**MATCH** Communications in Mathematical and in Computer Chemistry

# Autobiographical Notes 80 Years of Age, 68 Years of Chemistry

# Alexandru T. Balaban

Texas A&M University at Galveston, Marine Sciences Dept., Galveston, TX 77553, USA

## Childhood and Adolescence, 1931-1949

In Roumania,<sup>1</sup> where I was born, a weekly magazine called *Journal of Sciences and Travels* had a page for amateur chemists, which as a teenager I was eagerly awaiting to read. Every few months there was a competition with problems and prizes (I won a few times) alternating with brief communications submitted by youngsters. My first contribution was published there in 1943, and it described how one can observe "light flashes in a liquid – on dropping small crystals of potassium permanganate into molten naphthalene". My parents and I were living in a rented apartment on the upper floor of a house whose owners lived at the ground floor, and on the enclosed terrace I had an improvised laboratory: instead of running water I had a large metallic container with a faucet and a bucket for spent waste; instead of a Bunsen burner I had an alcohol lamp made from an inkpot with a wick made of cotton wool. Whenever my parents or relatives wished to bring me presents, I preferred to get money to buy chemicals from a pharmacy specializing in supplies for amateur chemists (there were almost no restrictions, which would be inconceivable nowadays – I was buying small amounts of concentrated acids, metallic mercury, and all other kinds of chemicals).

<sup>&</sup>lt;sup>1</sup>Roumania is a country in Eastern Europe between the Carpathian Mountains and the Black Sea. Roumania joined the European Union in 2007; it is the ninth largest country of this Union by area and with 21.5 million people has the seventh largest population of the European Union. Several spellings for it circulate; herein I use *Roumania*, although the current official denomination (since 1965) has been *Romania*.

My father, Teodor Balaban, was born in a village in the Roumanian region Moldavia<sup>2</sup> called Bălăbăneşti (with a station on the railway connecting the town Bârlad to the town Galați on the Danube; in 2010 this village commemorated its 550<sup>th</sup> documented anniversary). My paternal grandfather had been a teacher in that village. An older brother of my father, Alexandru, became a professor of Roumanian and French languages and literature at the Bârlad high school, and had helped financially my father during his studies in Bucharest to graduate as an electromechanical engineer. In gratitude, I bear the name of my uncle. My mother was born in Iaşi, the capital city of Moldavia, from a family of writers (my maternal grandfather, George Botez-Gordon, was a poet) and Orthodox Church high prelates (my maternal grandmother's last name was Scriban – two of her uncles were a well-known linguist and an Archimandrite (equivalent to Bishop). My mother had become an instructor for preschoolers, and had published studies on teaching methods for improved preschool learning.

My parents had met in Moldavia, and after their marriage they moved to Reşiţa,<sup>3</sup> where Roumania's locomotives and all metallic pieces that had been used for the Eiffel Tower were built, close to Timişoara where I was born on April 2, 1931. Till I was 13, I have been an only child. My parents had both become orphans at an early age. They paid a lot of attention to my education, encouraging my fascination with chemistry. After 1935 my parents moved to Bucharest, Roumania's capital city. During the summer holidays, I went for three months to a village, Odaia Bursucani, close to my father's birthplace, with my paternal aunts and my cousins (Professor Alexandru Balaban's children). In my parents' Bucharest home, we had lots of books in Roumanian and French, and my father prompted me to learn foreign languages. In middle school French was mandatory, and after 1942 also German, but then, after 1945, only Russian was taught. I will mention later how I learnt English. I had similar-age friends from neighboring houses (especially Silviu Teleman and his younger brothers) who shared my interests in chemistry, and in turn, they showed me how much charm there is also in mathematics.

In 1939, Hitler and Stalin signed a pact that allowed Germany to start the 2<sup>nd</sup> World War, and therefore I consider that these two monster-criminals are equally responsible for this war. This "Ribbentrop-Molotov pact" signaled the division of Poland between Germany and USSR, gave Roumania's Northern Transylvania to Hungary and Eastern Moldavia (Bessarabia, which became the Moldavian Republic in the Soviet Union) as well as the Baltic States to the Soviet

<sup>&</sup>lt;sup>2</sup>Roumania emerged historically from the union of three principalities/regions: Wallachia (South), Moldavia (East) and Transylvania (North-West). One needs to make a distinction between Moldavia and today's Moldova, an independent country, most of which had belonged to Moldavia till 1812 and to Roumania between 1918 and 1940.

<sup>&</sup>lt;sup>3</sup> In this text I am using for cities and names the Roumanian spelling with s = sh, t = ts, a and a slight variants for a.

Union. Roumania's entry into the war against USSR was partly motivated for recovering Bessarabia, but Roumania also provided Germany's petroleum, and thus it was forced to continue after the old border had been reached.

My father was drafted as an artillery lieutenant and for two years, he was on the front against USSR, from Bessarabia to Crimea. On comparing photographs, before he left and after his return, one can hardly believe that the difference is of only two years. In 1945, our family moved to the coal-mining district of Roumania, in Petroşani, where for four years I was in high school. My chemistry teacher entrusted me with the keys to the school's laboratory, where I finally had access to running water and Bunsen or Teclu gas burners. By now I was familiar with French and German, and my father insisted that I start with English, which was not taught in schools (although Russian was the only foreign language that was taught in schools, it was hard to learn because of its non-Roman alphabet).

At that time, the political situation in Roumania was becoming dominated by the increasing conflict between democracy and communism, and Roumanians were hoping for American support, without knowing that at the Yalta Conference Churchill had traded Roumania for Greece with Stalin. Then after 1946, the Iron Curtain fell over Eastern Europe. I started learning English by listening in for *English by Radio* from the British Broadcasting Corporation (BBC). Sometimes I changed wavelengths and listened to BBC programs in French. In 1947 I caused a great scare to my parents when I received from the BBC a book as a prize for a competition in which I had enrolled. It was a time when one would be imprisoned for listening to Radio Free Europe or BBC, but luckily for us nothing happened (however, one of my teenager friends in Bucharest was arrested during that time for having frequented the American library).

My uncle, who had been the mayor of Odaia Bursucani, was arrested during those years and died in prison. By falsifying elections with the blessing of Soviet occupying troops, communists seized power in Roumania in 1946, and a wave of terror started. Earlier prominent political officials, priests, and influential journalists or writers filled the prisons. The Roumanian Academy was "reorganized" by expelling all those that had a political past.

During the summer holidays, with either my parents or my school colleagues, we now admired the Carpathian Mountains close to Petroşani in long excursions. I also enjoyed various sports such as skiing or skating in winter, bicycle trips or jogging in the summer. Reading from my parents' library in Roumanian and French during rainy days and starting to love poetry was also a favorite occupation. I tried to solve mathematical problems that I had imagined, such as computing all the solid angles in regular and semiregular polyhedra (including stellated polyhedra), and I found a simple formula for solid angles formed by up to four straight lines emerging meeting at a vertex, that is probably known, but I did not find it in the literature. I also solved what now I know to be a naive problem (the geometry of a sequence of six identical regular tetrahedra, each sharing one vertex with two neighboring tetrahedra such that their centers form a planar regular hexagon in order to model benzene with bonds that are intermediate between single and double). During all my study years, I had always been at the top of my class, without effort, and I could memorize easily long poems that I recited at various festivities. Learning and speaking foreign languages came easily for me, although I am told that I speak with a slight lisp. When in 1949 the time came for choosing the direction for a career, I hesitated between mathematics, physics, and chemistry, I decided for the last one. Then again, there were two choices – either the Bucharest University (Faculty of Chemistry) or the Bucharest Polytechnic (Faculty of Industrial Chemistry), and again I chose the latter because an older friend had told me about the better professors there.

## Polytechnic University Bucharest, 1949-1956

After the war with its destructions, there was a shortage in housing. In Bucharest, I stayed with the family of my mother's sister, within walking distance from the Polytechnic. Housing and accommodation in Bucharest posed difficult problems, and when in 1951 my father's work required that my parents return to Bucharest, they had to wait until a distant relative vacated a part of an apartment. There was no place for me to stay with them; my sister, who is younger than me by 13 years, stayed in a room through which people who shared the apartment were passing (as in movies like *Doctor Zhivago*, or *Ninotchka*).

During the summer holidays, students were required to fulfill a one-month practice at industrial plants. I had the bad luck that during the summer of 1950 at the end of this practice period, when helping two women-technicians to carry a large glass container of concentrated nitric acid, this container broke and I got severe burns on my feet. The whole winter semester I was confined to bed and I still have the scars from those burns. When during the spring semester of the 2<sup>nd</sup> year and the next two semesters I listened to the enchanting courses of organic chemistry by academician Costin D. Nenitzescu (1902-1970) surnamed 'the Magister', I was bewitched. Together with a few colleagues selected on the basis of our grades, we were allowed to join in the Magister's research groups. We were encouraged to synthesize as many representatives of various classes of organic compounds as possible – this was the German system. Nenitzescu, after having obtained his PhD degree with Hans Fischer in Germany (Nobel

Prize for Chemistry in 1930) and returning in 1925 to Roumania, had already made important discoveries, namely three "name reactions": two indole syntheses and the reductive acylation of aromatics. I know now that one has to become an apprentice for learning how to make discoveries in science. During the last two years of my university studies, I was selected to be one of the very few students who were awarded a substantial allowance, on the basis of the grades I had got at all disciplines.

For several years during and after the war, doctorate studies had been discontinued, and western chemical journals became unavailable, but in the early 50s they started to arrive in a few libraries and it was again possible to learn whether a substance was new or not, by searching the repository of all known compounds. Nowadays this is facilitated by computer search engines, but at that time, chemistry was still mainly a German science via *Chemisches Zentralblatt* (however, soon this was going to be changed by *Chemical Abstracts* of the American Chemical Society). Knowing the molecular formula of a substance, one had to look at the indexes of these repositories, and one needed also to know the rules of chemical nomenclature for various isomers. What now can be achieved in one minute needed at that time several hours or days.

Doctorate studies were reinstituted for the first time after the war during the autumn of 1953, after I had completed the 4<sup>th</sup> year in the Polytechnic. The doctorate studies were modeled after the Soviet system with admission exams once a year for a three-year stipend. With Professor Nenitzescu's recommendation, I had the good luck to be allowed to graduate as chemical engineer in 1953 in order to participate in this exam and to become a PhD student ("aspirant"), being exempted from preparing the graduation thesis for one more semester, like all my fellow colleagues who graduated only in the summer of 1954. One of these colleagues, Cornelia (Nelly), was to become my wife in 1955, but then she was going to have a higher salary than my meager stipend. What had initially tied us together was her need to learn English for keeping up with chemical literature, and my offer to help by writing for her the English poems that I knew by heart and I cherished.

The topic of my PhD work was in a field that Nenitzescu had started before the war, namely reactions catalyzed by anhydrous aluminum chloride. After three years, when my stipend ceased, I was appointed as Assistant Professor and I needed three more years in order to finalize and defend my PhD thesis on April 2, 1959. They had been exciting, with full day's work (and sometimes also late into the night). I had clarified with experimental evidence the mechanisms of two AlCl<sub>3</sub>-catalyzed reactions: the reaction of alkanes and cycloalkanes with carbon monoxide, and the Scholl reaction (dehydrogenating condensation of two aromatic rings) which at present, in the laboratories of Klaus Müllen, with improvements due to using copper(II) cations, serves

for constructing giant aromatic molecules. Even more interesting, I had serendipitously discovered that alkenes could be diacylated to pyrylium salts, a "name reaction" known as the Balaban-Nenitzescu-Praill reaction. This was due to the observation that on studying the AlCl<sub>3</sub>catalyzed reaction of carbon monoxide with *tert*-butyl chloride I found (in addition to products that supported the newly proposed reaction mechanism) crystals of a mysterious product. Nowadays the structure would be found without difficulty by means of physical methods, but it took more than a year until I realized that it was a pyrylium salt formed in a single step by combining five molecular fragments together. The results of my thesis were published during 1960-1961 in 15 papers, three of which appeared in the Journal of the Chemical Society (London) back-to-back with a paper by Percy F. G. Praill who had also discovered independently the same reaction. We became good friends with Percy during the following years. I would like to mention that the vast majority of Nenitzescu's papers had been published in German language. in German chemical journals. The first three of the 15 papers went in the same direction, but for the following ones I suggested to have them in English, and Nenitzescu accepted (he could read English, but did not speak). Moreover, for the first time in his publications, most of these publications did not have Nenitzescu's name as first author. In 1961 Nenitzescu was invited by George A. Olah to contribute with two chapters to the multi-volume monograph that he intended to edit for the Wiley Publishers entitled Friedel-Crafts and Related Reactions, and the two extensively updated literature reviews from my PhD thesis (about the Scholl reaction and the aliphatic acylation) became two chapters in Olah's monograph that appeared in 1963, coauthored by Nenitzescu and me. In 1994 George Olah was awarded the Nobel Prize for Chemistry.

In the Scientific Genealogies of Physical and Mechanistic Organic Chemists (a kind of "paternal-doctor-relationship") which used to be distributed on the World Wide Web by Professor John Andraos from the University of York, Toronto, Canada, one could read the following scientific genealogy (one of Liebig's trees): Justus Liebig – Heinrich Will – August Kekulé – Theodor Zincke – Hans Fischer – Costin D. Nenitzescu – Alexandru T. Balaban.

In December 1955, Nelly and I tied the knot. My wife was at that time a research scientist in the largest chemical research institute in Bucharest. With the help of Nelly's brother (who is a famous Roumanian theater and movie actor), we were able to obtain a room in a two-bedroom apartment, shared with another family. One year later, we swapped that room with the person from my parents' apartment.

As an Assistant Professor in the Department of Organic Chemistry headed by Nenitzescu, I continued the study of pyrylium salts and published the future findings made with collaborators from this Department together with Nenitzescu. As will be seen below, I also studied other aspects of pyrylium salts, namely their physical properties, in another laboratory, publishing the results with my collaborators from that laboratory. I read with much interest books on quantum chemistry by Charles Coulson and Michael J. S. Dewar. Around 1958-1960 I tried unsuccessfully to attend Coulson's summer school in quantum chemistry in Oxford. In 1959 I published in Roumanian a study of the atom types that can form aromatic rings (more about this in the next paragraph), and I came to the conclusion that boron-containing aromatic rings should be quite interesting. Earlier, I had asked Nenitzescu if I may investigate such compounds, but he replied that I should concentrate on finishing my PhD thesis. However, I wrote a letter about this to M. J. S. Dewar at the Queen Mary College of the University of London, and from his reply I learned that he was already studying such compounds (indeed, he published about boroxaro and borazaro derivatives afterwards).

The systematics of monocyclic aromatic compounds mentioned above was an ambitious project, in which I intended to look for all possible combinations of atoms capable of forming aromatic rings. For simplicity I restricted the initial discussion to First-Row atoms such as B, C, N, and O, which may possess in the non-hybridized orbital 0, 1, or  $2\pi$ -electrons (according to the Pauli Principle, and denoted as Z-, Y-, and X-type). Then the ring  $X_x Y_y Z_z$  yields two Diophantine equations that result from the Hückel Rule and the ring size. I learned later that Alan R. Katritzky in England had submitted a manuscript with similar ideas for publication, but it had been turned down by the *Journal of the Chemical Society* (his notation had been almost the same, with reversed X and Z symbols (mine had intended to be mnemonic, with Z evoking zero).

Unknowingly, I had arrived at the famous graph-theoretical "necklace problem" for enumerating all possible necklaces formed by *m* beads of three colors, and Silviu Teleman had helped me but it was his suggestion to write to Frank Harary which brought the most substantial help. My efforts to collaborate with Roumanian graph-theorists were turned down; however, Frank provided considerable help during the following years. He travelled so often that he soon came to visit me in Bucharest, and we published together nine papers during the next years. I had already begun to read about graph theory but Harary's excellent treatise had not yet appeared. Two graph-theoretical problems had emerged out of Nenitzescu's research: (1) with Margareta Avram, he had initiated a program about synthetic approaches to butadiene, and as a side-product they had obtained the *Nenitzescu Hydrocarbon* (CH)<sub>10</sub>, a valence isomer of [10]annulene. The enumeration of all such isomers is equivalent to enumerating all cubic multigraphs with 10 vertices, and in 1966 I published a paper to that effect; (2) with Ileana Necşoiu, Nenitzescu had postulated a mechanism for hydrocarbon oxidations with hexavalent chromium derivatives that involved carbocations, and this gave me the idea to invent *reaction graphs*: unlike the common molecular graphs in which vertices symbolize atoms and edges symbolize covalent bonds, in -14-

reaction graphs vertices symbolize reaction intermediates, and edges symbolize elementary steps. The reaction graph of an ethyl carbocation with five substituents replacing the hydrogens leads to the Petersen graph (5-cage) if the two carbon atoms are not isotopically distinguishable and to the Desargues-Levi graph when they are. I made a cardboard model for this graph in the form of a regular dodecahedron whose pentagonal faces were replaced by inner edges so that there was no five-membered circuit, and this model stayed on Nenitzescu's desk for about one year, when finally he told me that I should publish this idea. Interestingly, soon after I had published this paper in 1966, Fausto Ramirez and coworkers published the reaction graph for the turnstile rotation of phosphoranes with five different substituents; this graph is identical to the Petersen graph when enantiomerism is ignored, and to the Desargues-Levi graph when one takes enantiomerism into account. This topic has drawn the attention of famous chemists: Vlado Prelog, Jack Dunitz, and Kurt Mislow, with the latter emphasizing my priority.

#### Institute for Atomic Physics (IFA), 1956-1966

Another stroke of luck happened in 1956, when Roumania imported from USSR a nuclear reactor and a cyclotron, and the authorities decided to initiate an Institute for Atomic Physics (IFA) in the vicinity of Bucharest. For training the personnel, about 150 young graduates in physics, chemistry, and electronics were selected and were offered intensive courses for a whole year in nuclear physics and radiochemistry (an abridged physical faculty, without nonscientific courses). I accepted the offer, and unlike my colleagues who were on leave from their jobs during this time, I continued my activity as Assistant Professor and research in the Department of Organic Chemistry, a position that I kept for several years along with my research scientist position in IFA. Then in 1957-1960, I assembled a group of about a dozen fresh radiochemists in the Laboratory of Isotopically Labelled Organic Compounds. Our aim was the synthesis of <sup>14</sup>C- and <sup>3</sup>H-labelled compounds (a sister laboratory was in charge of other radioisotopes) for studying reaction mechanisms or biochemical applications.

In 1958, my son, Teodor-Silviu, was born, and in the same year for the first time after the war, a scientific exchange took place with western countries when several Fellows of the Royal Society came to visit the Roumanian Academy. Two members of the delegation were chemists: G. R. Clemo and William A. Waters. I was asked to translate their lectures (and later to accompany them in a visit to the University of Iasi). My wife was quite anxious because this required me to stay close to the lecturer on the podium, to memorize what was said in several sentences, and then to translate. However, all went well. Later, when Alan Katritzky and his

family visited Bucharest, I also translated his lecture, and we became long-life friends, without knowing that our chemical paths would cross several times during our lives. The first collaborations with Alan were published in 1962, 1964, 1967 after he helped with NMR spectra of my new compounds. Alan decided to include me on the Editorial Board of the book series *Advances in Heterocyclic Chemistry* that has reached in 2010 its 100<sup>th</sup> volume.

For help in planning and building laboratories designed to handle radioactive products I made my first trip abroad for two weeks in November 1958, to visit the Central Nuclear Research Institute in Dresden-Rossendorf, and the several institutes in Leipzig and Berlin in Eastern Germany. Later, in 1961 I was for two months in Moscow for practice in working with <sup>14</sup>C-labelled compounds. However, back in the IFA laboratory we also attacked other purely organic-chemical topics that were relevant to physical research: (i) we synthesized 2,5-diaryloxazoles as scintillators for detecting nuclear radiations (in a collaboration with Professor Nenitzescu's wife, Ecaterina Ciorănescu, I discovered a new synthesis of oxazoles); (ii) for the IFA laboratory that was in charge with electron spin resonance instruments, I synthesized stable free radicals such as 2,2-diphenyl-1-picrylhydrazyl, and on the basis of new analogs with only two nitro groups I hypothesized on push-pull electronic stabilization of aminyl free radicals, but I found later that M. J. S. Dewar had published a comprehensive study on similar phenomena; (iii) I did investigate boron-containing compounds, and after synthesizing new tropophenylene chelates that I predicted to have high dipole moments, I sent samples to Sutton in England for measuring the dipole moments, verifying experimentally this prediction.

My third stroke of luck was in 1963, when I was announced that I had been elected as a corresponding member of the Roumanian Academy. As I understood later, academician Horia Hulubei, a prominent physicist who had worked with Perrin and the Curies in Paris and was then the director of IFA, had made the proposal, and professor Nenitzescu had seconded it. I was at that time the youngest of all newly anointed corresponding members (among them, two of my professors in the Bucharest Polytechnic – and one of them was Ecaterina Ciorănescu), and only once during the previous century had a younger person been elected as corresponding member. This election was a considerable honor, and it also brought several responsibilities, such as helping Professor Nenitzescu, who was the Head Editor of the Academy's chemical journals, to reformat them, raising their standards; till then *Revue Roumaine de Chimie* was publishing mainly in French and German, and now it was intended to become a mostly-English journal (with my polishing of all manuscripts).

After this election in the Roumanian Academy, most of my travels abroad were supported by the Academy during the next ten years. Now my presence in the Department of Organic Chemistry as Assistant Professor was something of an embarrassment for the older coworkers of Nenitzescu, so that I was offered a promotion as Associate Professor in the Department of General Chemistry. I had to present lectures on general chemistry to non-chemists, which I did for several years for students of Electronics and Mechanics of the Bucharest Polytechnic.

Other consequences of the election in the Academy were that I was allowed to attend international congresses (1963: 19<sup>th</sup> IUPAC Congress in London and 7<sup>th</sup> European Congress of Molecular Spectroscopy in Budapest where I talked about pyrylium salts). In 1964, after attending the Symposium on isotopically labeled compounds in Italy, I was one of the founders of the *Journal of Labelled Compounds* (now the name includes also *Radiopharmaceuticals*). I was also able to accept invitations for lecture tours (1964: West Germany and Czechoslovakia; 1965: India). In 1964 three members of the Roumanian Academy participated in the Symposium on Reaction Mechanisms in Cork, Ireland: C. D. Nenitzescu, his wife Ecaterina Cioranescu, and I. In 1965 I attended both symposia on aromaticity in West and East Germany in Bonn and Leipzig, respectively (with a plenary lecture at the latter symposium) occasioned by the centennial anniversary of Kekulé's theory. One year later I attended the London symposium on aromaticity, and two conferences on free radicals in solution in Ann Arbor (my first transatlantic travel) and in Schloss Elmau, Germany.

In 1965 Nicolae Ceausescu became the dictator of Roumania. His wife, Elena, was handed a diploma of chemical engineer and a PhD degree from the Bucharest Polytechnic without attending courses and had been appointed the Director of the country's largest applied research institute in Bucharest. An official visit to France took place in 1966 for a group of about 15 Roumanian scientists and industrialists that included me and Elena Ceausescu and was headed by a highly-situated person in the hierarchy of the Ministry for Chemical Industry. Since I had already published about 70 papers in refereed journals, my name was the only one known from the chemical literature by the hosts of the French National Center for Scientific Research. I was later told that along with the fact that I was the only person fluent in French from the group, this caused bitter animosity to Elena Ceausescu.

Nelly's health had deteriorated because of the toxic atmosphere in her laboratory due to mercury and vanadium. She changed jobs, and became Assistant Professor in the Department of Chemical Engineering of the Bucharest Polytechnic Institute. Her health improved rapidly, and in 1966, our daughter was born: Irina-Alexandra, who is eight years younger than our son. Then in 1967, we were presented with an unexpected offer: the International Atomic Energy Agency in Vienna had a vacancy in the Chemistry Section of the Division of Research and Laboratories, and my name could be included as one of the possible candidates. We were told that in order to

take care of the children, Nelly would be granted an extended leave, and that our parents would be allowed to join us. I would no longer teach, but every two months I would fly for a few days to Bucharest where I was still in charge of the IFA laboratory. I accepted, and was appointed as United Nations International civil servant (P5 research officer) for three years. Thus began a different type of existence, with more financial and political liberty than my family and I had experienced in the after-war years.

## International Atomic Energy Agency (IAEA), Vienna, 1966-1971

I could now travel with my wife (our parents came pairwise to stay with us in Vienna and take care of the children when we were away) after both of us acquired our first car and got our driver licenses. In 1968 I accepted invitations for lecture tours in Switzerland where we met Valdo Prelog, in Italy, in West Germany, in England (where Nelly would help me cross roundabouts when driving on the "wrong" side of the road), and in Czechoslovakia (where I gave a plenary lecture at the Conference on Heterocyclic Chemistry). However, she would not accompany me in airplane travels because of the risk for our children of remaining orphans. During the week, I flew to Israel to visit the institutes in Rehovoth another El-Al plane was blown up. In USA I visited and lectured at Argonne, Brookhaven and Oak Ridge National Institutes. My job at IAEA was mainly on radiopharmaceuticals and I traveled several times to the World Health Organization in Geneva as IAEA's representative for the monographs on labeled molecules and radiopharmaceuticals edited and published in Vienna. The negotiations with private companies such as Amersham concerning open disclosure of economically viable procedures were sometimes tedious but always polite. Also, as a consultant for Albania and Latin American countries I had to travel to Tirana, Mexico City, Sao Paulo, and Buenos Aires, being the scientific secretary for several meetings involving Latin American countries.

During my stay in Vienna, I attended the weekly chemical seminars in the University and Technical University. As a side remark, I remember that when Professor Gutmann introduced the lecturer at one of the seminars at the latter University announcing that there is a parallel between a scientist's name and his special field, he said, "I am Gutmann working in Inorganic Chemistry, and the lecturer is Bestman working in Organic Chemistry".

For her PhD work, my wife carried out occasionally experiments in chemical engineering at the Vienna Technical University. I also carried out some laboratory research at the IAEA laboratory in Seibersdorf, close to Vienna, and for NMR spectra, I collaborated with a chemist at the Vienna University. In collaboration with Professor Werner Schroth and his coworker Dr. Gerhardt W. Fischer from the University of Halle, I published in 1969 the first part of a review on pyrylium salts in volume 10 of *Advances in Heterocyclic Chemistry*. By an oversight on my part, I had sent to Alan Katritzky the manuscript indicating the address as East Germany instead of German Democratic Republic, and this caused some political trouble for my German friends.

In my spare time, I tried to solve graph-theoretical problems, and I became intrigued by the fact that trivalent cages were known for girths 3 to 8 and 12, but there was a gap for girths 9, 10, and 11. With symmetry as a guide and with my observation on how smaller cages can be obtained from larger cages I found a trivalent graph with 70 vertices and I conjectured that it was a 10-cage, but I did not publish this result until a few years later. Only much later was it proved to be indeed the first 10-cage (two other ones were discovered later) by mathematicians using arrays of computers working for long time; a similar computational effort proved that another conjectured trivalent graph with 112 vertices to be the unique 11-cage. Both these cages are known as "Balaban graphs"; the *Balaban 10-cage* appears on the cover of the book *Pearls in Graph Theory* by N. Hartsfield and G. Ringel. In an international effort that included Coxeter, Frucht, Harries, and Evans along with me, we had found several nice, highly symmetric graphs with 60 vertices and girth 9, but before anything was published about them, Norman Biggs published a paper about the first 9-cage with 58 vertices. It is now known that there are eighteen 9-cages, all with low symmetry.

I published a few papers together with Frank Harary on using Polya's Theorem for enumerations and on employing dualists (inner duals) of benzenoid graphs as simple means for distinguishing cata/peri/corona-fused benzenoids and for codifying catafusenes. Another joint paper reminded the chemical community that the characteristic polynomial of a graph does not characterize it uniquely.

Young chemistry professors in Roumania were publishing books and this activity helped in their promotion. When I was asked why I did not yet publish any book, I replied that I would not publish books on topics that could be found in other books. Also, because the Roumanian language is spoken by the smallest number of people from the five main Neo-Latin languages (French, Spanish, Italian, Portuguese, and Roumanian) I preferred publishing mainly in English. During the time I was in Vienna, I started editing a book on *Chemical Applications of Graph Theory*, the first of its kind, having contacted several specialists in the field, but it would be published only in 1976. However, mention should be made that Vlado Prelog signed his foreword to this book on July 18, 1975, and in October of that year it was announced that he was one of the 1975 Nobel Prize laureates for Chemistry. In the summer of 1970, Costin D. Nenitzescu died in his sleep. He was 69 years old. My three-year term at IAEA was going to expire soon, and I was one of the possible persons to assume one or both his positions as Chair of Organic Chemistry in the Bucharest Polytechnic and Director of the Research Center for Organic Chemistry of the Roumanian Academy (CCO). As it turned out and as I had written in the special issue of *Revue Roumaine de Chimie* dedicated to the 100<sup>th</sup> anniversary of Ecaterina Cioranescu (1909-2000), she wished to assume her husband's former position in CCO, and I had made a special effort in her favor with the Roumanian Ministry of Education. This had angered the Prorector of the Bucharest Polytechnic, and she appointed Professor Margareta Avram as Head of the Organic Chemistry Chair. Thus, I returned to Bucharest as one of the professors in this Chair, and kept my earlier position as Head of the IAEA Laboratory of Labelled Compounds.

In 1970 one of Nelly's two brothers, a famous actor who had played in Roumanian movies and on stage decided to leave Roumania (illegally, of course) with his wife and son. Independently, only one month later, my only sister with her husband did the same. The political situation in Roumania had become worse since Nicolae Ceausescu, after returning from visits in China and North Korea, became the object of a frenzied personality cult.

#### Back in Roumania, 1971-1990

With the handicap of close relatives who had left Roumania illegally, my travels abroad became a problem. I knew that if I chose to remain in the West there would be little chance to see my family again. Two fellow graph theorists, Dennis Rouvray and Robin Wilson (the son of the British Prime Minister, Sir Harold Wilson) tried to obtain from Nicolae Ceausescu the permission for me and my family to leave Roumania but nothing happened.

Throughout the 70s and 80s living conditions worsened in Roumania. A terrible earthquake in 1977 killed about 6000 inhabitants of Bucharest; our apartment was seriously damaged, and for a couple of months we had to stay with Nelly's parents. Food became scarce, and restrictions in natural gas for heating caused problems during the harsh Roumanian winters. It was in the early 80s that for several weeks in winter our apartment had no heating, and we had to move and stay with our son, who was also living in an apartment, but since it was situated close to residences of politically highly-situated people the natural gas supply was not cut off. When we returned to our flat in springtime, we found that ice had broken all heating installations so that the whole blockhouse needed drastic repairs.

Research institutes of the Roumanian Academy were now required to devote all their efforts to applied research, and those that did not or could not do that were closed, such as the Institute of Mathematics, causing an exodus of Roumanian mathematicians who left Roumania illegallly. In 1974 realizing that the IFA laboratory offered no longer any hope for research, I decided to leave it and remain only with my teaching activity. At universities, conditions for experimental research in organic chemistry precluded the possibility of opening new directions that needed expensive chemicals and modern instrumentation. We could compensate the former handicap by having undergraduate students synthesizing chemicals that would ordinarily be bought as part of their laboratory training. Also, we compensated the latter handicap by mailing our new compounds abroad for NMR spectra and publishing jointly the results. However, one cannot fight the huge handicap of not having the scientific literature.

Although I had no longer any official position in IFA, I continued to follow what happened there. With one colleague who still worked in IFA and two MDs using radioisotopes we decided to publish jointly a book on *Labelled Compounds and Radiopharmaceuticals Applied in Nuclear Medicine*, which was published in Roumanian by the Academy's Publishing House in 1979. However, we were told that there were restrictions for the number of pages. Then I contacted Wiley Publishers and the reply was positive, provided that Wiley administered only the book distribution if the printing would be done in Bucharest. It took seven years until all negotiations were finished and the English version appeared (now without page restrictions). An irony is that in the meantime one of the four authors had not returned from West Germany, and we all wished to keep this information as a secret, but I am certain that this "defection" was known but it was in the interest of the Roumanian publishers to act as if they did not know.

In 1981, I co-authored another book with two fellow chemists. About 15 years earlier, I had suggested as a PhD topic to Valeriu Dragutan the burgeoning field of alkene metathesis. He continued and had achieved a sound collection of literature data. Together with Professor Mihai Dimonie, who was teaching polymer chemistry at the Bucharest Polytechnic, we published a thin book in Roumanian on *Olefin Metathesis and Ring-Opening Polymerization of Cyclo-olefins* (Editura Academiei, Bucharest, 1981), the first review of this field in book form. The English translation (again with Wiley Publishers) with twice as many pages was published in 1985. Three facts about this book deserve to be mentioned. The first is that we had sent the Roumanian version to several chemists working in this field (including K. J. Ivin) and that in 1984 Ivin published with Academic Press his book *Olefin Metathesis* that was inspired by ours but did not cite it; with a better distribution, Ivin's book and its second edition published in 1997 is more cited than ours. The second fact is that the 2005 Nobel Prize for Chemistry was awarded to Y. Chauvin, R. H. Grubbs, and R. R. Schrock for the development of the metathesis method in

organic synthesis. The third fact is that around 1980 Professor Mihai Dimonie had received an invitation that he could not refuse, namely to move his laboratory to the institute directed by Elena Ceausescu, where he would benefit from many facilities and coworkers; of course, all his subsequent publications in scientific journals had E.C.'s name as first author.

Research on theoretical problems such as graph-theoretical applications could be carried out without worrying about lack of chemicals and spectrometers. I started collaborating with Roumanian mathematicians interested in chemical problems, notably Solomon Marcus (on isoprenoid graphs *via* picture grammars, context-free grammars and push-down automata) and Ioan Tomescu (on benzenoid graphs, especially catafusenes, fibonacenes, and coronoids).

After 1974 when I left IFA, I no longer had any permanent coworkers. I did have PhD students at the Bucharest Polytechnic, continuing some experiments on organic compounds, but I was not supposed to supervise theses on theoretical aspects. However, for PhD students at other Roumanian universities I was allowed to suggest theoretical topics and this is how I collaborated with Professor Zeno Simon at the University of Timişoara and one graduate student, Ioan Motoc. Unfortunately, after a few years Motoc left Roumania (illegally, of course), obtained a position at the University of Saint Louis and died soon afterwards.

In 1975 Professor Oskar E. Polansky, with whom I had established friendly relationships during the Vienna years (and who had offered his help in case I would choose to emigrate) decided to found a journal for chemical applications of discrete mathematics, and together with Professors Adalbert Kerber (Aachen, Germany), André Dreiding (Geneva, Switzerland) and with me, we launched *match* which was initially to serve for informal communications. After Polansky's passing away, this journal was edited by Kerber, is now edited by Ivan Gutman with Boris Furtula's able help, and is called *MATCH Communications in Mathematical and in Computer Chemistry*, one of the flagship journals in this field.

In 1975, I visited the University of Rostov-on-Don where Genadii N. Dorofeenko was the leader of a large group of chemists working on the chemistry of pyrylium salts. The next year I gave a plenary talk on pyrylium salts at the Symposium on Heterocyclic Chemistry held in Kühlungsborn, in East Germany. At that conference, with Werner Schroth and Genadii Dorofeenko, we decided that the second part of the review on pyrylium salts could be a book. Alan Katritzky agreed, and during the late 70s and early 80s, Gerhardt Fischer came repeatedly to Bucharest to help in drawing formulas for our part of the book, with German accuracy and precision. Thus Supplementary Volume 2 of *Advances in Heterocyclic Chemistry* published in 1982 is entitled *Pyrylium Salts: Syntheses, Reactions, and Physical Properties*; the seven authors

listed in alphabetical order are two from Roumania (Tony Dinculescu and I), two from Halle (Schroth and Fischer) and three from Rostov (Dorofeenko, A. V. Koblik and V. V. Mezheritskii).

Also in Rostov-on-Don, I met Professor Vladimir Minkin who was interested in our boron chelates and offered to measure their large dipole moments. With him and his collaborators we published in 1981 a study of low-temperature NMR spectra for analogous arsenic chelates that till now holds the record for the high rate of degenerate rearrangements.

A review on topological indices was written in Bucharest in collaboration with colleagues from Bulgaria – because people from all Eastern European countries could travel more easily abroad than those from Roumania – and had as authors Danail Bonchev and Ovanes Mekenyan from the University of Burgas, together with Motoc and me. It appeared in 1983 as a chapter in a book edited by M. Charton and I. Motoc.

Publishing papers in foreign journals became more and more difficult and expensive as I had to pay for all mailing costs. The following story will shed some light on the situation that prevailed at that time. With Professor Zeno Simon from Timisoara and his graduate students, we decided in 1980 to publish a book, Steric Fit in Quantitative Structure Activity Relations, Lecture Notes in Chemistry No. 15. Springer Publishers sent us by mail specially prepared white paper. We hired a professional typist and a specialist in graphics for preparing the camera-ready copy. When everything was ready, we sent the manuscript for approval by the political authorities in charge for supervising materials to be sent abroad. After several weeks, the manuscript was returned with each and every page having the stamp APPROVED. Of course, we had to restart from square one. Nevertheless, the more difficult it became to publish in foreign journals the more determined I was to continue publishing no matter how many hurdles were thrown in my way. I had Nelly support and I had also the support of my few young coworkers. Two of these are Antonie Dinculescu and Daniela Oniciu, with whom I published numerous papers on biologically active compounds obtained from pyrylium salts. I recommended them for fellowships with Alan Katritzky at the University of Florida in Gainesville, where they did also good work.

Many times, I prepared slides for invited talks, only to find out later that I would not be allowed to attend the corresponding scientific meeting. In such cases, I refused to follow the recommendation to motivate my absence by health reasons. When in less than half of the invitations I did succeed to travel, I had to bear all costs of transportation (and often also the other expenses unless they were included in the invitation). Thus, when I did travel to USA, I took the train to Luxemburg and boarded the less expensive Loftleidir Icelandic Airline propeller plane that flew to New York with a stop-over in Rejkiavik. Now I take the liberty to make a presumptuous parallel with one of the legendary figures of the 18<sup>th</sup> century chemistry, Sir Humphry Davy. He obtained for the first time the alkali metals by electrolyzing their molten salts, he constructed voltaic cells, he invented miners' safety lamps, he studied tanning compounds, and discovered boron, nitrous oxide (laughing gas), phosphine, and hydrogen telluride; his fame is responsible for the fact that the French Academy invited him for a lecture tour although Britain and France were at war during the reign of Napoleon. Yet posterity considers that his greatest discovery is none of the above, but is represented by Michael Faraday. I have the impression that all my graph-theoretical findings and writings are trumped by the chance participation of Milan Randić at the seminar I presented in 1975 in the Chemistry Department of Harvard University, which opened to him the perspective of discrete mathematics and graph theory, as he recounts in his Autobiographical Notes published in 2010 (issue 2 of *MATCH Commun. Math. Comput. Chem.*). I am proud of this "conversion" that benefitted the whole field of Mathematical Chemistry.

A constant preoccupation with aromaticity led to invitations to deliver a plenary lecture at the IUPAC International Symposium on Aromaticity held in 1980 in Dubrovnik. I was also invited to present a lecture at the IUPAC 4<sup>th</sup> International Symposium on the Chemistry of Novel Aromatic Compounds in Jerusalem and I sent my contribution that appeared in the 1982 volume of *Pure and Applied Chemistry*, without my being present at that meeting.

My first publication on topological indices involved applying the graph-theoretical notion of graph center in 1979. Then together with Ioan Motoc we showed that centric indices allow quantitative structure-activity/property relationships (QSARs and QSPRs, respectively) with octane numbers of alkanes. It was, however, another topological index that brought the most interesting results. I made two modifications to Randić's molecular connectivity index  $\chi$ , which varies both with the branching and the size of graphs. In order to model separately these two aspects I replaced the adjacency matrix by the distance matrix, and I added a factor to compensate for the number of edges in the graph. I called the resulting index the *average distance sum connectivity*, but it is now known as Balaban's index *J*. An interesting aspect is that for an infinitely long linear alkane *J* takes the value  $\pi$ . Although it varies with branching similarly to the first topological index W introduced by Wiener, *J* is much more discriminating (less degenerate) than both W and  $\chi$ . A rigorous proof that index *J* for alkanes starts to be degenerate with dodecane isomers was published in collaboration with Louis V. Quintas, a mathematician from Pace University, New York. Additionally, unlike the above two other indices, *J* can be easily adapted to encode the presence of multiple bonds and heteroatoms. As a

consequence I was invited to present a plenary lecture on topological indices at the IUPAC International Symposium on Theoretical Organic Chemistry held in Dubrovnik in 1982.

Among the uses of index *J*, I will relate only one of them. In a paper published in *Nature Biotechnology* in 1998, Roger Lahana and his coworkers designed immunosuppressive peptides by *in silico* screening starting from 19 known decapeptides (9 bioactive and 10 inactive). Three amino acids in positions 1, 4, and 10 were common to all bioactive peptides, but for selecting the amino acids in the seven other positions the authors chose six amino acids and formed a virtual combinatorial library of  $6^7 \approx 280,000$  decapeptides. This library was investigated using 13 molecular descriptors including log P, molar refractivity, molecular volume, ellipsoidal volume, dipole moment, number of O and N atoms, number of hydroxyl and ethyl groups, and four topological indices, one of which was the Balaban index *J*. By comparing the constraints of good and bad value ranges for these 13 descriptors, the above authors reduced the library by four orders of magnitude to 26 decapeptides that were analyzed by elaborate simulations. The top five decapeptides were synthesized, and it was found that one of them had approximately 100 times higher immunosuppressive activity than the lead compound.

In 1986, I took pleasure in accepting an invitation from István Hargittai for writing an essay about *Symmetry in Chemical Structures and Reactions*, which appeared in *Computers and Mathematics with Applications* as well as in a volume edited by him and entitled *Symmetry Unifying Human Understanding*. In this chapter I discussed symmetry aspects of the Periodic System and the nucleon magic numbers; of polyhedranes and their solid angles; of annulene valence isomers; of linear binary copolymeric macromolecules; of reaction graphs and trivalent cages. In a subsequent essay also prompted by Hargittai and published in 1989, I discussed *Carbon and Its Nets*, although at that time it was not easy to guess the future importance of fullenes, nanotubes, and grapheme (in 1968 I had published what may have been the first paper about relative stabilities of several planar and tridimensional carbon lattices).

In January 1986, I was invited to attend an International Conference on Substituent Effects in Radical Chemistry in Louvain-la-Neuve, Belgium, organized by H. G. Viehe within the NATO Advanced Series Institute. When submitting the request for travel to this meeting, I had cut off the NATO heading, and surprisingly I was allowed to lecture at that conference. My name (but not the lecture that I had presented) is included in the volume under my home address so that any unpleasantness would not be reflected on the Bucharest Polytechnic if one would discover that I took part in a NATO conference.

In the late 70s, I suggested reviewing all possible valence isomers of annulenes with up to 24 carbon atoms to a PhD student, Vasile Ciorba, as topic for his thesis. He did a good job;

Mircea Banciu, my younger colleague in the Polytechnic, had synthesized several valence isomers of benzoannulenes. With my enumeration of cubic multigraphs and with the inclusion of a graph-theoretical-based discussion of aromaticity, a three-authored monograph was published in 1986 by CRC Press, Boca Raton, Florida, under the title *Annulenes, Benzo-, Hetero-, Homo-Derivatives and Their Valence Isomers*. Most of the smaller annulene valence isomers were known, although they were sterically strained and much less stable than the annulenes, but in the book one could find structures of many larger ones that had a good chance to be stable and interesting. This fact brought many citations of this book in the 1990s.

An invitation came from the University of Leipzig in East Germany to accept a six-month appointment as Wilhelm Ostwald Chairperson for Theoretical Organic Chemistry. For my wife and me, an apartment in the guesthouse of the university would be provided. With the promise that my wife would be allowed to join me later, I arrived in Leipzig in June 1989. My duties involved lecturing to advanced students and writing jointly in German with Werner Schroth a chapter on pyrylium salts for the prestigious Houben-Weyl monograph series. I started with the lectures in Leipzig, Berlin, Halle, and Merseburg, but after less than two months, I was recalled to Roumania without any clear reason.

A few details about my family will now be included. My wife had defended her PhD thesis in 1972 and was working as assistant professor for chemical engineering in the Bucharest Polytechnic. She could not be promoted to associate professor because of her brother's defection. In 1988 at the age of 59 she took her retirement. Our son graduated there as chemical engineer in 1983 and was working as Research Scientist in the Center for Organic Chemistry of the Roumanian Academy (where he got his PhD degree under the supervision of Professor Ecaterina Cioranescu); his wife was an Assistant Professor at the Department of Organic Chemistry, and their daughter Silvia-Carmen was born in 1986. Our daughter, who had married when she was 18 a fellow medical student, finished her medical studies in 1989.

Then in December 1989, Ceausescu's dictatorship came to a bloody end. During the days and nights of the so-called revolution (very likely orchestrated by the second-tier died-in-thewool communists who would become Roumania's next leaders with USSR's blessing), we watched on TV the events and the shootings on the streets that had started in Timişoara and extended to other cities, including Bucharest. University students and faculty were guarding day and night over flammable and toxic chemicals. In the chemical institutes of the Roumanian Academy, primitive defense measures using gaseous chlorine were ready to be used in case of need. Political trouble continued well into 1990 when the true facts about the revolution gradually became better understood. Before the flight of Ceausescu, prominent members of the Roumanian Academy and Orthodox Church had been approached by the communist authorities for declaring their support of the regime, and such a letter of support from Romania's Patriarch had indeed appeared in newspapers. Having refused to comply with such a request to make a written statement of support, I had gone with Nelly into hiding before Christmas 1989, because we had heard the rumor that my name was among the black list of the authority's troops.

#### Destination USA, 1990-1995

Finally, Roumanians were allowed to have at home their passports, and I was allowed to continue my collaboration with the German friends in Leipzig, this time accompanied by Nelly. From our 6<sup>th</sup> floor apartment in Leipzig (without elevator) overlooking Nikolaiplatz, we could see every Monday how the police were arresting numerous political protesters, probably releasing them soon afterwards. I worked with Werner Schroth for the Houben-Weyl chapter on pyrylium salts, which was finalized and published in 1992.

With sponsoring from the Roumanian Ministry of Education, I attended the  $2^{nd}$  Congress of the World Academy of Theoretical Organic Chemists (I had been a member for several years) and I presented a plenary lecture on topological indices in Toronto. Then I was invited to travel from Canada to Fairbanks, Alaska, where a conference entitled *Quo Vadis, Graph Theory?* was organized by Louis W. Quintas, John W. Kennedy (from Pace University, New York), and John Gimbel (from the University of Alaska). Two chemists were invited to attend this meeting namely Milan Randić and I. My lecture, entitled *Solved and unsolved problems in chemical graph theory* (discussing graph centers in connection with chemical nomenclature, sequences in stereoregular polymers and in copolymers, cages, spectral graph theory, *k*-factorable graphs with k > 1, and perfect matchings) appeared in a special issue of the *Annals of Discrete Mathematics* and was reprinted in a volume.

In 1991, I received an invitation to collaborate for three months with Professor Lemont (Monty) B. Kier at the Medical College of Virginia in Virginia Commonwealth University, Richmond. In an earlier collaboration with Milan Randić, Monty Kier and Lowell Hall had generalized index  $\chi$ , which had been computed by Milan from all edges (1-paths). The Randić, Kier and Hall's indices take into account longer paths. Then Kier and Hall modified index  $\chi$  for heteroatoms. I accepted the invitation and came with Nelly, being financed as a consultant for Sterling Drug Company. It was Nelly's first transatlantic flight. In three months the collaboration

with Monty Kier led to two QSAR studies involving topological indices for normal boiling points of haloalkanes, ethers, and peroxides published in the *Journal of Chemical Information and Computer Science*. At the end of the three months we were prepared to return to Roumania, when I received an invitation from Professor Douglas J. Klein to come for another three months to Texas A&M University at Galveston (TAMUG); he had invited me several times in the past, but I was never able to come earlier. Thus is how my commitment with TAMUG has started.

An arrangement was agreed upon, starting in the Spring Semester of 1992, whereby I would teach undergraduate organic chemistry one semester in Galveston and one semester in Bucharest (in addition to graduate courses that I usually taught in Roumanian). With the gradual opening towards Western countries, I also started in the late 1990s to have classes in English in the Bucharest Polytechnic. By this arrangement, I was able to attend some of the National American Chemical Society Meetings or Gordon Conferences. In August 1994, the Division of Chemical Information of the American Chemical Society honored me with the Herman Skolnik Award "in recognition of outstanding contributions to the field of chemical information". Although in 1973 I had published *Confessions and reflections of a graph-theoretical* chemist in *MATCH Communications in Mathematical and in Computer Chemistry*, I had to include again some autobiographical data in my acceptance speech, which was published in 1975 in the *Journal of Chemical Information and Computer Sciences* under the title *Chemical graphs: looking back and a glimpse ahead*.

At the invitation of André Rassat, Nelly and I came for one month in 1996 to the École Normale Supérieure in Paris. Then, on visiting Lyon, I met James Devillers who edits the journal SAR and QSAR in Environmental Research, and we discussed editing a monograph on topological indices, as will be shown below. With Christian Roussel from the Marseille University I have had a long friendship and we had published since the 1980s several joint papers on pyrylium salts.

In 1997, I edited a book: *From Chemical Topology to Three-Dimensional Geometry*, Plenum Publishing Corporation, New York; the authors of its chapters have reviewed their theoretical or experimental contributions to three-dimensional chemical structures.

Collaborations with faculty in Galveston include research on theoretical aspects of fullerenes, nanotubes, nanocones, and other carbon nets such as diamond-graphite hybrids (with Douglas J. Klein and occasionally his post-doctoral students); on benzenoids that we called *claromatics*, which have only Clar sextets and empty rings (with D. J. Klein and T. G. Schmalz); and on nitric oxide donors (with William A. Seitz and Melanie Lesko).

In 1978, I had developed a graph-theoretical approach for the systematic enumeration of all possible diamond hydrocarbons based on dualists by analogy with benzenoids, and I had published it in a joint paper with Paul von Ragué Schleyer who had discovered the synthesis of adamantane. Now this enumeration was found to be useful for the recently discovered "diamond hydrocarbons" consisting of fused adamantane units, occurring in petroleum by chemists from Chevron. In collaboration with Professor D. J. Klein and Dr. Robert Carlson from Chevron, I published a correlation between the structure of these hydrocarbons and their retention times in gas-chromatography and high-performance liquid chromatography. Other studies on carbon nets were published with Roald Hoffmann, whom I had met first at American Chemical Society Meetings and who is an old friend.

I have also collaborated with several of my PhD students in Bucharest who have come to Galveston and are now permanent U. S. residents: with Dr. Ovidiu Ivanciuc and his wife, Teodora Ivanciuc, we have published results on using mathematical operators for topological indices in order to improve QSAR methodology. At present, Dr. O. Ivanciuc edits the *Internet Electronic Journal of Molecular Design*. He is a major contributor to the book I edited in collaboration with James Devillers: *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon and Breach, The Netherlands, 1999. Another former PhD student of mine is Dr. Marc Antoniu Ilieş, who is at present assistant professor at the School of Pharmacy, Temple University, Philadelphia; with him and Dr. W. A. Seitz, we have explored the use of pyrylium salts for obtaining pyridinium-based liposomes (cationic lipids) for gene transfer.

In the summer of 1992 I presented a plenary lecture at the 7<sup>th</sup> International Symposium on Novel Aromatic Compounds held in Victoria, British Columbia, Canada entitled *Benzenoid catafusenes: perfect matchings, isomerization, automerization.* With two other lecturers (H. Staab and J. Frazer Stoddart), with music accompaniment, I had to dance a jig in the plenary session. I reported in my lecture on recent theoretical discussions of cata-condensed benzenoids and on experimental data (obtained in collaboration with Drs. Mircea Gheorghiu and his wife in Bucharest) showing that anhydrous aluminum chloride catalyzes a degenerate rearrangement (automerization) of <sup>13</sup>C-isotopically-labelled phenanthrene. Earlier I had coined the term automerization for reactions that rearrange covalent bonds without yielding a different structure and used it for <sup>14</sup>C-isotopically-labelled naphthalene but on checking with Dan Farcasiu with the more reliable <sup>13</sup>C-isotope we could not reproduce the results and we had to withdraw that paper.

Starting with 1994 the Natural Resources Research Institute of the University of Minnesota at Duluth invited me periodically for one or two months as a consultant; I published several

papers in collaboration with Subhash C. Basak from this institute on using topological indices for QSAR studies of biologically active compounds.

#### Vice President of the Roumanian Academy, 1995-1998

In 1995, the President of the Roumanian Academy called me asking if I would agree to be a candidate for replacing one of the four Vice-Presidents who had died unexpectedly. I agreed, and I was elected for a period of three years. This involved the supervision of the Academy's scientific research institutes in the fields of physics, chemistry, biology, and medicine, as well as other administrative duties such as the introduction of a competitive system for all the Academy institutes to obtain research grants. Together with Professor Florin T. Tanasescu from Roumania's Ministry for Science and Technology and with Eustratios N. Carabateas from the Science and Technology Directorate of Greece, we organized a four-day NATO Advanced Workshop (ARW) on Science and Technology Management in Sinaia, Roumania on May 20-24, 1997. The 3-editor volume published by IOS Press in 1998 (NATO Science and Technology Policy Series No. 24) contains the 30 lectures presented by scientists and managers from 18 countries with various degrees of development, including my lecture entitled: R&D in universities, academic and technological institutes: marriage, cohabitation, or divorce? Soon afterwards, I attended another NATO ARW (in Prague) on Science Evaluation and Its Management where I spoke about Science evaluation in universities and academy research institutes: Similarities and differences.

# Texas A&M University at Galveston, 1998-2011

The Texas University at Galveston renewed its invitation to have me back, I decided to return to the USA, and in 2001 I was accepted as full professor with tenure. My American friends tell me that awarding tenure to someone who is 70 years old happens very seldom. At present, I am teaching organic chemistry and general chemistry courses to undergraduates. In addition, I mentor postgraduate students, fellows and young faculty. Together with my friends and collaborators, I continue to write and publish.

The Hungarian Academy of Sciences elected me as an Honorary Member in 2001, and in my acceptance speech, I discussed the artistic face of chemistry. In 2005, the International Academy

of Mathematical Chemistry was founded in Dubrovnik, with me as the first President and with Milan Randic as Vice-President. We decided to serve only for a three-year term. At present, this Academy has 89 members from the whole world.

In 2002, Professor Haruo Hosoya had an anniversary celebration, and he invited Milan Randić and me to come to Japan in 2002, and took great care of us. Hosoya had invented the term *topological index* and applied it to his *Z* index; he also showed that Wiener's index is the half-sum of all entries in the distance matrix of a molecular hydrogen-depleted graph. In Europe a godfather is a person who gives a name to a child, and because of that I had given to my talk the title "Haruo Hosoya, the godfather of topological indices"; however, the Japanese audience was perplexed because they knew only about Marlon Brando's and Al Pacino's title roles in the movies *The Godfather* and failed to see any similarity between them and Haruo.

Starting with 2004, I began a fruitful collaboration with my old friend Milan Randić on how the  $\pi$ -electrons in formulas of benzenoids or other fully conjugated compounds are partitioned between rings. According to Milan's proposal, a double bond shared by two rings contributes with one  $\pi$ -electron to each ring, whereas an unshared double bond contributes with two  $\pi$ electrons. We published together a series of papers on this topic and found also another way of characterizing benzenoids by their " $\pi$ -electronic signature". On similar lines a close collaboration with Professor Ivan Gutman and his coworkers started more recently, analyzing parallelisms and differences between Randić's  $\pi$ -electronic partition and Gutman's energy effect.

Before ending with more personal notes, a few more details on scientific publications will follow. A new review on pyrylium salts was co-authored in 2003 with my son, T. S. Balaban in *Science of Synthesis; Houben-Weyl Methods of Molecular Transformations*", Georg Thieme Verlag, Stuttgart, and an up-date has recently been submitted. In a book (*Nanostructures: Novel Architecture*) edited by my friend M. V. Diudea from the University of Cluj in Roumania, I contributed in 2005 with a chapter on theoretical investigations of single-wall nanocones. In 2009, I have also written two book chapters on aromaticity in books edited by Alan Katritzky (*Advances in Heterocyclic Chemistry*, centennial volume 99, 2009) and by T. M. Krygowski and M. K. Cyranski (*Aromaticity in Heterocyclic Compounds*).

Being on Editorial Boards of a dozen scientific journals, I am conscious that refereeing manuscripts is a necessary activity as gatekeeper, so that I try to be helpful both to the authors and to the journals by spending a considerable time for this task.

In the summers of the last five years, Nelly and I spent one to three months in Slovenia, where I have an official collaboration with Professors Marjan Veber and Matevz Pompe from the University of Ljubljana on research involving environmental chemical problems. In August 2010, Nelly and I visited China where I had been invited to present lectures in Xiamen and Tianjin on *chemical applications of graph theory*, and where I was offered my book with that title that had been translated into Chinese. Together with other representatives of mathematical chemistry (Douglas J. Klein, Milan Randić, Ivan Gutman, and Pierre Hansen who had also been invited) I realized that this field of research has been popular in Eastern Europe, China, and Iran because it can lead rapidly to new interesting results without any other investment than computers. In Beijing, Nelly and I were guests of Dr. Chan Laiwa and Dr. Daniel Chen (with whom I had collaborated in connection with the U. S. patent I had taken with Professor W. A. Seitz from Texas A&M University in Galveston and Dr. Robert Garfield from the University of Texas Medical Branch for nitric oxide donors).

A few details about life in Galveston: winters are very mild, with snow perhaps once in 20 years. Among natural disasters, hurricanes are less dangerous than earthquakes, tornadoes, or tsunamis because one knows in advance their direction and one evacuates the island. We did that in 2008 when hurricane Ike caused severe floods. For two months we had to evacuate our apartment which had been slightly flooded and needed remodeling. For the whole remaining winter semester of 2008, Texas A&M University had provided lodging space for students in the main campus at College Station, and the faculty commuted (3-hour drive) from Galveston to College Station where we had all our classes, spending there one day and two nights per week.

On a personal note, I find that Texans are nice and friendly people. Ironically, my only "problem" since coming to live in USA was when applying for U. S. citizenship. Neither my Roumanian passport nor my US permanent resident card had my middle initial, so I asked the immigration officer if I could include it on my American passport. After filling in my middle name, Teodor, I was told that this might cause some delay; when I tried to withdraw this request, I was told that this could not be done. As a consequence, I got the US citizenship four years after my wife, and only after hiring a lawyer who filed a lawsuit against the US government.

I see myself fortunate that both my son and daughter pursued research careers. My son, Teodor Silviu Balaban, graduated from the Polytechnic Institute in Bucharest and was a Research Scientist in the Academy's Institute of Organic Chemistry. In 1991, he obtained a Humboldt scholarship and went to Germany to work with Professor Günther Snatzke at the Ruhr University Bochum and Professor Klaus Hafner at the Technical University Darmstadt, then worked at the Max Planck Institute for Radiation Chemistry in Mülheim an der Ruhr. Subsequently, he took his habilitation degree with Professor Jean-Marie Lehn in Strasbourg, and with his support was appointed as Senior Research Scientist at the Institute for Nanotechnology at the Karlsruhe Research Center. Since 2010, he is a Professor at the University Aix-Marseille III (Paul Cezanne), Department of Supramolecular Organic Assemblies, in France. His daughter graduated in 2010 as a lawyer in Germany.

My daughter, Irina Alexandra Buhimschi (MD from Carol Davila School of Medicine, Bucharest) became a physician specialized in Obstetrics-Gynecology. Together with her husband, Catalin Sorin Buhimschi, she had come in 1993 to the US as research fellows at the University of Texas Medical Branch in Galveston. Their son, Alexandru Dan Buhimschi, was born in 1995 and is proud to be a Texan and a *BoI* (meaning *Born on the Island* of Galveston). After working through the ranks in Baltimore and Detroit, Irina and Catalin are now faculty (Associate Professors) at Yale University School of Medicine in New Haven, Connecticut and lead together a laboratory pursuing translational research on complications of pregnancy. Their noninvasive *Congo Red Dot Test* for high-risk pregnancy has been in the news recently.

I could say that my family is much larger. At different times in my career both in Roumania and in USA, I have mentored many individuals at undergraduate, PhD, or postdoctoral level, as young faculty collaborators, and for a few at all the above stages. Many of them shared with me their questions, thoughts and ambitions as with parents. In turn, I hope their interaction with me made a difference in their carrier and a bit easier to pursue their dreams.

One has to consider that the lifetime-accumulated knowledge of a person is destined to go to the grave unless it is transmitted to the next generations by raising children, by teaching, or by writing. And one must remember that *teaching enriches the students without making the teacher poorer*. Like my friend Milan Randić, I also collect aphorisms and other pieces of wisdom. Among my favorites are Alfred North Whitehead's "Panic of error is the death of progress", and Michael Faraday's maxim "Work, finish, publish". And I like what Polonius tells his son, Laertes: "And this above all, to thy own self be true!"