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Confessions and reflections of a graph–theoretical chemist

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Introduction. In writing a personal account of my involvement in chemical graph theory, I am faced with the necessity of providing the readers with the background information about general and private circumstances starting with the '40's.

In high school I had been equally attracted by chemistry, physics and mathematics. At home in Bucharest I had a small terrace that I had converted into a chemical laboratory (without gas or running water, however). When I was 12 to 14 years of age, I spent most of my free time there, except for winters, of course. Two friends and neighbours of the same age shared my interests, namely Nelu Burculeț and Silviu Teleman. When peace came to Europe in 1945, our group of three "amateur chemists" made on our street a successful fireworks demonstration. I had won a few prizes in competitions for "high school amateur chemists" and sent several contributions to the weekly journal which organized this competition.

In Eastern Europe the post–war years were grim. My father, an electromechanical engineer, had been drafted in the army in 1942 and fought on the Russian front for two years. During this time his hair turned completely white. After his return our family moved away from Bucharest, which probably was a fortunate event because the material and political situation was worst in Bucharest. One of my two closest friends mentioned earlier, Nelu, was sent to prison because he had frequented the American Embassy's library in 1945, before the communist regime took hold of the power in 1945–46, and he died shortly thereafter.

Earlier, I had learnt French and German at school and, after leaving Bucharest, my parents had encouraged me to become fluent in these languages by reading literature from the books we had at home. I started learning English and spent many hours listening to BBC's "English–by–radio" programmes. With the carelessness of youth I participated in BBC competitions and earned a book as a prize, causing the panic of my parents (in Bucharest such a "crime" as listening to the BBC would not have remained unpunished). I had hoped to be able to study in the West (as had usually been done by many youngsters before the war), but that proved to be impossible. Later, I declined offers to study in the USSR.

Organic chemist. What decided me in 1949 to become a student of the Bucharest Polytechnic's Industrial Chemistry Faculty was the fame of C. D. Nenitzescu's research school in organic chemistry. Costin D. Nenitzescu had obtained his Ph.D. with H. Fischer before Fischer had been awarded the Nobel Prize for his research on porphyrins. Back in Roumania, the young Nenitzescu had discovered two new indole syntheses which to this day bear his name.

Having always been ranked first in my class during all my studies, I was fortunate to be invited to join this research group and obtained a Ph.D. fellowship for three years in a competition after graduating as a chemical engineer in 1953. It was the first time after the war that doctoral studies were again allowed. This competition also allowed me to finish the studies one semester ahead of my class, so that my future wife, Cornelia, who had performed her studies with me for four years, obtained her degree six months later. This Ph.D. fellowship was one of the three opportunities that chance had offered me in an otherwise very rigid system where shortcuts for gifted people were almost impossible.

At the same time, I had teaching duties for organic chemistry seminars and laboratories. The topic of my Ph.D. thesis was "Reactions catalysed by aluminium chloride", a field in which Nenitzescu's school had already attained international recognition.

In 1955 Cornelia (Nelly) and I were married. During the three years that I had the Ph.D. fellowship, my income was the lowest among all my ex–fellow–students, but I think it was a good idea to require from future scientists a higher interest for research than for money. In 1956 I was appointed laboratory assistant and was promoted several years later to a position of lecturer (assistant professor) in organic chemistry. Though my Ph.D. thesis was not yet ready, I had obtained some interesting results and worked in the laboratory for 12–14 hours a day. In 1956 I registered as a first year student for Mathematics but in the same year the second opportunity knocked: a one–time offer for a one–year study of atomic and of nuclear physics, as well as of radiochemistry. An institute of Atomic Physics was to be created for the Roumanian Academy, having as director professor Horia Hulubei who had been a coworker of the Curie family in Paris, and during the wartime had obtained the "Legion d'Honneur" distinction for his bravery in the French Air Force.

This second opportunity was quite rewarding because it gave me the possibility to get an intensive training with excellent professors, avoiding the dull uninteresting lectures a regular student had to take. At the same time, the teaching duties, the preparation of my Ph.D. dissertation, and the birth of a son, Teodor–Silviu, in 1958 made me give up the attempt to finish Mathematics. Looking back, I think it was a right decision, but nevertheless it left me with regrets.

In 1959 I obtained the Ph.D. degree and also my first papers started to appear: with C. D. Nenitzescu, we published in 1958 the demonstration of mechanisms for the Scholl reaction (dehydrogenating condensation of aromatic rings catalyzed by $AlCl_3$) [1] and (in 1959) of the reactions between alkanes [2] or cycloalkanes [3] with carbon monoxide in the presence of $AlCl_3$. A new synthesis of pyrylium salts was found by the $AlCl_3$–catalyzed diacylation of alkenes [4]. The latter reaction had been simultaneously and independently discovered by Praill in England, and we published in 1961 in the same issue of *J. Chem. Soc.* our generalization of this reaction [5–7].

These papers, as well as Nenitzescu's international prestige, led to an invitation by G. A. Olah to write two chapters for his well–known monograph "Friedel–Crafts and Related Reactions"; with Nenitzescu we coauthored the chapters on the "Scholl reaction" and on the "Aliphatic acylation" [8,9].

Throughout our whole cooperation, relationships with Nenitzescu remained more than cordial; he was the godfather of my son. As head editor of the Roumanian Academy's chemical journals (*Revue Roumaine de Chimie* is the only one which survived Ceausescu's era), Nenitzescu co–opted me as deputy head editor, and I was happy to implement some of the editorial practices I had learnt by publishing in such journals as *Tetrahedron*.

In the Laboratory of Labelled Compounds of the Institute of Atomic Physics, I started research areas of my own, with a few young coworkers. We could attack in this Institute of Atomic Physics organic chemical problems, in addition to preparing isotopically labelled compounds and radiopharmaceuticals. Thus, we published the first studies on push–pull stable aminyls [10–13], a topic which later was extended to carbon free radicals ("merostabilization" discussed by Katritzky [14] or "capto–dative stabilization" discussed by Viehe [15]). Another area was that of heterocyclic organoboron compounds [16–19], a topic about which I had mused since 1955 when I had written to professor M. J. S. Dewar about this idea; he replied that he was working just on such compounds about which he published later [20].

In collaboration with professor Ecaterina Ciorănescu (C. D. Nenitzescu's wife) we developed a new oxazole synthesis (2,5–diaryloxazoles are good scintillators) by using the $AlCl_3$–catalyzed reaction between azlactones and aromatics [21–24]. In addition, I continued the study of spectral properties and reactions of pyrylium salts working with my small research group at the Institute of Atomic Physics, while on pyrylium syntheses I continued to publish with C. D. Nenitzescu. The work on pyrylium salts was reviewed [25–28]. Some of the isotopic labelling topics were connected with pyrylium chemistry, since I observed the very easy exchange of methyl hydrogens between 2,4,6–trimethylpyrylium salts and deuterium oxide [29–34] (we reviewed the subject [35,36]). Our tritiation method [37–40] for organic compounds was based on the catalytic activity of $HTO.AlCl_3$; this work is closely related to independent observations on

tritiations with HTO and strong acids.

Graph–theoretical interests. During the late 50's and 60's, I came across several problems connected with chemical structure. They were actually graph–theoretical problems, but I learnt this later. In 1959 I published in Roumanian a long paper [41] on a theoretical approach to aromatic monocyclic systems: an sp^2–hybridized atom in an aromatic ring can contribute 2, 1, or 0 electrons to the delocalized set of $4k + 2$ π–electrons (Hückel's rule). These three types of atoms, denoted by $\ddot{X}$, $\dot{Y}$, and Z, then form the $\ddot{X}_x\dot{Y}_yZ_z$ system with the following constraints in an m–sized ring:

$2x + y = 4k + 2$ $(k = 0, 1, 2, ...)$; $x + y + z = m$ $(m = 3, 4, 5, ...)$

In addition, as pointed out in 1961 in a first collaboration with Z. Simon, local and global electronegativity constraints exist [42]. These ideas were further developed later [43,44]. (Interestingly, I learnt later that Alan R. Katritzky had forwarded to *J. Chem. Soc.* a manuscript describing similar ideas, but it had been turned down by referees). This approach has been incorporated into several books and reviews [45,46].

In the 1959 paper [41], the enumeration of $X_xY_yZ_z$ systems (i.e. the graph–theoretical "necklace problem" of an m–membered necklace with beads of three colours) had been worked out, using combinatorial and algebraic methods, with my life–long friend Silviu Teleman, who in the meantime had graduated as a mathematician. (At present he is an American citizen, and is a professor of mathematics at the University of Puerto Rico.)

The third opportunity occurred in 1963 when I was 32 years old: I was elected as corresponding member of the Roumanian Academy, which was the highest honour that could be bestowed by this country on a person. Only one or two people had been elected in the past to the Academy at such an early age. I was still an associate professor (from 1962–1966 in General Chemistry for non–chemistry majors in the Bucharest Polytechnic, and I became a full professor in 1967).

In the early 60's I came upon two other graph–theoretical problems. Both are connected with research then carried out by Nenitzescu and coworkers: the first multiply–connected valence isomer of annulene is a hydrocarbon $(CH)_{10}$ known as Nenitzescu's hydrocarbon; isomerizations of phenylalkanes under the action of $AlCl_3$, as well as of aliphatic chains on oxidation with Cr(VI), can be rationalized by a series of 1,2–rearrangements which may be better presented as reaction graphs. Now I was aware of the topic, and I read with interest graph–theoretical books and papers by Berge, Ore, and Harary. To my surprise, I learnt that the chemical problems of enumerating and finding the structures of valence isomers of annulenes $(CH)_{2k}$ (cubic graphs) and of polycyclic aromatic hydrocarbons (hexagonal cell animals) were then unsolved. I published in 1966 two papers as the first two parts in the series "Chemical Graphs": "Enumeration of $(CH)_{2k}$ valence isomers" [47], and "Reaction graphs" [48]. With a better mathematical technique, two follow–ups of the first paper appeared in 1970 [49], one of which, on cubic identity graphs, involved cooperation with several mathematicians and, unlike all my previous papers, appeared in a mathematical journal [50].

In Roumania, my attempts to find graph–theoreticians willing to collaborate with me proved unsuccessful. Then in the early 60's I wrote to Frank Harary, and a fruitful cooperation resulted. During his first visit to Bucharest, we discussed the "necklace problem" and the "hexagonal animal cell problem". Several joint papers were published with him between 1967 and 1976 [51–52] solving necklace problems by means of Pólya's theorem. A seminal joint paper with Harary introduced in 1968 the characteristic or dualist graphs of polyhexes (see next paragraph), which are useful for many applications in the field of polycyclic benzenoid hydrocarbons [53]. Another paper with Frank, published in 1971, is among the earliest ones on isospectral graphs, i.e. non–isomorphic graphs having the same characteristic polynomials, hence the same eigenvalues [54].

In 1976, with R. W. Robinson and F. Harary, for the centennial of LeBel–Van't Hoff's introduction of stereochemistry into organic chemistry, we described mathematical approaches for computing the numbers of chiral and achiral alkanes and alkyl groups [55].

The dualist (or inner dual) of a polyhex has as its vertices the centers of the polyhex, and its edges connect centers of condensed hexagons, i.e. hexagons sharing an

edge. This approach leads to a simple partition of polyhexes into three classes namely: (i) catafusenes, whose dualists are acyclic (trees), (ii) perifusenes, whose dualists have three–membered rings, possibly in addition to acyclic appendages, and (iii) coronafusenes (coronoids) whose dualists have larger rings which are not peripheries of aggregates of 3–membered rings (possibly in addition to acyclic appendages and 3–membered rings). In addition, dualist graphs allow an easy approach for the coding and nomenclature of benzenoids [56]. I reviewed later various uses to which dualists can be put [57], and these dualists (which are different from normal graphs because their angles do matter) have become accepted by the international community [58–60]. After 1980 I learnt about the existence of an early publication which had made use of such dualists [61]; my and Frank's development of dualists for polyhexes was an independent approach.

In the early sixties, I had started thinking about editing the first book about chemical graphs. A group of authors agreed to contribute to this monograph. In 1966 I visited Frank Harary in Ann Arbor, Michigan for one month, and we drafted a joint chapter for this book, as well as plans for future joint work. However, the book would probably have taken a long time for becoming published because of postal restrictions (censorship) in Roumania; luckily, however, I was offered a position of senior research scientist in the Chemistry Section, Division of Research and Laboratories, International Atomic Energy Agency, Vienna, Austria, for three years (1967–1970). My duties there were of editing scientific books [62], organizing international symposia [63–64], and acting as liaison officer for radiopharmaceuticals between IAEA and the World Health Organization in Geneva for drafting recommendations for the International Pharmacopeia. For these years I had to give up teaching in Bucharest, but I still maintained a close contact with my research associates in the Laboratory of Labelled Compounds from the Institute of Atomic Physics; I flew for three days to Bucharest six times per year, giving up some of my vacation time from the IAEA, and taking advantage of the 5 working days in Vienna versus 6 working days in Bucharest.

Life was pleasant in Vienna, and my family could enjoy a better living: my son attended the English school and became fluent both in English and in German. My daughter, born in 1966, was well taken care of by my wife who stayed at home. Occasionally, either my parents or my wife's parents came to stay with us for extended periods. My wife could finally accompany me when I was at scientific meetings or lecture tours. We exchanged visits with chemists from Germany (K. Dimroth) or England (P. F. G. Praill, A. R. Katritzky).

Being away from the chemical laboratory (not completely, however, because I was in contact with the chemists from the University and from the Technical University in Vienna, and we published jointly several papers during this period), I had more time to devote to theory. Chemical graphs were practically untrodden ground, and I could raise and solve a variety of interesting problems which attracted later the attention of many fellow graph–theoretical chemists. Thus in 1968, the first paper was published on alternative 2– and 3–dimensional infinite networks for elemental carbon (unfortunately omitting fullerenes) [65]; later on, these ideas were continued either alone [66], or in collaboration with Roald Hoffmann [67,68].

A curious incident is worth relating as concerns my paper on reactions with 6–membered transition states; initially, I sent it to *Angew. Chem.*, but the referees turned it down, and I had it published in *Revue Roumaine de Chimie* [69]. Several years later, Hendrickson published in *Angew. Chem.* a review [70] containing the same ideas, without citing my paper; I then corresponded with him, and he regretted not having known it, but I believe that the editorial office of *Angew. Chem.* should have done better. So far, I have abstained from publishing in this journal.

Benzenoid hydrocarbons, which correspond to what mathematical graph–theorists call 'polyhexes' or 'hexagonal–cell animals', continued to constitute a source of interesting problems. They had been much investigated previously by quantum chemists, but graph–theoretical correlations still offered interesting challenges. I was able to show [71] that a correlation previously advocated by Sahini [72] (between the number of 'imperfect benzenoid rings' and the resonance energies of catafusenes) was easily explained by means of zeroes in the 3–digit notation using dualists (each zero indicates an anthracenic triplet

of benzenoid rings). In addition, non–benzenoid cata–condensed polycyclic conjugated hydrocarbons raised interesting problems, such as the generalization of an earlier observation by Bochvar [73] that there exist such systems with $4n+2$ π–electrons with vacant bonding MO's or occupied antibonding MO's [74,75].

Even geometrical diastereoisomerism can be treated, as I showed when discussing the configurations of annulenes [76]; for this purpose I proposed a notation for the two directions on the three orientations of the edges on a graphite lattice, which is equivalent to the boundary code (later converted into a computer program by Trinajstić, Knop and coworkers [77]).

In 1970 C. D. Nenitzescu, then aged 68 years, died in his sleep of a heart attack. He had been the best Roumanian chemist. Having the choice between returning to Roumania (where I was promised his position as head of the chair of organic chemistry and director of the Institute of Organic Chemistry belonging then to the Roumanian Academy) or continuing for a further term of office in the IAEA, I decided to return (though the salary decreased by more than one order of magnitude). There are a few other comments that should be borne in mind: (i) research and teaching were closer to me than administration and coordination, as I was doing in the IAEA; (ii) the post–war situation in Roumania seemed the best so far, both economically and politically: Ceausescu had taken office in 1965, but in 1968 when the "Czechoslovak spring" was defeated, he had taken an anti–Warszaw Pact attitude which deceived many people; only after 1972 would the overall decline and the 'hard' dictatorship begin in Roumania.

After returning to Bucharest, I was professor of organic chemistry at the Polytechnic but not head of the chair (actually this spared me from many unpleasant administrative duties, as I was to learn when I held that position in the late 80's), and I still led the Laboratory of isotopically labelled organic compounds. I volunteered to advocate the nomination of professor Ecaterina Cioranescu–Nenitzescu as Director of the Institute of Organic Chemistry.

After 1974 when political pressure against intellectuals was reflected in compulsory applied research for all research institutes which were transferred from the Academy to economic ministries, I gave up my position in the Institute of Atomic Physics and thus my experimental research possibilities were limited to a very small group of occasional voluntary associates. Lack of computing facilities also limited my theoretical possibilities. I tried to compensate these handicaps by cooperation with foreign scientists, but the worst blow was the lack of scientific documentation, which could in no way be compensated.

In 1971 my only sister and one of the two brothers of my wife left Roumania with their families (they live now in USA and Canada, respectively); illegal defection was then considered a crime and the result for these persons was a prison sentence ('in absentia') and persecution against family members left behind.

During several years between 1973 and 1976 I was not allowed to travel abroad at any scientific meeting where I was invited. Afterwards, I succeeded sometimes to attend such scientific congresses, but more often I was absent from symposia where I was expected.

However, despite all these problems I remained an optimist trusting that the situation would improve (actually, it went worse and worse till December 1989). With the help of Ph.D. students of my own (previously I had *de facto* supervised a few Ph.D. theses for Nenitzescu's students), I opened new areas of research. One of these caused me a great worry, namely the automerization (a term I introduced for degenerate isotopic rearrangement) of [1–^{14}C]–naphthalene, where some still obscure radiochemical impurity in the degradation altered the radioactivity measurements and caused us to believe that such a reaction takes place under mild conditions in the presence of $AlCl_3$ [78]. Reinvestigation of the reaction with ^{13}C–labelling by means of ^{13}C–NMR (which at that time had to be performed abroad) compelled us to publish a disavowal of our previous results [79]. Luckily, we had observed the error in our preceding measurements at the right time, because H. A. Staab and coworkers had also detected that error [80]. Only more recently was it possible to show that such a reaction does indeed take place with phenanthrene [81] (and maybe with naphthalene under more drastic conditions, but still

far removed from those employed for thermal automerizations by L. T. Scott [82]). The whole story (so far) is presented elsewhere [83].

In the graph–theoretical area, when still in Vienna, I had been fascinated by the high symmetry of trivalent cages such as the Petersen graph with 10 vertices ([5]cage). These [*n*]cages are the minimal graphs with girth *n*. The reaction graph for rearrangements of pentasubstituted ethyl carbenium ions is a trivalent graph with 20 vertices [48], and if no isotopic labelling is present, it reduces to the Petersen graph [48,84]. An isomorphic reaction graph describes the pseudorotation of phosphoranes which have two apical and three equatorial ligands; the latter graph, described by Lauterbur and Ramirez [85], was shown by Mislow [86] to be isomorphic with the graph I had published earlier, which some chemists started to name after me till I wrote that this 20–vertex graph should be called the Desargues–Levi graph.

Further chemical applications of such reaction graphs continued to interest me, e.g. rearrangements of complexes with five [87,88] or six different ligands [89], or degenerate rearrangements of cyclic carbenium ions such as homovalenium cations [90]. Moreover, I found (by spending many pleasant hours) the first examples of [10]cages with 70 vertices [91] and what is conjectured to be the unique [11]cage with 112 vertices; I published these results in mathematical journals [92], but I know that my style is that of a chemist rather than a mathematician's approach. When I tried to apply the approach I had used for finding the still unknown [9]cages, I came upon trivalent graphs with 60 vertices, some of which have nice high symmetries and were to be published in cooperation with a few mathematicians; however, these results remained unpublished because by means of computer programs, Biggs [93] and then Evans [94] found examples of conjectured [9]cages with 58 vertices; till now, almost 20 such [9]cages have been found, none having high symmetry (unlike all other cages).

Editorial duties started to emerge. In addition to having in charge *Revue Roumaine de Chimie*, I had been one of the founding editors for the *Journal of Labelled Compounds* (after 1985 when in its title the words "*and Radiopharmaceuticals*" were added, I continued to be on the editorial board for a few years). With professors O. E. Polansky, A. Kerber and A. Dreiding, we founded "*Mathematical Chemistry – MATCH*", published in Mülheim/Ruhr where Polansky was the director of the Max–Planck–Institute für Strahlenchemie. I was then invited to be on the editorial boards of a few other journals, and I consider that constructive refereeing of papers is a significant contribution to the progress of science.

Interactions with fellow graph–theorists started to appear both in Roumania and abroad. Professors of mathematics at the Bucharest University (S. Marcus [95–97] and I. Tomescu [98–103]) asked me to propose for their students chemical problems that they could solve by using graph–theoretical or computational approaches, and as a result several joint publications emerged. I was particularly glad to arrive (with Prof. I. Tomescu [98–103] and Dr. C. Artemi [104]) at rigorous results concerning particular classes of benzenoid catafusenes using mathematical rather than chemical methods.

As a side–remark, graph–theoretical chemists have been mostly trained as physical chemists or quantum chemists, with a strong mathematical background. As an organic chemist, I have been an exception, and I had the advantage to know many relevant problems for organic chemistry. Graph theory has as one of its origins an organic–chemical problem proposed to Cayley, namely the enumeration of alkane isomers. Thus, graph theory is an ideal instrument for dealing with such problems.

In particular, graph theory facilitates the application of the "Sherlock–Holmes strategy" (encoded in several of Conan Doyle's stories about his character) which states: "When excluding the impossible, whatever remains, no matter how impropable, must contain the truth". Indeed, by means of graph–theoretical algorithms, one can find the set of all imaginable possibilities such as chemical structures or reaction pathways: then by applying chemical criteria one can exclude the impossible and select from whatever remains the most plausible alternatives.

Professor Milan Randić told me that after attending a lecture I had presented on chemical application of graph theory in R. B. Woodward's seminar at Harvard University, he decided to enter this area with now many impressive results.

With few exceptions, my Ph.D. students in Bucharest must have theses connected with experimental organic chemistry. Among the exceptions have been a few chemists graduated from other Roumanian Universities. The best of them was the late I. Moţoc, who had graduated in Timişoara with professor Z. Simon. Together we developed applications of topological indices [105–108], a field which had been initiated by H. Wiener in USA [109], M. Gordon in England [110] and the Zagreb group (M. Randić, N. Trinajstić, I. Gutman and others [111]). Among the Roumanian coworkers with whom I interacted in this field, I would like to cite O. Ivanciuc [112–114], P. Filip [115–117] and my son, T. S. Balaban [116–119] (all from Bucharest), professor Z. Simon [120,121], D. Ciubotariu [112,121,122] and M. Medeleanu [122] from Timişoara, and M. Diudea in Cluj [123]. With co–authors from Timişoara, a book entitled "Steric Fit in QSAR" was published in 1990 by Springer–Verlag as *Lecture Notes in Chemistry Series* No. 15 [124].

A fruitful collaboration with professors D. Bonchev and O. Mekenyan from Bulgaria resulted in more than 15 publications: we generalized to cyclic graphs the notion of graph center [125–126] (one paper in this field is in cooperation with Prof. M. Randić [125]), we investigated applications and intercorrelations of topological indices [127], and we published a series of 8 papers entitled "Unique description of chemical structures based on hierarchically ordered extended connectivities (HOC procedures)" [128,129]. We also published a review of topological indices [130].

With professors L. V. Quintas and J. W. Kennedy from the Mathematics Department, Pace University, New York, I published a paper on a new topological index, described further below [131], and on how to apply Pólya's Theorem for enumerating alkanes and alkyl radicals as a function of both the total number of carbon atoms and the number of carbon atoms in the longest unbranched chain [132]; the latter factor, which lies at the basis of IUPAC nomenclature, had not been taken into consideration earlier by chemical graph theoretists.

An interesting collaboration, resulting in a few joint papers on enumeration of polyhexes, was with professor S. J. Cyvin [133–136], whom I never met so far. I hope to do so in the future, because travel restrictions no longer exist.

With Dennis Rouvray (whose elegant and easily readable style did good service to the community of graph–theoretical chemists), we published a joint paper [137] and we reviewed some chemical applications of graph theory in a book chapter [138]. I published a few other reviews on this topic [139,140], one of which [140] appeared in the Silver Jubilee issue of the *Journal of Chemical Information and Computer Sciences* (before I was invited to join its editorial board).

With professor Paul Schleyer, a joint paper was published on all possible isomers of diamond hydrocarbons [141]; earlier, I had devised a coding system and an enumeration procedure for staggered conformers (rotamers) of alkanes [142]; this system was applicable to adamantane–like hydrocarbons by analogy with coding polyhexes via their dualist graphs. Actually, there are some minor differences and many analogies between the numbers of staggered alkane rotamers and those of catafusene isomers with the same numbers of vertices in their dualist graphs as the number of alkane carbons [143]. Some other collaborations with Paul Schleyer were purely quantum–chemical rather than graph–theoretical [144–146].

With professor M. Banciu (who had been a student in my first year as assistant) and the late V. Ciorba (who had his Ph.D. with me in Bucharest), we applied a systematic graph–theoretical approach for reviewing in a three–volume book the valence isomers of annulenes, benzo–, hetero– and homo–derivatives [147]. With professor Z. Simon from Timişoara and with two co–authors from the Oncological Institute Bucharest, we published a book on "Modeling of cancer genesis and prevention" in which I contributed the part on using topological indices for correlation with biological activities [148]. Earlier, I had published a paper with professors K. Balasubramanian, W. S. Koski and Joyce J. Kaufman on how to compute structures of carcinogenic polycyclic hydrocarbons [149].

Present areas of interest in theoretical chemistry. There is a great difference between pre– and post–1989 life in Eastern Europe. Political freedom makes it now possible to travel

abroad without an internal exit visa (of course one has to obtain entry visas and to have the financial support for travel and subsistence). Research and teaching, as well as day–to–day existence in Roumania, still have to overcome economic hurdles. Although personal computers have become almost commonplace in research institutes and universities, there are still no computers at home.

There are three major handicaps against which one has to fight. Lack of chemicals can be compensated by long syntheses starting from simple materials. Lack of advanced instrumentation (or, what is more depressing, of spare parts for existing instruments because of the scarcity of hard currency) can be compensated by cooperation with foreign universities; many of my younger coworkers are now on doctoral or post–doctoral stages abroad, mainly in France and USA, and this is one form of such cooperations. Lack of documentation, however, cannot be compensated at all. The present situation is worse than before the 1989 Roumanian Revolution because earlier one could buy books and journals from Eastern Europe in "soft currency", while now everything has to be bought in hard currency.

Personally, I have been blessed by the possibility to stay abroad for several months each year in the company of my wife. My teaching duties in the Polytechnic University Bucharest have been concentrated in the winter semester; I am now teaching organic chemistry in Roumanian, and we also have classes entirely in English, French and German so that I am also teaching general chemistry and organic chemistry in English. I am also consulting for two new private universities in Bucharest (the Hyperion University and the Ecological University).

In the spring–summer semester of 1990 I spent two months at the University of Leipzig completing my assignment as "Wilhem–Ostwald Lehrstuhl–Inhaber für Theoretische Chemie". During that time I completed writing the monograph on pyrylium salts for "Houben–Weyl's Methoden der Organischen Chemie" with professor Werner Schroth from the Martin–Luther–University, Halle [150].

Though our friend from Lund (Sweden) Salo Gronowitz and I never co–authored a paper, I owe him and his wife, Rella, my gratitude for providing me for many years with a beta–blocker and anti–arythmic drug that could not be found in Roumania.

An earlier cooperation in theoretical chemistry with professor Jose Elguero from Madrid continued recently with several joint papers on aza–derivatives of cage hydrocarbons [151].

Since 1991, I have spent six months per year in the USA: three months in 1991 with professor L. B. Kier from the Virginia Commonwealth University, Department of Medicinal Chemistry (with whom we published three joint papers on QSAR using topological indices) [152–154] and the remaining time at the Texas A & M University in Galveston, with professors D. J. Klein, W. A. Seitz and T. G. Schmalz. In Texas, I also met an old friend, professor D. Bonchev from Bulgaria, who is on an extended stay in the USA. Several joint papers were published with the Texas colleagues [155–160]. It was also of interest to be able to attend several meetings and symposia in the USA, France and Germany. This brings the discussion to its conclusion, by indicating the present areas of interest in theoretical chemistry.

Topological indices (TIs) are numbers associated with chemical structures, i.e. with constitutional graphs. This is not a one–to–one association because several nonisomorphic graphs may have the same TI, i.e. may be degenerate. For QSAR/QSPR this degeneracy is not as critical as it is for other uses of TIs, such as for discriminating among, and ordering of, isomers, or (as an ultimate goal) for coding molecular structures.

Topological indices are useful tools for quantitative structure activity (property) relationships (QSAR, QSPR). In 1979 I had proposed a new approach for centric topological indexes of alkanes [161], followed by generalization to arbitrary graphs [162]. In 1982, I devised a new TI, denoted by J, which at that time was the most discriminating one [163]. Unlike previous TIs, it was devised so as not to increase automatically with the number of the vertices in the graph, but to take into account only the degree of branching. Interestingly, for an infinite linear alkane, J becomes equal to the number π [164]. The low degeneracy [131] and the correlational ability of J in multiparametric correlations make it useful for QSAR studies [152,165], especially since it

can be modified to take into account the presence of multiple bonds, molecular fragments, and/or heteroatoms [115,166,167]. I reviewed some properties of TIs at an IUPAC symposium [168], and showed that octane numbers of alkanes correlate well with simple TIs [105]; more recently, such correlations were extended to alkenes and aromatics [154].

So far, all new TIs were based upon traditional approaches, starting from the simplest numerical invariants that could be associated with molecular graphs: *vertex degrees* are associated with the adjacency matrix, and indicate whether an atom is primary, secondary, tertiary or quaternary as in the case of alkanes, by assigning degrees 1, 2, 3, or 4, respectively; *distance sums* are associated similarly with the distance matrix, but have no other limitation than being integers. Such numbers do not depend on vertex numbering, and are therefore called local vertex invariants (LOVIs). The integer TIs based on integer LOVIs have high degeneracy and are considered to be first–generation TIs. Second–generation TIs are real (non–integer) numbers, and are also based on integer LOVIs, but are derived from them via more sophisticated operations; they are therefore more discriminating; examples are Randić's molecular connectivity, Kier and Hall's extended molecular connectivities, and my index, *J*.

Lately, the efforts of my group of coworkers in this area have tried to develop new methodologies for devising real–number LOVIs for third generation TIs [169,170]. Six types of such non–integer LOVIs were invented, thereby extending greatly the available tools from which new TIs may be assembled. Indeed, so far only two integer LOVIs had been used, but now a whole battery of real–number LOVIs is at the disposal of theorists.

A brief enumeration of the new LOVIs follows: (i) solutions of linear equation systems, based on triplets of a matrix and two column vectors [114,117,171]; (ii) regressive vertex degrees [123] and regressive distance sums [172], which take into account the decreasing contributions of more remote vertices; (iii) eigenvectors for selected eigenvalues of the adjacency of distance matrices [122]; (iv) information–based LOVIs obtained from topological distances on each of the graph vertices [119,173]; (v) LOVIs in the real–number range from zero to one, obtained by combining exponential operations with sums and products of vertex degrees [174]; (vi) by changing the concept of topological distances, one can reason in terms of reciprocal distances [175,176] or of resistance distances [176], and obtain from them new TIs termed Harary numbers and Kirchhoff numbers, respectively.

All new TIs based on distances or on modified distances [112,175,176] may easily account for the presence of multiple bonds and/or heteroatoms. For molecular fragments (substituents, widely used in molecular modeling and drug design) [166] it is also possible to devise mathematical models either by weighting the attachment atom (root vertex) [115], or by constructing the symmetrical dimer molecule from two identical substituents [177].

Another theoretical area of interest has continued to be centered on benzenoids (polyhexes). In addition to cooperations with professor I. Tomescu and Dr. C. Artemi from Bucharest, as mentioned earlier, I benefitted from collaborating with professor S. Cyvin and his research associates, and we published jointly a significant number of papers, taking into account the symmetry group of the corresponding benzenoid [131,134,136,156,178,179]. One of these papers, based on a computer program specially devised by professor D. J. Klein and Dr. X. Liu from the Texas A & M University [156], reports an interesting 3– and 4–periodicity in terms of the number h of condensed benzenoid rings, for the benzenoids possessing the largest numbers of the Kekulé structures for a given h. I was invited to lecture on this finding at the International Symposium on Novel Aromatic Compounds held in Victoria, B. C., Canada in 1992 [83].

The interaction with the colleagues at the Texas A & M University involves mainly research on fullerenes and on other forms of carbon such as diamond–graphite hybrids [157], or graphitic cones (a topic that I also presented in Victoria) [83].

Professor Tibor Braun from the Budapest University, a long–time friend (we had been fellow radiochemists in the Institute of Atomic Physics in Bucharest) who edits the new journal "Fullerene Science and Technology" invited me and two colleagues from Galveston, professors D. J. Klein and W. A. Seitz, to join its editorial board.

Professor István Hargittai, a member of the Hungarian Academy of Sciences,

asked me to contribute to his volumes on symmetry, so I published one paper on "Symmetry in chemical structures and reactions" [180] and another one on "Carbon and its nets" [166].

On the mathematical side I was invited by professor J. W. Kennedy and L. V. Quintas to attend the symposium "Quo Vadis Graph Theory?" in Fairbanks, Alaska in 1991. In the company of professor Milan Randić, we were two graph–theoretical chemists interacting with first–rank mathematical graph theorists [181].

I would like to conclude with trying to provide a reply to a question that I was asked several times, namely why I did not leave Roumania. There were several reasons for this, the first one being that I felt I could do for this country what some predecessors like Nenitzescu had done. When the situation in Roumania became so bad after 1973 that many people emigrated, I could not contemplate the idea to become separated for a long time from my family, to be condemned "in absentia", and to give up for an undetermined period of time both teaching and research that I enjoyed so much. Luckily, having close relatives that lived abroad, I was spared "invitations which one could not refuse" for becoming involved politically. Like Heisenberg or Laue during Hitler's time in Germany, I and other Roumanian intellectuals had waited for Ceausescu's dictatorship to end, in order to provide a continuity link for the younger generation.

I had never been able to study abroad during my scientifically formative years, and now I try to facilitate such studies for young people either via personal contacts in France, USA and Germany, or by using official channels such as the TEMPUS programme offered by the European Community.

Looking back, I think that there may be some truth in the motto we had on the wall of our laboratory: "For weaker characters, difficulties provide opportunities for excuse; for the stronger ones, they are challenges stimulating efforts to overcome them."

Four years ago the future seemed almost hopeless, as it had for over a decade. But now I am confident that Eastern and Central European countries (if they will be able to avoid becoming involved in military conflicts such as those occurring in ex–Yugoslavia and confronting the ex–USSR), will overcome their present economic difficulties: their young and creative minds will then join efficiently the international community engaged in the never–ending collective effort of deciphering our universe.

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