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A Life in Science

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A Life in Science

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The spoken word vanishes into air –
The written words stand time.
Anonymous

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Abstract

The author describes his family background, schooling, research, his teachers, his students, his co–workers and scientists he met in the course of his life.

Keywords. Chemical graph theory; combinatorial enumeration; computer chemistry; mathematical chemistry; quantum chemistry; history of Croatian chemistry.

1 FAMILY BACKGROUND

I was born in Zagreb (Croatia) on October 26, 1936. My parents were Regina (née Pavić) (April 17, 1916, Zagreb–March 9, 1992, Zagreb) and Cvjetko Trinajstić (September 9, 1913, Volosko–October 29, 1998, Richmond, Australia). My maternal grandparents came to Zagreb in the last decade of the 19th century from northern Dalmatia whilst my paternal grandparents lived all their lives in Volosko, a small town located between Rijeka and Opatija. Rijeka is a large seaport and Opatija is a well–known summer and winter resort. My younger brother Ivan (born in 1938 in Zagreb) and I spent the five years during the Second World War (1941–1945) in Volosko with our paternal grandparents. Our parents were divorced in 1946, father moved first to Italy, where he remarried and emigrated to Australia, whilst Ivan and I remained with our mother in Zagreb. Mother encouraged Ivan and me to read books, learn languages and be good students. My brother took degrees in physics and mathematics, moved back to Volosko and taught in Rijeka, Opatija and finally in Matulji, a place above Volosko, where he is presently the principal of a primary and junior secondary school. He is married, has two sons (Slaven and Nenad) and a granddaughter (Emma). His older son Slaven has lived in Toronto since 1993, he is a Canadian citizen and his

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daughter Emma was born in Toronto.

The origin of the family name Trinajstić is linked to the number 13. This number appears as the root word in the family name Trinajstić: 13–ić – 13 = trinajst in the Čakavian dialect of the Croatian language; the Croatian language has 3 dialects: Čakavian, Kajkavian and Štokavian [1]. The family name Trinajstić is an old Croatian family name (it can be traced back to the 12th century in the place called Trinajstići, located above Rijeka) and belongs to a class of Croatian family names with numbers in their roots [2]. Šimunović [2], an authority on the origin of Croatian family names, hypothesized that the Croatian family names reflecting a certain number were motivated by the order of birth in old patriarchal families. Thus, the thirteenth born child got the nickname *Trinajstić* (the thirteenth, 13 and *ić* meant the smallest), which later became the family name of the child's descendents and has remained so until today. Šimunović [2] also mentioned very briefly the possibility that the family name Trinajstić originated from the folk belief in the magic of the number 13. Anyway, whatever the origin of the family name Trinajstić, the number 13 is a lucky number for the Trinajstić clan, which is now dispersed over five continents, although in some cases the name has undergone changes, *e.g.*, the part of the clan in California is now called Trinast (presumably an immigration clerk on the Ellis Island had trouble spelling the name Trinajstić and consequently americanized it to Trinast).

Professor Sven J. Cyvin (Trondheim, Norway) liked the idea of using the alphanumeric family name of mine so much that he and his co–workers dedicated a paper to me, using 13–ić as my family name [3], on the occasion of my appointment to the position of Editor–in–Chief of *Croatica Chemica Acta*, the chemistry journal published by the Croatian Chemical Society since 1927.

2 SCHOOL DAYS

I started primary school in 1944 in Volosko and in Trieste, but because of the bombing of Rijeka and Trieste by the Allies, especially in the spring of 1945, this was a highly irregular schooling. For the second form I was already in Zagreb where I attended a downtown primary school. In those days, primary schooling in the former Yugoslavia lasted 7 years and was modeled after the Soviet system of seven–year elementary school called *sedmoljetka*

At about the age of nine I started doing chemical experiments. Several friends in the house where we lived in downtown Zagreb (I was born in that house) decided to make gunpowder. I joined them and we produced some lovely explosions in the cellar. These experiments lasted until our parents forbade us to continue after a particularly violent explosion that shook the whole building.

I finished the seven–year school in 1951. One of the many changes in the Croatian school system happened in that year and the seven–year school was extended to the eight–year primary school (educational legislators now want to extend primary schooling to nine years). Thus, all of us who

finished the seven–year primary school had to do five years of secondary school (instead of four like the several generations before us) that ended in the final examination called *matura*. One good point of the type of schooling I had was that we had lectures in chemistry from the fifth form of the seven–year school and throughout all five years of high school, making a total of 8 years of chemical education. Later generations had at best 5 years of chemical education. At high school I met my future wife Judita née Juričev (born in Zagreb in 1938); she was in the same class with my brother Ivan. I even remember the date we met – September 21, 1954. We have remained together ever since that day. We were married in 1960 and have two children (Regina, born in 1960, and Dean, born in 1965; both born in Zagreb) and thus far two grandchildren (Sebastijan, born in 1979, and Mateo, born in 1984; both born in Zagreb). Dean lives in Copenhagen and is married to a Danish girl. Regina is presently in Buenos Aires with her husband.

I have remained in close contact with many of my former schoolmates (three graduated in chemistry) and we meet on a yearly basis (recently we celebrated our 47th graduation anniversary).

I graduated from high school in 1956 and the same year entered the University of Zagreb, enrolling in the Department of Chemical Technology at the Technical Faculty. Years of my primary and secondary schooling were difficult because of the postwar shortage of practically everything. Nevertheless, with the little money we had my mother always bought books that Ivan and I needed for school and books we liked to read. In this way, Ivan and I became acquainted with a number of literary masterpieces and since those days I have been an avid reader and collector of books. My personal library has nowadays reached some 15,000 books, including several hundreds of scientific books and journals.

3 UNIVERSITY

Chemistry was only my second choice. I actually wanted to study philosophy. A few days before enrolment, I went to the Alps with a group of friends and asked my mother to take my documents to the Department of Philosophy. I spent two weeks climbing various Alpine peaks. Upon returning to Zagreb, I found to my astonishment that my mother had entered me into the Department of Chemical Technology at the Technical Faculty. We had a long talk and my mother convinced me that chemistry was a better choice for me.

During my school days, I read biographies of Louis Pasteur and Justus von Liebig, and their lives and achievements in chemistry and science influenced me so much that I wanted to imitate them. I, therefore, started to read chemical books and to do experiments in our school lab and in the analytical laboratory of the nearby Faculty of Pharmacy (now called the Faculty of Pharmacy and Biochemistry). Our apartment was fairly large and my mother, in need of money, used to rent a room to two students studying pharmacy who were undergraduate lab assistants. Thus, almost every weekend I went to their lab with them to do simple analytical experiments. This activity lasted

about a year and a half. Then, the room was rented to a student attending the Department of Chemical Technology, who was an undergraduate lab assistant in organic chemistry. Thus, I occasionally went with him to his lab (which again was located close to our house) and did some simple organic syntheses and purification of solvents. Those visits to the organic chemistry lab went on for about a year until the student left Zagreb. Then my interest suddenly focused on philosophy. I accidentally came by a book on Plato and his philosophy and my enthusiasm for chemistry was shifted to philosophy. I became a Platonist and have remained the Platonist ever since. I read and reread *Timaeus* and even started to learn Greek to avoid translations that I did not trust.

It should be pointed out that in those days Marxism was the official philosophy of the former Yugoslavia. I had a number of arguments with my philosophy teacher by contrasting Plato's beautiful philosophy and his masterly writings to Marxism as an economic theory and not a sound philosophical foundation upon which to build the society. My mother warned me that if I wanted to study philosophy and oppose Marxism, which was the basis of the communist ideology, I would end up in prison. In those days one could be imprisoned for any kind of opposition to the communists, even philosophical. My mother also said that, as a chemical engineer, I would be safe even if I sometimes said something that the communists disliked. Thus, I started chemical studies and returned to my first love, to chemical research. I should also mention that Vladimir Prelog (1906–1998), the Croatian Nobel laureate in chemistry for 1975 (sharing the Prize with John Warcup Cornforth), was professor of organic chemistry in the Department of Chemical Technology from 1935 to 1941, when he moved to Eidgenössische Technische Hochschule (ETH) in Zürich.

I studied chemical technology uneventfully from 1956 to 1960 and did research in polarography for my degree thesis under Professor Ivan Filipović of Heldenthal (1911–1998) [4], whose undergraduate lab assistant I became in the second semester. The degree thesis was entitled *Influence of pH on the Half–Wave Potential of Bismuth in Solutions of Sodium Acetate and Acetic Acid* ("Utjecaj pH na poluvalni potencijal bizmuta u otopinama natrijeva acetata i octene kiseline", University of Zagreb, 1960). Filipović taught me the elements of the resonance theory and introduced me to the Schrödinger equation. After getting a degree in chemical technology, at the beginning of November 1960 I joined the research department of PLIVA, then and now the largest pharmaceutical company in the southeast of Europe. The powerful broad–spectrum antibiotic called azithromycin was discovered in PLIVA. It is sold in Croatia as SUMAMED and was licensed by PFIZER as ZITHROMAX.

In the early 1962, I left PLIVA and joined the Rugjer Bošković Institute in Zagreb. I did this because I wanted to enroll in the graduate school at the University of Zagreb and the Rugjer Bošković Institute was in those days an ideal place for graduate research. This move of mine was largely influenced by a good friend from student days – the late Krešimir Humski (1939–1997) [5] (later professor of organic chemistry in the Faculty of Technology and at the Faculty of Pharmacy

and Biochemistry). When Humski got married, I was his best man. He suggested I should join the Laboratory of Physical Organic Chemistry in the Institute whose head was Dionis Emerik Sunko (later professor of organic chemistry in the Department of Chemistry at the Faculty of Natural Sciences and Mathematics). Besides Sunko, the leading chemist in this laboratory was the late Stanko Borčić (1931–1994) (later professor of organic chemistry at the Faculty of Pharmacy and Biochemistry), who got his Ph.D. from ETH doing research under Leopold Ružička (1887–1976) and Prelog, two Croatian Nobel laureates in chemistry (Ružička shared the Nobel Prize in 1939 with Adolph F. J. Butenandt).

4 M.Sc., Ph.D. DEGREES AND POSTDOCTORAL RESEARCH

I started M.Sc. studies in organic chemistry and biochemistry. But, after a year I switched to physical chemistry, the reason being that both Humski and I got in trouble with the late Professor Krešimir Balenović (1914–2003) [6]. At that time, he was the leading Croatian organic chemist, collaborator of three Nobel laureates: Albert Szent–György (1893–1986), Ružička and Prelog, and head of the M.Sc. program in organic chemistry and biochemistry. Božo Težak (1907–1980) [7], the leading Croatian physical chemist at that time, was the head of the M.Sc. program in physical chemistry. He accepted us into his program and this change was also approved by Sunko.

During coffee breaks, a regular visitor to our lab was Milan Randić [8], who had come back to the Institute in 1958 after getting his Ph.D. from the Cambridge University. Research for his thesis *Some Studies in Infrared Spectra of Molecules* was carried out under Professor Norman Sheppard, FRS. In Cambridge, Randić met John N. Murrell who was working for his Ph.D. degree under Professor H. C. Longuet–Higgins, FRS. They became good friends and, besides Randić, Murrell played a crucial role in the early development of quantum chemistry in Croatia [9]. At the graduate school in Zagreb, Randić lectured on *Quantum Chemistry* and *Symmetry in Chemistry* in the M.Sc. program in physical chemistry. His lectures were very stimulating and during coffee breaks we talked a lot about quantum chemical problems. At that time, Randić was developing the maximum overlap approach to strained systems using a paper by Coulson and Moffitt [10] as the starting point. I liked his lectures and I liked to talk with him so I finally decided to do research for my M.Sc. degree under his supervision. Most of the work for my M.Sc. degree was completed by the summer of 1963. I applied the Coulson–Moffitt maximum overlap approach, in a modified form, to all possible methyl–substituted cyclopropanes. However, before I could get the master's degree, I was called up for the compulsory army service in autumn of 1963.

I could not avoid it, though I tried, and thus I spent the next 11 miserable months in Banja Luka (Bosnia and Herzegovina). That time was not completely wasted, because I read a lot – I read more than 150 books on science, philosophy and literature. Near the end of my army service, while I was waiting to be discharged, I was on guard duty at the army car depot guarding thousands of cars and

tons and tons of gasoline. One day while on guard duty I was thinking about what to do after the army – should I get my master's degree and work in industry or perhaps continue to do research for a Ph.D. degree, but with whom, since Randić was abroad and I had learnt he was moving from Sheffield to Ottawa, when suddenly a car appeared with the officer in charge of the depot. He brought me a telegram from the Institute. The message it contained changed my destiny. The Institute's authorities asked me if I would like to go to the University of Sheffield and do predoctoral research under John Murrell. My answer was an emphatic Yes!

It appears that somebody else was asked this first, but his wife did not want to leave Zagreb and her job. I was the second on the list of possible candidates. I returned from the army in late August of 1964 and already in early October I was in Sheffield in Murrell's group. Since I left Zagreb so quickly, I again had to postpone the orals for the M.Sc. degree.

This position was offered to the Rugjer Bošković Institute upon Randić's suggestion. While I was in the army, Randić spent a year with Murrell in Sheffield and when Murrell told him that he had got this Royal Society grant, Randić suggested that it be given to somebody from Zagreb. When the Institute proposed me for this position, Randić strongly recommended me to Murrell and I was accepted. After several years in Sheffield, in 1965 Murrell moved to the new University of Sussex in Falmer near Brighton, where he became professor of physical chemistry and stayed there until his retirement, being, among other things, the chair of the Chemistry Department and the Vice–chancellor of the University. He was also elected to the Royal Society. I stayed with Murrell from October 1964 to June 1966, first at the University of Sheffield and when he moved to Sussex, I went with him and a part of the group to the University of Sussex. Later on, several young people from the Institute spent some time with Murrell (*e.g.*, Tomislav Živković) and some even won Ph.D. degrees working with him (*e.g.*, Slobodan Danko Bosanac). After I left Sussex, I occasionally visited Murrell and he came many times to Zagreb and to the theoretical chemistry meetings held in Croatia (Dubrovnik, Brijuni).

In Sheffield I met Harry Kroto, the future Professor Sir Harold W. Kroto, FRS, a Nobel laureate for chemistry (he shared the 1996 Prize with Robert F. Curl and Richard E. Smalley for their discovery of buckminsterfullerene). Kroto was and has remained a nice friendly person. He did Ph.D. research in spectroscopy under Richard Dixon. The late Professor George Porter, FRS (1920–2002) [11], also a future Sir and Nobel laureate for chemistry (he shared the 1967 Prize with Ronald W.G. Norrish and Manfred Eigen for their work on ultrafast reactions), was head of the Physical Chemistry Department at the time. In Murrell's group I met several people with whom I have remained in contact ever since. One of them is Stuart Carter, later a postdoctoral fellow with Randić in Zagreb. In the ensuing years, he visited my brother and me several times in Volosko. In Sheffield, Stuart Carter patiently taught me the correct pronunciation of many English words. I came to England with a good passive knowledge of the language but had never before spoken to an

English person. Carter has a natural gift for languages and during his stay in Zagreb learned to speak decent Croatian. From 1986 to 1989 I used to spend three weeks each year in the Department of Chemistry of the University of Reading on a British Council grant. There I was located in the lab of the well–known molecular spectroscopist Professor Ian Mills, FRS. Carter was also associated with Mills and during my stays in Reading we did a lot of collaborative research [*e.g.*, 12]. Alan Hinchliffe helped me with programming. In Sheffield we had used an old Feranti computer, and that was my first encounter with computers. After getting a Ph.D. from the Sheffield University, Hinchliffe joined the University of Manchester Institute of Science and Technology where he is presently reader in chemistry. After both of us left Murrell's group, we published several papers together [*e.g.*, 13,14]. He did important research in chemical modeling and wrote, to my mind, the best book in the field, which has already had two editions [15]. He is also senior reporter for the specialist periodical report entitled *Chemical Modelling – Applications and Theory*, published the by Royal Society of Chemistry.

I studied several problems with Murrell – I did some experimental work on determining the kinetics of unsymmetrical quinone–hydroquinone redox reactions [16], used the Pariser–Parr–Pople (PPP) SCF MO method to interpret the UV/VIS spectra of alternant hydrocarbon anions and cations [17] and reported a few original criteria for obtaining localized orbitals [18]. Altogether, I produced 7 papers during my stay with Murrell and he agreed that this productivity and its quality would make an acceptable Ph.D. thesis.

I returned to Zagreb and obtained and M.Sc. degree first, because in those days an M.Sc. degree was a prerequisite for the Ph.D. The title of my M.Sc. thesis was *The Method of Maximum Overlap and Its Application to Calculation of Hybrids in Some Methyl–Substituted Cyclopropanes* ("Metoda maksimalnog prekrivanja i primjena na izračunavanje hibrida nekih metil–supstituiranih ciklopropana", University of Zagreb, 1966). Part of the M.Sc. thesis was published in 1965 and this was my first published research paper [19]. This was also the first of many papers that Randić and I published together over the years.

As soon as I got my M.Sc. degree, I submitted my Ph.D. thesis, based on the papers published while I was with John Murrell, to the Faculty of Natural Sciences and Mathematics. The thesis was accepted and I defended it in early January 1967. My Ph.D. thesis was entitled *Electronic Structure of Some Polyatomic Molecules* ("Elektronska struktura nekih poliatomnih molekula", University of Zagreb, 1967). My M.Sc. and Ph.D. theses were the first theses in quantum chemistry in Croatia.

In 1967, Randić organized the first quantum chemistry school in the former Yugoslavia and I helped him with the organization. The school was held at Herceg–Novi, a city in the Bay of Kotor. At that school I met the late Professor Michael J. S. Dewar, FRS (1918–1997) [20], who invited me to join his group at the University of Texas (Austin) as a Robert A. Welch postdoctoral fellow. I described how I met Dewar in my article under the same title. This article appeared in *A Group*

Memoir (University of Texas, Austin, 1988) containing a collection of memories and tributes written by his present and former students and colleagues, which was dedicated to Dewar on the occasion of his 70th birthday and given to him at the *International Symposium on Physical Organic/Theoretical Chemistry* held in his honor in Austin on February 25–28, 1988. I wonder why Dewar was never awarded a Nobel Prize in chemistry? He was a brilliant scientist, developed the PMO theory and a semiempirical MO method of high accuracy that was and is still widely used. He was also a highly educated person who possessed a vast knowledge of art and literature, who appreciated good food and wine, but with his sharp criticisms easily made enemies (perhaps this is the reason why he was never given the Prize!).

In Austin, my family and I spent two wonderful years (1968–1970). I was doing the SCF MO and MINDO studies of various large molecular systems and their properties [*e.g.*, 21–24] and produced 16 papers with Dewar. This research of mine and of Dewar's other postdocs was a precursor of the AM1 (Austin Model One) method – the paper introducing the AM1 is the second most cited paper published in the *Journal of American Chemical Society* (JACS) in its 125 years [25]. The list containing the 125 most cited papers published in JACS can be found on the Web: http://pubs.acs.org/journals/jacsat/125promotion/articles/html. Dewar has several more papers on this list. For example, his paper with Walter Thiel on the MINDO method is the third on the list.

In Austin, I met Douglas J. Klein, who was at that time doing Ph.D. research under Professor F. A. Matsen. After being a postdoctoral fellow in several places, Klein settled down as a professor of chemistry in the Department of Marine Sciences, Texas A & M University at Galveston. I have visited him there many times and on several occasions I spent three months working with him and several other professors in the Theoretical Chemical Physics Group that Klein was heading. Collaboration with Doug Klein and his colleagues was very productive and we have so far published a number of research papers [*e.g.*, 26–28].

5 YEARS AT THE RUGJER BOŠKOVIĆ INSTITUTE

After returning from England in 1966, I joined the Theoretical Chemistry Group in the Department of Physical Chemistry of the Institute and stayed there until mandatory retirement at the end of 2001. The retirement age in Croatia is 65. The Theoretical Chemistry Group was founded by Randić on his return from Cambridge.

My advancement in the Department was as follows: I became a research scientist in 1967, an associate research professor in 1971 and a full research professor in 1977. I was head of the Theoretical Chemistry Group for many years and chairman of the Physical Chemistry Division from 1997–2001. I was also lucky to be continuously supported by grants from various Croatian granting agencies and after 1991 from the Ministry of Science and Technology of Croatia. Croatia

became independent in 1991. Even now that I am retired, I am still supported by a modest research grant from the Ministry of Science and Technology, since I have continued to do what is, I hope, competent research [*e.g.*, 29].

When Randić left Zagreb for good in 1971, I took over his lectures in quantum chemistry in the Department of Chemistry of the Faculty of Natural Sciences and Mathematics. There I was first elected to the position of assistant professor in 1970, then associate professor in 1973, and finally in 1977 I was promoted to the rank of full professor. I also lectured on molecular orbital theory in the graduate school. To help graduate students, I wrote a book entitled *Molecular Orbitals in Chemistry* ("Molekularne orbitale u kemiji", Školska knjiga, Zagreb, 1974; the book was translated by my doctoral student Gani Jashari into Albanian for the use of students in Albania and at the University of Prishtinë in Kosovo). This was the first book on molecular orbital theory in the Croatian language. Later, Leo Klasinc, Zvonimir Maksić and I wrote a book for undergraduate students on the use of symmetry in quantum chemistry, entitled *Symmetry of Molecules* ("Simetrija molekula", Školska knjiga, Zagreb, 1979).

I supervised 15 B.Sc. degree theses, 12 M.Sc. theses and 20 Ph.D. theses. I still have several students working with me. Among the students who were awarded their B.Sc degrees under my supervision, Zlatko Bačić is now a professor at the New York University and one of the leading chemical physicists in the USA. He got his Ph.D. degree from the University of Utah and received the Camille and Henry Dreyfuss Fellowship. Boris Sinković got his B.Sc. degree with me, his Ph.D. degree from the University of Hawaii and is presently professor of physics at the University of Connecticut (Storrs). He runs highly regarded research in surface physics. Milorad Milun, who got all three degrees, B.Sc., M.Sc. and Ph.D., under my supervision, is now director of the University Institute of Physics in Zagreb and a leading Croatian researcher in vacuum physics and nanotechnology. Ivan Gutman obtained M.Sc. and Ph.D. degrees with me and later he was also awarded a Ph.D. degree in mathematics from the University of Belgrade (Serbia). His M.Sc. thesis (*Graph Theory and Molecular Orbitals*, University of Zagreb, 1973) and his Ph.D. thesis (*Investigation of Topological Properties of Conjugated Hydrocarbons*, University of Zagreb, 1973) were the first theses in mathematical chemistry in Croatia. Gutman is one of the international leaders in mathematical chemistry and professor of physical chemistry at the University of Kragujevac (Serbia). He is also a current Editor–in–Chief of *MATCH – Communications in Mathematical and in Computer Chemistry*, an international periodical, established in 1975 by late Professor Oskar E. Polansky (1919–1989) [30], for the publication of research work in the overlapping area between discrete mathematics and chemistry as well as for its applications in computer chemistry. Borka Džonova–Jerman–Blažič is head of the computer networking research at the Josef Stefan Institute in Ljubljana (Slovenia). Her Ph.D. thesis *Computer–Aided Solutions of Some Nonnumerical Problems in Chemistry* (University of Zagreb, 1981) was the first thesis in computer chemistry in Croatia. Sonja Nikolić is a distinguished associate research professor in the

Institute. Her Ph.D. thesis *Chemical Graphs – Conjugated–Circuit Model*: *Selection of Parameters and Applications of the Model* (University of Zagreb, 1988) contains a scholarly review of the conjugated–circuit model, gives its quantum–mechanical basis and presents its extension to heteroconjugated polycyclic molecules. Bono Lučić has an interesting background: he got his bachelor's degree from the Department of Electrical Engineering, his master's degree from the Department of Physics and his Ph.D. degree from the Department of Chemistry of the Faculty of Natural Sciences and Mathematics. He did research for his Ph.D. degree in chemistry under my supervision, whilst his M.Sc. thesis was supervised by the well–known Croatian biophysicist Professor Davor Juretić. In his Ph.D. thesis, entitled *Quantitative Structure–Property–Activity Relationships of Molecules*: *The Use of Ordered Orthogonalized Descriptors* (University of Zagreb, 1997), Lučić took advantage of his broad education. Iva Maria Tolić–Norrelykke got the first Croatian Ph.D. in theoretical biology with her dissertation *Cells as Tensegrity Structures* (University of Zagreb, 2002). She completed the experimental part of the thesis at Harvard University working with Professor Ning Wang. Tensegrity is a contraction of tensional integrity. The word was coined by Buckminster Fuller (1895–1983). Buckminsterfullerene, named after him [31], the now famous C_{60} molecule with the structure of a truncated icosahedron, is also a tensegric structure.

6 RESEARCH

I have been lucky to have good teachers (Filipović, Randić, Murrell, Dewar), gifted students from Croatia and abroad, good co–workers all my life and to have done joint research with most of the leading mathematical chemists of our time. Some of them have already been mentioned and some will be mentioned below. From the early days, I learnt to cooperate and appreciate the results of my colleagues and I have published research papers jointly with more than 200 scientists of various backgrounds. I have published extensively with some of them because I liked to collaborate with them because they were and are very nice persons, and research has always been an enjoyable occupation for me. In this way, doing science was like an exciting journey into the unknown in good company.

My research interests lie in the fields of quantum chemistry, mathematical chemistry, computer chemistry, history of chemistry and especially in the history of Croatian chemistry. Two topics prevailed in quantum chemistry: development of the semi–empirical molecular orbital (MO) theory applicable to large (heterocyclic) molecules [13,14,17,21–24,32,33] and setting up, in collaboration with Douglas J. Klein, Milan Randić and Sonja Nikolić, a valence–bond model, named the conjugated circuits model (originated by Randić [34] in 1976), on a firm quantum–mechanical basis, its parameterization and application to different classes of conjugated molecules and fullerenes [35–40]. I also did some *ab initio* computations with the late Andrej Ažman (1937–1980)

[41], who was a senior scientist at the then Boris Kidrič Institute in Ljubljana (now the Slovenian National Institute of Chemistry; Slovenia became independent in 1991) and MO interpretations of photoelectron spectra of biologically active molecules with Leo Klasinc [*e.g.*, 42]. With Klasinc and our doctoral students Branko Ruščić (presently a senior scientist at the Argonne National Laboratory, Argonne, Illinois) and Aleksandar Sabljić (presently head of the Physical Chemistry Division and a full research professor at the Rugjer Bošković Institute) we took the first photoelectron spectra of opiates, interpreted them and even discussed how their structure affects their activity [43].

In the field of mathematical chemistry, I worked on the development and application of graph theory to chemistry with several of my doctoral students (*e.g.*, Ivan Gutman, Milorad Milun, Maria Barysz, Sonja Nikolić, Albin Jurić, Dragan Amić) and many colleagues (*e.g.*, Dragoš Cvetković, Milan Randić, Doug Klein, Tomislav Živković, Roger B. Mallion, Danail Bonchev, Ante Graovac, Dejan Plavšić, István Lukovits, Subhash C. Basak). Gutman came to Zagreb with the knowledge of graph–spectral theory and the Sachs theorem (introduced in 1964 by Professor Horst Sachs [44], a distinguished mathematician from Ilmenau in the then East Germany; a recent issue of MATCH [45] is dedicated to him on the occasion of his 75th birthday), which he learnt from Cvetković in Belgrade. When Gutman told me that Cvetković calls C.A. Coulson's and A. Streitwieser's *Dictionary of π–Electron Calculations* (W.H. Freeman & Co., San Francisco, 1965) the book of graph spectra, it became clear to me that there was an isomorphism between the Hückel MO (HMO) theory and graph–spectral theory and we started to analyze the simple HMO theory in terms of graph–theoretical concepts and the Sachs theorem [46]. In the MATCH issue dedicated to Sachs, Gutman described the impact of the Sachs theorem on theoretical chemistry [47].

Later, during my visit to the Department of Theoretical Chemistry, University of Oxford, early in 1974, I collaborated with Mallion and A.J. Schwenk in applying the Sachs theorem to weighted graphs representing heteroconjugated molecules [48,49]. My visit to Oxford coincided with a sad occurrence – Charles Coulson's demise – in fact, he died on the very day that I arrived at the Oxford University Department of Theoretical Chemistry: January 7, 1974. That Department had been created especially for Coulson, who held a Personal Chair in Theoretical Chemistry and had transferred to the position after 20 years as the Rouse Ball Professor at the Mathematical Institute and a Fellow of Wadham College, because the Rose Ball Chair is permanently attached to that College. By a private arrangement between him and the College, Coulson remained the Fellow of Wadham College until he died. Charles A. Coulson, FRS (1910–1974) was the leading theoretical chemist of those days in the United Kingdom and was a father figure to theoretical chemists all over the globe [50]. I met Coulson during the Herceg–Novi School and shared long walks with him during which we discussed about many topics including the future of quantum chemistry.

In the aftermath of Charles Coulson's death, Mark Child, FRS became *Inter Regnum* Head of

Department. Then, Norman March, FRS was elected to the first Coulson Chair of Theoretical Chemistry (with an associated Fellowship at University College). When March retired, Mark Child became Coulson Professor of Theoretical Chemistry in his own right. At about that time (in 1994) the Theoretical Chemistry Department was amalgamated with, and absorbed into, the Physical Chemistry Department. However, the Coulson Chair of Theoretical Chemistry remained.

When I was in Oxford in 1974, Mallion was in the course of completing his second Ph.D. thesis (called, in Oxford, a D. Phil.) under Coulson, his first having been obtained from the University of Wales at Swansea, under Claude W. Haigh. At Oxford, Mallion was a Research Lecturer of Christ Church. Schwenk got his Ph.D. degree from the University of Michigan (Ann Arbor), under Professor Frank Harary and was a postdoctoral visitor to the Matematical Institute in Oxford. I met Harary there and he made me a gift a copy of the second edition of his now–famous book *Graph Theory* (Addison–Wesley, Reading, MA, 1971, 2nd edition). The well–known graph–theoreticians E.M. Palmer and L.W. Beineke were in the same group of visitors. Another well–known graph–theoretician, Robin J. Wilson, then Lecturer of Jesus College, was also a member of the Mathematical Institute.

After publishing our first paper on the relationship between the HMO and graph–spectral theory [46], we soon found that research in chemical graph theory was also being done by Alexandru T. Balaban in Bucharest, Dennis H. Rouvray in South Africa, Haruo Hosoya in Tokyo, William C. Herndon in El Paso (Texas), Roger B. Mallion in Oxford and that, before them, Edgar Heilbronner was very productive in this area while he was at ETH and that Coulson and Klaus Ruedenberg were also interested in this type of research. In his reminiscences about the Z–index Hosoya [51] described how he came to Zagreb and met Gutman and me there. In July of 1973, Hosoya attended the *International Conference on Quantum Chemistry* in Menton. There he met Rouvray and Mallion. From Menton Hosoya proceeded to Basel to visit Heilbronner. From Basel he came to Zagreb and then went to see Balaban in Bucharest. Interestingly enough, I had a choice of attending either the conference in Menton or going to Prague to attend the *Conference on Chemical Structure–Biological Activity Relationships*: *Quantitative Approach*. I went to Prague and met there Corwin Hansch, Lemont B. Kier, William B. Purcell, Rudolf Zahradnik, the late Peter A. Kollman (1945–2001) and many other QSAR practitioners. This was the *first* international meeting on QSAR. I wonder why Hosoya did not go to Prague instead of to Menton – the Conference in Prague would have been a much more rewarding meeting for him in the light of his work on the Z–index and its use in QSPR [52]. Randić learnt about all this activity first from Balaban when he delivered a lecture at Harvard University – at that time Randić was visiting Professor E. Bright Wilson in the Department of Chemistry [53]. Randić immediately realized the potential of chemical graph theory and started doing highly creative research in this area of theoretical chemistry, soon to become the leader in the field.

Our most interesting result in the graph–theoretical analysis of HMO theory is the formulation of topological resonance energy (TRE) as a measure of aromaticity of conjugated systems [54,55]. The TRE theory was developed in collaboration with my doctoral students Ivan Gutman and Milorad Milun and its applications were extended to conjugated ions, radicals, ion–radicals and bridged annulenes with my diploma student Sinković and doctoral students Predrag Ilić [56] and Sabljić [57]. The TRE theory was based on the concept of acyclic polynomial. We had problems with calculating this polynomial, thus with the help of Bojan Mohar, a mathematician from Ljubljana, a computer program was devised for computing the acyclic polynomial and the TRE values [58]. Approximately at the same time, Jun–ichi Aihara in Japan derived the same type of theory [59], although he called the acyclic polynomial reference polynomial and TRE the A–II method. He later accepted our terminology whilst the acyclic polynomial became known as the matching polynomial [60]. The TRE theory is nowadays accepted as a reliable theory of aromaticity [*e.g.*, 61].

I summarized our activities in analyzing the HMO theory with graph–theoretical tools in my article *Hückel Theory and Topology* [62]. Professor G.A. Segal (University of California, Los Angeles) was visiting Oxford and heard my lecture with the same title. He was just editing volumes 7 and 8 of the series of books on modern theoretical chemistry and he liked my lecture and thought that, if written, it would nicely fit in his volume 7, in which a theoretical framework of a number of semiempirical methods for computing electronic structures of molecules would be presented. I cast my lecture into the requested form and the article was printed in that book.

I was also involved in the development of molecular descriptors known as topological indices, a term introduced by Hosoya in 1971 [52] and quantitative relationships between the structure, properties and activities of organic molecules and biomolecules (QSPR and QSAR modeling – I believe that the term QSPR – quantitative structure–property relationship – was first used in print by Sabljić and me in 1981 [63]). I was prompted by the lectures on QSAR that I heard at the Prague Conference in 1973 to start doing QSPR and QSAR modeling. In collaboration with Randić, my doctoral students Dragan Amić, Bogdan Bogdanov, Bono Lučić and Sonja Nikolić, my younger colleagues Drago Bešlo, Zlatko Mihalić and Dejan Plavšić and a graduate student–volunteer, Ante Miličević, I introduced several novel molecular descriptors, such as the Harary index [64] and the modified Harary index [65] in honor of Professor Frank Harary, the detour index [66–68], the three–dimensional Wiener number [69], the connectivity index with a variable exponent [70], a modified Wiener index [71] and a variable Wiener index [72]. Some of these descriptors have also been independently introduced by other people. For example, the Harary index was at about the same time derived by Ovidiu Ivanciuc, Teodor–Silviu Balaban and Alexandru T. Balaban, but was given a different name – the reciprocal distance sum (RDSUM) index. Their report was published in the same issue of the *Journal of Mathematical Chemistry* as our paper [73]. Later, Balaban and his co–workers accepted the suggested name – Harary index [74]. This index is based on the chemists' intuitive expectation that distant sites in a structure should influence each other less than the near

sites. Randić *et al*. [75] also considered the connectivity index with selected values of the exponent, while we considered all possible values in search of the optimal exponent, that is, an exponent that would produce the QSPR model with the lowest value of the standard error of estimate. Gutman and Žerovnik had considered the modified Wiener index before us [76], but only its mathematical properties, while we investigated its use in the QSPR modeling. Such oft–repeated research in this highly competitive area is easy to understand.

Gutman and I also developed a pair of rather simple topological indices, which are often referred to in the literature as Zagreb indices [e.g., 77,78]. One index represents summation of all vertex–degrees squared and the other summation of edge–weights in terms of multiplied degrees of incident vertices. In our early work on the topological basis of the π–electron energy, these two indices appeared in the topological formula for the total π–energy of conjugated molecules [79] and were first used as branching indices [80] and later as topological indices in QSPR and QSAR studies [77,78]. We should also mention that the famous connectivity index of Randić was also introduced as a branching index [81] and only later used as a molecular descriptor, which in due course became the most exploited of all topological indices in QSPR and QSAR [77,78]. Zagreb indices, similarly to the modified Wiener index, were also modified [82] in such a way that the outer atoms and bonds gave a larger contribution to indices than the inner atoms and bonds, because the outer atoms and bonds are associated with a larger part of the molecular surface and are consequently expected to make a greater contribution to physical, chemical and biological properties. Variable Zagreb indices were also proposed [83].

Danail Bonchev paid a visit to Zagreb in the spring of 1976. We used his stay to study the branching of acyclic structures using information–theoretic indices that we had derived from the distance matrix [84] (we could do that because Bonchev was familiar with information theory). In 1981, in collaboration with Ovanes Mekenyan, we derived the topological superindex as a sum of six information–theoretic indices that were derived from the orbits, chromatic properties, edges (and vertex–degrees), distances, radial distribution of vertices and the non–adjacent numbers of a graph [85]. This index has shown a considerable discrimination power. A few years later (1983) Bonchev summarized all these efforts in a book in which he gave a survey of the application of infomation–theoretic indices in chemistry [86].

With my doctoral student Lučić, I developed a CROMRsel procedure [87]. This is a very efficient computational procedure for selecting relevant descriptors for the property modeled and for obtaining the best possible QSPR models for a given number of descriptors within the multivariate regression. The procedure was then used for modeling several molecular properties in collaboration with Professor Dragan Amić from the University of Osijek [88], Professor Alan R. Katritzky, FRS and his group from the University of Florida (Gainesville) and Damir Nadramija and his group from PLIVA [89–91].

My strategy for building the structure–property–activity models is delineated in a paper prepared in collaboration with Mihalić and published in the *Journal of Chemical Education* [92], which appears to be used by quite a few researchers in QSPR and QSAR modeling.

I was also involved in combinatorial enumeration of various classes of molecules. In collaboration with Professor Jan von Knop and his group from the University of Düsseldorf, I developed several efficient algorithms for characterization, generation and enumeration of chemical structures. These efforts were summarized in our two books [93,94]. Our most valuable results are the development of an algorithm based on the N–tuple code for constructive enumeration of acyclic structures [95] and an algorithm based on the DAST (dualist angle–restricted spanning tree) code for generation and enumeration of certain classes of polycyclic structures [96]. The N–tuple code lead to the development of compact codes [97–104] and induces a unique labeling of atoms in acyclic structures [97]. Every digit in an N–tuple code belongs to a single atom; thence, the sequential appearance of the digits indicates sequential labeling of atoms.

Some enumerative work was also carried out in collaboration with Professor Sir Harold W. Kroto, FRS [105]. This happened in the following way. I was visiting the University of Sussex in May 1982 and gave a series of lectures on enumeration in chemistry. The lectures were well attended; Murrell was there as well as Harry Kroto. Throughout the lecture series I had an uneasy feeling I was boring my audience with such exotic concepts as the N–tuple code, the boundary code, the DAST code, 1– and 2–factors or the counting trigonal, square and hexagonal animals. They were probably asking themselves what all that was good for? However, one person was diligently taking notes and asking penetrating questions during coffee breaks. This person was Kroto. A few years later, in the spring of 1985, I got a letter from Kroto asking if I could generate all the possible polyynes C_nH_m and related cyanopolyyenes C_nH_mN, which I did. Polyynes (cyanopolyynes) are molecules consisting essentially of long chains of carbon atoms (and one nitrogen atom) and it appears that our understanding of interstellar chemistry depends on their existence in the interstellar medium. Kroto wanted to know the size of each family of these structures and I supplied the requested data. Later on, we (Kroto, von Knop and his group and I) introduced the concept of a physical tree [106]. This work was directly linked to our above–mentioned effort, since in it we proposed a simple mechanism by which acyclic molecules could be formed in interstellar space and circumstellar shells. To do this, we introduced trees with the memory of their origin (*e.g.*, physical trees to differentiate them from chemical trees, that is, trees without memory) and we indicated this by assigning labels to the vertices of a physical tree consecutively and each vertex to be labeled must be adjacent to an already labeled vertex. Certain interest was later shown in physical trees and it was pointed out that Morgan–trees [107] were a subclass of physical trees [108]. I hope that through my collaboration with Kroto and von Knop, I was able to show the usefulness of constructive combinatorial enumerations in chemistry even before the combinatorial libraries proved to be an imperative tool in chemical modeling, preparation

of novel compounds and drug design. Furthermore, I did all kinds of enumerations such as the counting of Kekulé structures, conjugated circuits, various classes of graphs, etc. using a variety of original and transplanted methods [109]. The first time I encountered the problem of enumerating Kekulé structures was in 1967 when Randić and I tried to extend our method for computing bond lengths in cyclopentadienyl ligands in the half–sandwich structures containing transition metals [110] to various benzenoid ligands. We did not do much because at that time we did not know how to generate all valence structures (Kekulé, Dewar, excited structures) of a benzenoid hydrocarbon except by hand.

For some time I was also interested in producing criteria for accounting molecular complexity. The complexity [111] (or as Mallion and I call it, the intricacy [112]) of a molecule is characterized by its size (in terms of either the number of atoms and/or bonds), branching, cyclicity, the presence of heteroatoms, multiple bonds, chirality, symmetry, etc. We (Nikolić, Tolić, Ivo Baučić and I) used various definitions of Zagreb indices in considering the two–dimensional complexity of molecules [113,114], and Mallion and I used a reciprocal spanning–tree density as a new index of complexity (intricacy) [112]. Later, we (Nikolić, Tolić and I) prepared in collaboration with Gerta and Christoph Rücker a summary of currently used complexity indices, which appeared in a book *Complexity – Introduction and Fundamentals*, edited by Bonchev and Rouvray [115].

In 1983, I wrote the first single–author book on chemical applications of graph theory *Chemical Graph Theory* (first edition in two volumes: CRC Press, Boca Raton, Florida, 1983, second revised edition in a single volume: CRC Press, Boca Raton, Florida, 1992). According the *Science Citation Index*, this book has been cited over 1250 times to date.

Regarding the history of chemistry, I mostly studied the events and persons relevant to Croatian chemistry [4,9,116], but I have also written about the history of quantum theory [117,118], about Roald Hoffmann and his research [119] and translated some of his poems into Croatian [120], and commented part of my correspondence with Vladimir Prelog [121]. With Randić I have written about a dozen less known early developments of chemical graph theory [122]. I have also written several articles on the history of numbers and their uses in science and chemistry, *e.g.*, with Lionello Pogliani and Randić on zero [123] and one [124] (the computer age is based on these two numbers) and alone on the number five [125], and with Tolić on the manifestations of the number five in biology [126]. Thus far, Pogliani, Randić and I have not succeeded in publishing our article on the number 13 [127].

I was given several awards for my research, such as the City of Zagreb Science Award in 1972, the Croatian National Award for Science in 1982 and the Mid–America State Universities Association Distinguished Foreign Scholar Award in 1986. On the occasion of my 60th birthday, my former and present students and colleagues from Zagreb and abroad organized on October 25, 1996 a day–symposium in conjunction with the Croatian Chemical Society, Faculty of Chemical

Engineering and Technology and Matrix Croatica (Matica hrvatska).

7 OTHER MATTERS

I have served and am still serving on editorial boards of several journals: *Croatica Chemica Acta* (1967–1994), *Journal of Molecular Structure–Theochem* (1985–1995), *Journal of Mathematical Chemistry* (1986–1989, and again since 1994), *Computers and Chemistry* (1989–2002), *Symmetry* (1989–1990), *MATCH – Communications in Mathematical and in Computer Chemistry* (since 1997), *SAR & QSAR in Environmental Research* (since 1999), *Gazophylacium* (since 2000) and *Computational Biology and Chemistry* (since 2003). I am also a member of advisory boards of the *Bulletin of the Chemists and Technologists of Macedonia* (since 1995) and *Polimeri* (since 1998). Additionally, I was a co–editor–in–chief of the *Journal of Mathematical Chemistry* (1990–1993; the other editor was the well–known mathematical chemist Paul G. Mezey who has been the only editor–in–chief since 1993), the editor–in chief of *Croatica Chemica Acta* (since 1994) and of *Prirodoslovlje* (since 2001).

I am a member of a number of societies, such as *Matica hrvatska* (Matrix Croatica) – the central Croatian cultural and publishing society established in 1842 (since 1955), *Croatian Chemical Society* established in 1926 (since 1960), *Croatian PEN Club* (since 1987), *Brethren of the Croatian Dragon* – an old Croatian fraternal and cultural society established in 1408 as the *Knights' Order of Dragon* (since 1991). I was elected to the *Croatian Academy of Sciences and Arts* (established in 1861) in 1992 as the 12th chemist (out of 14) who became a regular member of the Academy and the first theoretical chemist ever.

Since my two–year postdoctoral stay at the University of Texas in Austin and return to Zagreb, I visited for shorter periods of time, from one to six months, the University of Trieste (visiting Professor Vinicio Galasso), the University of Utah in Salt Lake City (staying there with Professor Frank E. Harris in the Department of Physics), the University of South Carolina in Columbia (staying there on several occasions with Professor Benjamin M. Gimarc in the Department of Chemistry. Gimarc also twice spent some time in Zagreb with me), the University of Missouri at Kansas City (staying there on several occasions with Professor Jerry Ray Dias in the Department of Chemistry), the University of Düsseldorf (staying in the Computing Center with Professor Jan von Knop at least once a year since June 1973. I probably spent *in toto* more than three years there; thus, Düsseldorf became my home away from home). I also visited Texas A & M University at Galveston (staying on several occasions with Professor Douglas J. Klein in the Department of Marine Sciences), the Natural Resources Research Institute in Duluth (staying with Dr Subhash C. Basak in the Center for Water and the Environment. I met Basak in 1983, when we attended the *Symposium on Chemical Applications of Topology and Graph Theory*, held at the University of Georgia, Athens, April 18–22, 1983 and organized by Professor R. Bruce King), the Chemical

Research Center of the Hungarian Academy of Sciences in Budapest (visiting Dr István Lukovits), etc. A funny thing is that, although I am older than many of these fine scholars, somehow I have always felt them to be not so much my colleagues as the older brothers I have never had.

Retirement has not removed me from science and research. I hope to continue to do modest research for a few more years to come.

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