and L. M. DeAlba, which is more than half of the faculty of the Department of Mathematics and Computer Science. In addition I had two outstanding undergraduate students, G. Krilov and S. Bobst, with whom I published few papers [27]. During my stay at Drake I also had three postdoctoral visitors, Dr. Borka Jerman-Blažič from the Josef Stefan Institute in Ljubljana, Slovenia, two visits of Professor Xiofeng Guo from Wulumuchi, Xinjiang, China, and Dr. Jan Cz Dobrowolski from Industrial Chemistry Research Institute, Warsaw, Poland.

After two years at Drake I obtained tenure, became Professor, then Distinguished Professor, and was later nominated by the President of the University for Governor's of Iowa Annual Science Award, which I received and which became also distinguished recognition for Drake University. With University of Iowa and Iowa State University, each having over 25,000 students, while Drake having at most 5,000, it must have been hard competition for Governor's Science Award, because this is not award for chemistry, but all natural sciences. In retrospect, I am sure that I would not be even close in competition was it not for very strong recommendation of outstanding supporter that I was able to attract: Professor E. Bright Wilson of Harvard, Professor R. G. Parr of John Hopkins; Professor R. S. Hansen, Director of Ames Laboratory, Professor Roald Hoffmann, at Cornell University, Nobel Prize in Chemistry 1981, and Professor Per Olov Löwdin of University of Florida in Gainesville

and Uppsala, who signed his letter by indicating to be the secretary of Nobel Prize in Physics (1970-1980).

I received few other public recognitions of which I will mention only two, which are to me very dear. In 1996 I received the Herman Skolnik Award (annual award given by the Division of Chemical Information of the American Chemical Society), I believe that I was nominated for this prestigious award by Sandy Balaban, who received it two years before me. Both these awards are a nice recognition not only for both of us but also for Chemical Graph Theory.

The other unexpected recognition came in 2000, when within the Division of Computers in Chemistry of the American Chemical Society Professors L. L. Hall and L.B. Kier organized “Molecular Connectivity – The First Quarter Century Symposium” to celebrate 25 years of publication of my article on the connectivity index. The symposium grouped some 25 scientists for a two day meeting.

From 1995 I started collaboration as Visiting Scientist at the National Institute of Chemistry, Laboratory for Chemometrics, Ljubljana, Slovenia for three months per year with Marko Razinger, which after his sudden untimely death continued for almost 20 years by collaboration with Jure Zupan, Marjana Novič and Marjan Vračko from the same laboratory, which is still in progress.

I became (foreign) Member of the Croatian Academy of Sciences and Arts on the initiative of Professor Ivan Supek. When I came to the Academy a secretary of Professor Supek, who was at that time the President of the Croatian Academy of Sciences and Arts, she brought a diploma document and was to give it to me but Professor Supek told her to keep it till he organizes a small ceremony so that it is given at that time. Few days later we invited dozen guests, which included Professor D. J. Klein who was then in Zagreb. Professor Supek was saying some good words about me and how I started Quantum Chemistry in Croatia. I should add here that often I am getting credit for founding Theoretical Chemistry in then Yugoslavia and now Croatia, but Quantum Chemistry was the initiative of Professor Supek – and I was just the messenger. In the audience there were three academicians, my younger sister (she was at the time Dean of Faculty of Construction and Naval Architecture of the University of Zagreb) and few others and at the informal part I raised a question: How is that the founder of the Academy, Archbishop Josip Juraj Strossmayer, has two names when everybody in Croatia has just one name? Nobody knew the answer, except for the President of the Academy Professor Ivan Supek. So I told them the story how Strossmayer was one of two identical twins and two days after their birth one of the twin has died and parents did not

know who died, they were so similar, so the survivor carried both names! I used to tell this story sometimes in my quantum chemistry class when lecturing on H_2 molecule to indicate that identical particle cannot be individually named and that is why we have for wave functions $\psi_a(1)\psi_b(2) \pm \psi_b(1)\psi_a(2)$.

Additional recognitions include being the Honorary Member of Croatian Chemical Society and Honorary Member of the National Institute of Chemistry in Ljubljana.

I formally retired with December 31, 1999, because I wanted with time left to continue with research, which was difficult at Drake University under the heavy burden of teaching three courses each semester. For a while I established collaboration with Subhash C. Basak and would spend some time in Duluth, MN, at NRRRI (Natural Resources Research Institute) of the University of Minnesota at Duluth. It is there that I attended a seminar of Ashes Nandy (a theoretical physicist, a visitor from Calcutta, India), who presented his work on graphical representation of DNA sequences. It immediately struck me that his graphical representations of DNA can be accompanied by numerical representations, which would thus not only transform qualitative representations of DNA to quantitative, but would make it possible to manipulate with such data by computer. Not long after we published paper on numerical characterization of DNA [28] and thus opened a new direction of research in Bioinformatics, the area of research that I was following for the next ten years and continue to pursue.

In collaboration with S. C. Basak, and people from the National Institute of Chemistry in Ljubljana (Zupan, Novič and Vračko) and from the Institute Rudjer Bošković in Zagreb (D. Plavšić), I continued expanding this work to include numerical characterizations of proteomics maps [29], characterization of the secondary structure of RNA [30], and finally we were the first to come up with opening the field of graphical and numerical representation of proteins [31]. We all should be pleased that our work in Bioinformatics apparently has been well received, which can be contrasted to unwarranted ill-reception of much of our earlier work in Chemical Graph Theory by most quantum chemists, and physical chemists and medicinal chemists involved in QSAR (Quantitative Structure-Activity Relationship). I should mention here also my one-month visit to Santiago de Compostella, as a guest of Ernesto Estrada, a younger Cuban scientist who left Cuba in search for better opportunities for research outside Cuba. I have been in contact with him for a while and I consider him to be one of the youngest and still outstanding researchers in application of Discrete Mathematics in Chemistry and Bioinformatics. While in Santiago we re-examined the data on proteomics maps dose response and were able by focusing only on abundance (ignoring

mass and charge information on proteins) to detect J-shaped dose-response which signified hormesis [32]. The phenomena of Hormesis (stimulation by use of low concentrations of toxin), which has been reported for whole organism (animals and plants) was in dispute for a while [33], but is now generally accepted. Our work has demonstrated for the first time the presence of hormesis at the cellular level. The evaluation of the manuscript of an anonymous reviewer of *Journal of Proteomics Research* recommended publication by a single sentence: "This paper will be highly cited." Maybe? I could add that this result, detection of hormesis at cellular level, could have been discovered two years earlier in a paper by myself in collaboration with M. Vračko and M. Novič analyzing the same data by a different approach [34], but we missed it! However, when I recently plotted part of data we reported two years before work with Estrada, in preparation of a review article on graphical representation of proteins (to appear in *Chemical Reviews*) in collaboration with Jure Zupan, A. T. Balaban, Dejan Plavšič and Dražen Vikić-Topić [35], I got J-shaped curve for dose response.

After my formal retirement most of my research was directed to DNA, RNA, proteins and proteomics, though occasionally I would return to old love: molecular descriptors and Kekulé valence structures. Most significant novelty in that area in my view are the path/walks shape indices [36], which give the basis for very good regressions of numerous physico-chemical properties; and partitioning of π -electrons to individual rings in benzenoid hydrocarbons [37] and an systematic approach to interpretation of topological indices by calculating their bond contributions [38]. To this I should also add one of my latest works in collaboration with Marjana Novič, Tomaž Pisanski and Dejan Plavšič on "natural" distance matrix [39], in which graph on n vertices is represented by n points in n -dimensional space. If I am asked which of my papers in extending graph theoretical approaches to bioinformatics I consider most significant, besides the already mention paper with E. Estrada on hormesis at cellular level I would mention three themes; (1) Spectral representation of biosequences [40]; (2) Use of the Chaos Game approach of Jeffrey [41] to short sequences and codons [42]; and (3) Introduction of matrices which count amino acid adjacency, and their generalization to count amino acids separated by k amino acids [43]. Spectral representation of DNA and proteins lead to graphical approach to DNA and proteins alignments, respectively [44].

I should end this overview of research activities by mentioning collaboration with one of me latest coworker, younger mathematician Professor Damir Vukičević, and one of my oldest acquaintance, from the time of my visit to Sheffield, and later Brighton (Sussex), Sir Harry Kroto, with whom I published two papers in more recent time [45]. When visiting John Murrell at the University of Sussex at Brighton, the University was so new that there were no

guest rooms or motels in the vicinity of the University. Were it not for Harry Kroto and Lady Margaret, who took me into their home for three months, I would have serious problems of staying there.

I would like to end this outline of my life in science by mentioning few of my interests that are outside theoretical chemistry. I have from time to time entered into the domain of chemical information. My latest adventure in that area is a proposal for generalized Hirsch index, which may or may not be of interest – the time will tell. In this generalization information on the citations numbers for papers contributing to one's Hirsch index having variable number of citations is taken into account [46].

Another interest of mine was collecting quotes of scientist and quotes about science (involving also non-scientists). I have been doing this for some 25 years, collecting few quotes each year not searching for them, but recording those that came to my attention. So the collection is relatively small, almost 200 quotes (about 35 pages text). Parts of these have been published (about half or less) in an Indian mathematical journal [42], but I was not given proofs so there are some omissions of lines causing confusion and misquoting.

I have also been interested in developing scientific terminology for Croatian language based on three principles: (1) One should not use foreign ordinary words (folk language) in science, these have to be replaced by Croatian ordinary words; (2) One should not use foreign grammatical endings; (3) One should strive to construct Croatian term for foreign scientific terms when possible but one should not exclude foreign technical terms even when there is adequate Croatian substitute. The above may be noble intent, but apparently against time we are losing the battle, because by the time one arrives for a new solution for some term, meanwhile in the literature there are ten new technical terms! However, the alternative, not to try to develop national nomenclature, would be even worse. Much of Croatian early scientific nomenclature was based on Czech practice. Despite difficulties I may say that I came to few solutions, like composing a Croatian equivalent for "symmetry" which I once mentioned to Professor Ivan Supek. Supek, besides being scientist, was also writing numerous literary books, and he approved of my suggestion – which I smuggled in one of my book review for *Croatica Chemica Acta* (written in Croatian), which I believe nobody notices, which was good, otherwise it could be deleted!

Finally my great interest is in construction of graphical universal language, which engaged me now for almost 25 years, all the time since my first three weeks visit to China to attend the First USA – China Conference in Graph Theory and Applications in Shandong, China in 1986, followed by five weeks in Japan where I started to work on it. While in

Shandong (about two million inhabitants) I felt helpless because there are so many writings in downtown of the city and I could not understand a single sign. Well, after some time I noticed some signs that appear more often and in particular I could identify sign for entrance and exit on busses, as being rather simple. What surprised me when coming to Ochanomizu in Japan (where my wife has been visiting for six months the National Institute for Pharmacology) that in Japan busses have the same written signs for entrance and exit. But Chinese and Japanese languages are unrelated (in contrast to say English and Croatian being related, belonging to the group of Indo-European languages that all can be traced to Sanskrit). Japan adopted Chinese characters in the 11th century (to which they refer as kanji) but although pronounced differently they have the same signs for many same concepts – which demonstrate universality of Chinese characters. The problem for many is that it is difficult to learn numerous Chinese characters and I was interested to come up with simple signs instead. Already while in Japan I constructed my first 100 signs, which gradually grew to some 20,000. My book, entitled *Nobel – Universal Graphical Language* (almost 550 pages), to be published by Xlibris (Bloomington, IN), is coming out any day, where interested readers can get more information on Nobel, named after Alfred Nobel and his concern about peace on this Globe, reflected in annual Nobel Awards for Peace.

Coming back to chemistry let me end by telling also my latest activity – writing a book “*Discrete Mathematics Applied to QSAR and Beyond*” contracted with CRC Press, which evolved from a sizable manuscript summarizing my invited talk on a conference organized by James Devillers (the Editor of *SAR and QSAR in Environmental Research*) in Lyon, France, in 2007, which was too long for the proceeding of the conference. Dr. Devillers, who is also Editor of a series of books on QSAR for CRC suggested that I expand this manuscript into a book, which not only I accepted, but accepted his suggestion for a title, as the publishers insisted that “QSAR” be part of the title of the book, which was not in my original: “*Mathematical Chemistry in Structure-Property-Activity Studies.*” I particularly liked “Beyond” in the title, as this give me possibility to include in the book some of our work in bioinformatics that goes beyond chemical graph theory. I have to admit that I enjoy writing this book (over 450 manuscript pages have been completed), which will in several ways be different from the standard monograph and text in Theoretical Chemistry, and which ought beyond doubt to demonstrate the great future for Mathematical Chemistry in Chemistry. Mathematical Chemistry, as Professor Ivan Gutman has said on an occasion, is going to become the dominant part of chemistry in the future when one counts number of molecules that are experimentally available and that a computer can consider.

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