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Essay

Nenad Trinajstić – Pioneer of Chemical Graph Theory*

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We present a brief overview of many contributions of Nenad Trinajstić to Chemical Graph Theory, an important and fast developing branch of Theoretical Chemistry. In addition, we outline briefly the various activities of Trinajstić within the chemical community of Croatia. As can be seen, his scientific work has been very productive and has not abated despite the hostilities towards the Chemical Graph Theory in certain chemical circles over the past 30 years. On the contrary, Trinajstić continued, widened the areas of his research interest, which started with investigating the close relationship between Graph Theory and HMO, and demonstrated the importance of Chemical Graph Theory for chemistry. In more than one way he has proven the opponents of Chemical Graph Theory wrong, though some continue to fail to recognize the importance of Graph Theory in Chemistry.

INTRODUCTION

We will review the selected work of Nenad Trinajstić in the area of Chemical Graph Theory, but first of all we want to say that the development of Chemical Graph Theory, since its revival in the early 1970s up to today, some thirty years later, continues to be hindered by certain hostile circles unfamiliar with Chemical Graph Theory. This is not to challenge such »critics«, but response has been given elsewhere.[1] Here, it suffices to point out that Trinajstić had to work and endure in such adverse conditions – and he has worked and he has endured and contributed significantly to the development of Chemical Graph Theory.

Graph Theory is deceptively »simple«, which may cause some to have incorrect perceptions of Chemical Graph Theory. In other words, there are problems in Graph Theory that are easy to formulate and easy to understand, but nevertheless some of such problems are not so easy to solve. Let us illustrate this with The First Theorem of Graph Theory:

Any graph contains an even number of vertices of odd degree.

When »translated« to molecular structure, this becomes:

Every molecule contains an even number of atoms of odd valence.

The next two theorems are not difficult to understand either:

Every X-Y walk in a graph contains an X-Y path

and

The entry i, j of the n-th power of the adjacency matrix gives the number of walks of length n between vertices i and j.

These simple theorems may lead a novice to regard Graph Theory as an »elementary« subject, yet one of the important problems in modeling polymers, proving that

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* Dedicated to Professor Nenad Trinajstić on the occasion of his 65th birthday.

the average length of n-random walks over a grid is smaller (or at best equal to) the average length of n-random paths, is still unsolved, despite the deceptive simplicity of the conjecture.[2]

NENAD TRINAJSTIĆ

Nenad Trinajstić was born in 1936 in Zagreb, the capital of Croatia, but his family on the father's side comes from Volosko, a small coastal town of a few thousand people in the northern Croatian Littoral. The town of Volosko, despite the fact that during the Communist rule in the former Yugoslavia it was deleted from the map as a separate entity, and is still awaiting to regain its identity, was already on the map of Croatian science. It is the birthplace of Andrija Mohorovičić (1857–1936), a world-known Croatian geophysicist, who predicted the existence of the »Moho« discontinuity at the boundary of the earth's crust. Trinajstić studied chemistry at the University of Zagreb, the Faculty of Chemical Technology. Upon completing his degree, he joined the Rugjer Bošković Institute, a newly founded Institute for Physics, Chemistry and Biomedical Research, a »masterpiece« of Professor Ivan Supek. Soon after his arrival there was apparently an explosion in the laboratory where he was to work and Trinajstić, as the story goes, decided to leave experimental chemistry and become a theoretical chemist, a much safer alternative! He then joined my »Theoretical Chemistry Group« at the Institute. By this decision, in fact, Nenad Trinajstić became the first theoretical chemist of Croatia, since others were theoretical physicists by education. At that time, one of my interests was to quantify the qualitative model of the maximum hybrid orbital overlap,[3,4] which in my view was a suitable topic for the introduction of organic chemists to theoretical chemistry. In fact, during the next few years about a dozen younger organic and physical chemists were involved in calculations of the maximum overlap hybrids of various organic compounds[5–26] that I initiated in 1962.[3]

Trinajstić spent the years 1964–1966 with Professor John N. Murrell at the University of Sheffield and University of Sussex, Brighton (England), where he got a more thorough education in theoretical chemistry. In 1967 he got his Ph.D. from the University of Zagreb based on part of his work in England. Trinajstić spent the years 1968–1970 as a Robert A. Welch postdoctoral fellow with Michael J. S. Dewar (1918–1997) in Austin, TX, USA. There is no doubt that the excellent initial training that Trinajstić received in England and the USA was a great asset, which as we will see, Nenad Trinajstić used wisely and proficiently to establish himself as one of the leading theoretical chemists worldwide with the well-defined and novel research area of much overlooked applications of Discrete Mathematics to Chemistry, and specifically applications of Graph Theory to Chemistry.

Trinajstić's work was recognized about twelve years ago within Croatia by his election into the Croatian Academy of Sciences and Arts, a distinction that is not easy to earn, especially by relatively young persons. There is no doubt that his revised second edition of the book Chemical Graph Theory, [27] published in 1992, may have helped and that having on the back cover of the book the Croatian national flag in full colors could not hurt. This was the time when, besides Slovenia, only the three Baltic countries (Lithuania, Latvia and Estonia), Ukraine, Island, and Vatican recognized Croatia as an independent state – a dream to become true after the kingdom of Croatia had lost its independence at the beginning of the 11th century.

For more complete account of Trinajstić's life we direct readers to his recent autobiographical account »A Life in Science,« published in *Internet Electronic Journal of Molecular Design* (July 2003, vol. 2, number 7, pp. 413–434 at http//www.biochempress.com).

PIONEERS OF CHEMICAL GRAPH THEORY

We have to justify the title of this article, in which we characterized Nenad Trinajstić as one of the pioneers of Chemical Graph Theory (CGT). Trinajstić continued his very active participation in CGT for over 35 years. The other early pioneers of Chemical Graph Theory were (alphabetically): Alexandru T. Balaban, Ivan Gutman and Haruo Hosoya.

They were soon to be joined by Douglas J. Klein and myself, and then several other researchers. My involvement in CGT started with the lecture given by Balaban in the middle of May 1973 at the Department of Chemistry of Harvard University. In that lecture Balaban outlined a selection of unsolved problems of Chemical Graph Theory, which caught my attention. At that time, there were in all some 20 papers in CGT, almost all by the four pioneers mentioned above. Balaban, one of the »leading figures« of Chemical Graph Theory, carried at that time all the available literature on CGT in his briefcase!

One may compare this with the present situation with respect to the count of papers in CGT. Adding my contributions and those of D. J. Klein to those of the »gang of four« for a period of over 30 years, the count is about 2000, which is a factor of hundred compared to the early years of Chemical Graph Theory. This amounts to about dozen papers per person per year, or one paper a month. In fact, the number is smaller because most papers have two or more authors of the six mentioned ones. This is by no means excessive, but may have contributed to the growth of the hostile attitudes among some chemists, including those on editorial boards of chemical journals, towards Chemical Graph Theory. We have mentioned this with a reason and will come back to elaborate on this issue. In defense of the prolific output of CGT chemists, let us here quote E. Bright Wilson:[28]

»The most rewarding work is usually to explore a hitherto untouched field. These are not easy to find today. However, every once in a while some new theory or new experimental method or apparatus makes it possible to enter a new domain. Sometimes it is obvious to all that this opportunity has arisen, but in other cases recognition of the opportunity requires more imagination« (underlined by M. R.).

The »new theory« here is not so new but it is widely unknown among chemists: the branch of Discrete Mathematics known as Graph Theory. By searching the literature over a long period of over 50 years one finds that among theoretical chemists only Ruedenberg,[29] Heilbronner,[30] Schmidtke,[31] and Primas and Günthard[32] have made a reference to Graph Theory in their publications on HMO, a topic that thousands of chemists embraced for considerable time!

Before ending this section, we ought to mention also Dennis Rouvray among the early pioneers. He not only realized that CGT was a new untouched field of theoretical chemistry but also made a continuing effort to inform others about this. He authored some 60 reviews on Chemical Graph Theory (in several languages), which culminated in his article on topological indices in *Scientific American*.[33]

The first book on the application of Graph Theory to chemistry appeared in 1976.[34] It was edited by Balaban and contained a selection of contributions written by well-recognized authorities in the field. From this first monograph on Chemical Graph Theory anybody could have learned already in 1976 that graphs support metrics, that graphs are not confined solely to hydrocarbons, and that Chemical Graph Theory is not a synonym for Hückel Molecular Orbital Theory. The three most common fallacies concerning graphs and chemical graph theory are ignorance of graph distances and metrics, unfamiliarity with graph coloring, and identifying the adjacency matrix with HMO. If those who are »critical« of Chemical Graph Theory had only opened Balaban's book, they would have seen that applications of graph theory go beyond the study of properties of hydrocarbons, that graph theory is not HMO,[35] that »primitive,«[36] conjugated circuits reflect combinatorial properties of Kekulé valence structures and that the trivial fact that all diatomic molecules have the same graph (K_2, the complete graph on two vertices) does not mean that Graph Theory is of limited use in chemistry.[35]

PROFESSIONAL ACTIVITIES OF NENAD TRINAJSTIĆ

Before we focus on the scientific activities of Nenad Trinajstić, we would like to list some of his professional activities, which cover at least 13 different directions, as listed below:

(1) Writer of the first monograph on Chemical Graph Theory;
Twenty years ago, in 1983, Trinajstić published a two-volume monograph: *Chemical Graph Theory*, (CRC Press, Boca Raton. Florida, USA), which is not only the first single-author monograph on Chemical Graph Theory but also the only such monograph even today! The book was revised ten years later as a single volume book.[27]

(2) Editor of *Croatica Chemica Acta*;

(3) Co-author of several books on selected topics of Chemical Graph Theory;

(4) Editor and co-editor of several books on various topics of Chemical Graph Theory;

(5) Author of several chapters in books on selected topics of Chemical Graph Theory;

(6) Organizer of the international annual MATH/CHEM/COMP (Mathematics, Chemistry & Computers) meetings in Dubrovnik over a number of years;

(7) Professor at the University of Zagreb for undergraduate and graduate courses;

(8) Advisor for Master of Science and Ph.D. degrees at the University of Zagreb;

(9) Examiner for Ph.D. theses submitted to the University of Zagreb by foreign candidates living and working abroad;

(10) Co-author of textbooks;

(11) Author and co-author of several popularizing articles on Chemistry and Chemical Graph Theory;

(12) Reporter on current events, books, obituaries, *etc.*, related to the Croatian Chemical Society and the Chemical Community of Croatia;

(13) Reporter on topics related to the History of Chemistry in Croatia.

We should add that Trinajstić has additional interests beyond chemistry, which include literature and poetry among his other genuine interests. In Table I we have listed the titles of several of Trinajstić's articles, which reflect his wide interests and even philosophical traits.

The above activities of Trinajstić are characterized by the quantity of results and the quality of such results. For instance, he discovered the not known fact that a well-known Croatian writer, Milutin Cihlar Nehajev, was a chemist;[37] Trinajstić has written over 100 book reviews,[38] recorded events associated with the Croatian Chemical Society,[39] including about two dozen obituaries of Croatian chemists.[40] Again, there is so much to write about that I have selected to focus just on one of his recent books: One Hundred Croatian Chemists.[41] This book lists 100 chemists from Croatia who, in the author's opinion, deserve to be mentioned. I was told that Professor Smiljko Ašperger (one of the hundred) made the following com-

TABLE I. Some general topics of interest to Nenad Trinajstić

Title	Co-authors	Journal
The formula for rating scientists	A. Sabljić	*Periodicum Biologorum* **90** (1988) 397.
»If you want to be a leader, think!«		*J. Mol. Struct. (Theochem)* **200** (1989) 219.
The magic of the number five (Conference paper)		*Croat. Chem. Acta* **66** (1993) 227.
Experimental and theoretical research in natural sciences		*Encyclopaedia moderna* **14** (1993) 359
On the nature of theoretical research		*Croat. Chem. Acta* **69** (1996) 13.
On the Concept of Chemical Model	S. Nikolić	*Croat. Chem. Acta* **70** (1997) 777.
What is life? Is it just a physicochemical process of high complexity?	I. M. Tolić	*Periodicum Biologorum* **99** (1997) 295.
Origin of life: Earth or outer space?	I. M. Tolić	*Periodicum Biologorum* **100** (1998) 405.
Much ado about nothing – an introductory inquiry about zero	L. Pogliani, M. Randić	*Int. J. Math. Educ. Sci. Technol*. **29** (1998) 729.
About one – an inquiry about the meaning and uses of the number one	L. Pogliani, M. Randić	*Int. J. Math. Educ. Sci. Technol.* **31** (2000) 811.

ment: »Colleague Trinajstić, with this book you have made 100 friends and 1000 enemies!«. Actually, if I may add, there are even fewer friends because more than half of those listed died in recent years or have been dead for some time.

Clearly, such lists are always to some extent subjective, so in trying to be fair Trinajstić introduced strict criteria for a chemist to qualify to be »one of the hundred«. The list is to include:

(0) Nobel Prize winners;
(1) All chemists members of the Croatian Academy of Sciences and Arts;
(2) All editors of Croatica Chemica Acta during its 75 years of existence;
(3) All chemists who initiated any of chemical disciplines in Croatia;
(4) All professors of chemistry at Croatian Universities;
(5) Important chemists of the Rugjer Bošković Institute.

There was one additional condition though to be satisfied: a photograph of each person to be included in the list should be available to accompany the biographical and scientific description of that person. On that account, the chemist Zvonimir Pučar, who was the first in Croatia to build a laboratory for electrophoresis, was unfortunately not included! The list of 100 includes several people (including myself) who are theoretical physicists by education while some chemists that deserve to be included are missing. But those who want to blame the author should go through the trouble of collecting information on 100 chemists of their choice, their own criteria for selection, and come up with their own lists. I would add to this theme that I would like to include additional conditions for the selection of »chemists« deserving attention. I would add people who are on the editorial boards of chemical journals and all chemists who have many citations. In such cases, I would then include yet another theoretical physicist, Ante Graovac (who is on the editorial boards of the *Journal of Chemical Information and Computer Science* and *Croatica Chemica Acta*) though most chemists may view theoretical physicists as intruders. Be that as it may, if you accept the plausible definition of a »chemist« being a person who has published a scientific paper on a chemical subject in a chemical journal, then one should realize that the labels »physicist« and »chemists« are rather limiting because most physicists are more than physicists and most chemists are more than chemists. I certainly do not object to being called a chemist, it is a privilege that I cherish.

It is not difficult these days to make a list of the »most cited chemists.« In fact, Lučić and Trinajstić[42] published such a list of most cited chemists of Croatia not long ago, which we have reproduced in Table II.

It is interesting that four out of the 14 people, Andrea Bakač, Vlasta Bonačić-Koutecky, Stjepan Marčelja and Ivan Gutman are not included in the selected »100«. Hopefully they will be included in the second edition, if it ever appears! Their inclusion, besides raising the quality of the »average Croatian chemical paper«, by including photographs of the two ladies, Andrea Bakač and

TABLE II. The most cited Croatian chemists from 1981 to 1997[(a)]

Position	Name	# of citatons	# of papers	Quotient
742	E. Matijević	2613	173	15.1
1541	N. Trinajstić	1750	215	8.1
1779	M. Randić	1608	137	11.7
1842	Z. Bačić	1571	53	29.6
1866	A. Bakač	1561	126	12.4
2063	V. Bonačić-Koutecky	1476	56	26.4
3724	S. Marčelja	1038	26	39.9
4552	B. Ruščić	914	49	18.7
6217	I. Gutman	742	171	4.3
7173	B. Kaitner	672	67	10.0
7340	N. Kallay	661	56	11.8
8334	V. Prelog	604	18	33.6
10 154	M. Eckert-Maksić	527	67	6.6
10 800	L. Klasinc	502	80	7.5

[(a)] The number of papers refers to paper cited (and not to the total number of papers).

Professor Vlasta Bonačić-Koutecký, it would certainly also raise the quality of the »average face« of Croatian chemist. »Average face« of a person can be obtained by combining the Principal Component Analysis of Hotelling[43] and Wavelets Analysis,[44] and following the procedure outlined in one of the publications of Mladen Victor Wickerhauser.[45]

The list of »Croatian most cited chemists« is based on the list of all chemists in the world who received 500 or more citations for publications that appeared from June 1981 to June 1997, which was compiled by D. A. Pendlebury[46] of the Institute for Scientific Information, and which has over 10 000 names. The analysis covers a period of 16 years regardless of whether the person is the first author or not. The count of citations excludes self-citations, citations of review articles and books, and papers published in journals not covered by the Institute for Scientific Information. Clearly, papers published before June 1981 are not included, which »hurts« those who had been active a decade earlier and may have retired or even died during 1981–1997, and favors those who had been very active in the indicated period. Thus, for instance, Vladimir Prelog (1906–1998), the most illustrious chemist of Croatian origin, who published more than 500 papers, is represented by only 18 papers from that period, and is near the end of the list of the most cited Croatian chemists instead of being at its beginning.

To do justice to chemists whose photographs we may not have at the moment, or who may have been overlooked by not qualifying according to the »rules«, I have added a few »forbidden« names of chemists missing from the selected »100« in Table III, which lists the »dominant chemists« of Croatia. I used the four colors of the playing cards, since this appears politically »correct« at the moment, so each column lists 13 persons. No one should desire to be in the first column (spade) because those chemists are no longer alive! I left part of the third and the whole fourth column for readers to add whom they consider worthy of their attention. Anyone can thus fill in his or her »favorite« 13 chemists if they are not on my list!

TABLE III. The leading chemists of Croatia: The first column includes the deceased, those indicated by asterisk are not among the selected »100«

Spades	Diamonds	Hearts(a)	Clubs(a)
Stanko Borčić	Petar Alaupović	*Ante Graovac	...
Fran Bubanović	Smiljko Ašperger	*Andreja Bakač	...
Eugen Cerkovnikov	Dina Brovet-Keglević	*Vlasta Bonačić-Koutecky	
Slobodan Đokić	Dragutin Fleš	*Stjepan Marčelja	
Dragutin Kolbah	Drago Grdenić	*Ivan Gutman	
Zdenko Majerski	Željko Kućan	*Dejan Plavšić	
Vladimir Prelog	Egon Matijević	*Sonja Nikolić	
Mihovil Proštenik	Dionis Sunko		
*Zvonimir Pučar	Vinko Škarić		
Leopold Ružička	Vitomir Šunjić		
Božo Težak	*Viktor Thaller		
*Velimir Vouk	Nenad Trinajstić		
Karlo Weber	Hrvoj Vančik		

(a) I leave the »heart and clubs« for readers to fill in their beloved chemists, so as to minimize backlash of critical and angry remarks. Asterisks indicates chemists not included among the 100 listed in Trinajstić's book.

RESEARCH INTERESTS OF NENAD TRINAJSTIĆ

We have already mentioned the number 13 several times and this has been done with a purpose. As some may know, the family name »Trinajstić« in translation means »thirteenth son«, which probably originates from a family having 13 children at one time, not uncommon at the time of medieval Europe. In ancient Rome, names such as Quintas, Sextes, Septimus, Octavius, *etc.* were common. The given name »Nenad,« which is not an unusual name in Croatia, means in translation basically »unexpected« and indeed Nenad Trinajstić came onto the chemistry scene of Croatia unexpectedly. Trinajstić is not a follower of any particular predecessor, as it can be said of numerous leading »atomic physicists« of Croatia (including myself), all students of Ivan Supek, himself a student of Werner Heisenberg. Similarly, many »atomic physicists« in Germany were students of Arnold Sommerfeld (1868–1951) (including also chemists such as Hermann Hartmann, the founder and the first editor of the *Theoretica Chimica Acta*).[47,48]

With over 500 publications, it is difficult to give full justice to all of Trinajstić's contributions, so instead we will just mention some of his major scientific interests:

(1) Semi-empirical MO calculations;

(2) Adjacency matrix, characteristic polynomial;

(3) Enumeration of alkanes and benzenoids, N-tuple code (a prolonged collaboration with von Knop *et al.* from the Computer Center of University of Düsseldorf);

(4) Topological indices – Zagreb indices and their variants, detour index, distance indices, and 3-D Wiener index;

(5) Fast and exhaustive calculations of regressions;

(6) Topological resonance energy;

(7) Isospectral graphs, subspectral graphs, and endospectral graphs;

(8) The Conjugated-circuit Model;

(9) Clar π-sextets and fractal benzenoids;

(10) Fullerene properties;

(11) Hückel rules and electron correlation;

(12) Detour matrix;

(13) Resistance distance.

This, of course, is only the »tip of the iceberg« but we have to limit the length of this article, so 13 topics appear appropriate for a 13th-son person. Readers ought to examine the list of Trinajstić's publications to get a better picture of his various scientific interests and activities. A person having published some 500 papers clearly has to accept that not all of these many contributions are equally important or very important. But before one criticizes his neighbor, as an American Indian proverb says, one should walk a mile in his neighbor's moccasins!

Scientists differ in their attitudes and one should not criticize a person because he/she may be publishing well over the average. At least this fact should not be the basis for hostility towards CGT, even though comments can be heard, of course, from those who have not read a single paper on Chemical Graph Theory, that publishing in CGT is »easy.« In contrast, though at one time Herbert C. Brown (Nobel Laureate of 1979, in part for the development of very useful new reagents) was publishing one paper per week, not a month, I have not heard anyone complaining about »organic chemistry« being »easy.« And rightly so, because papers should be read first and then their content rather than their count can be criticized and commented on. Clearly and rightly, papers of H. C. Brown are beyond superficial critics who may not understand all subtleties involved in various chemical reactions, and by silence they either agree with the author or alternatively admit their ignorance. However, when it comes to Chemical Graph Theory, everybody seems to feel to be qualified to pass opinions as if Graph Theory had no hidden subtleties and non-trivial complexities that can be appreciated only by those initiated in Discrete Mathematics.

From time to time one hears complaints that chemical literature is cluttered with »insignificant« contributions, *etc.* The intent of such critics is to »slow down« the activities of others, who may have different views on science and scientific publications. The two extremes are, of course, »continual publications of incremental results« as opposed to »wait for a mature major contribution« that would then make a breakthrough in science. Again, it is a misconception that this ought to be »either/or«. For some chemists one alternative works better, for others the other. While I have nothing against those who think that one should »wait for a mature major contribution«, I want to defend the position of incremental contributions to science – if this is the choice of some authors. The argument in support comes from none less but Friedrich Engels (1820–1895), a natural philosopher (who was used, if not misused, by Karl Marx (1818–1883) for his political dogma). Engels summarized his many observations into the well-known axiom: Quantity changes into quality. Many important chemical accomplishments can be traced to this philosophy, including the celebrated paper of Woodward and Hoffmann on orbital symmetry.[49]

From the pragmatic point of view, I recall an obituary written by Professor Zaffarano, the former vice-president of Iowa State University (ISU) for graduate research, who on the occasion of the death of the late Professor Spedding (one of the founders of the Ames Laboratory in Ames, Iowa) described a meeting with Spedding upon his arrival at ISU as a young physicist. Spedding was giving advice to the then young instructor of physics along the following lines: As a young scientist, you ought to publish each year 3–4 papers that need not be important at all, but that will give you some experience in scientific writing and add to your publication list, which you need when applying for grants. In addition, you should work on some important problem in your discipline and publish one paper each year that will bring you recognition among physicists in the same field. Finally, you should consider some very important problem in physics that may take 3–4 years to complete but when completed will make you nationally known.

I am sure Trinajstić has not heard of Professor Spedding's advice, but he has adhered to it 100 percent, and he is not alone in following the prudent advise of the late Professor Spedding.

Personal View on a Selection of Important Scientific Results of Nenad Trinajstić

With such a voluminous scientific output even after filtering out annually »3–4 papers that need not be important at all,« which in the case of Trinajstić would make about 100, this still leaves a sizable volume of scientific output. Again, neither do we have space nor readers will have time for a litany of contributions to Chemical Graph Theory that could be mentioned here, so we have to make a very selective choice. I will therefore briefly mention only a few of Trinajstić's results that have enriched Chemical Graph Theory in particular and theoretical chemistry in general. I have decided to restrict this list to five, which, as those who know Nenad Trinajstić know, is his second most favorite number (13, of course, being the first).[50]

Topological Resonance Energy. – The idea that resonance energy (RE) can be defined solely using contributions to the molecular Hamiltonian that come from acyclic fragments[51] is not only simple, elegant, but also profound. This is so because it eliminates ambiguities and difficulties that have accompanied evaluation of RE since the early days of quantum chemistry. The same idea was independently proposed by Aihara at the same time.[52] Although in both cases the outline of RE was expressed within the HMO model, which was about that time getting out of »fashion«, the notion of the topological RE is very sound and still awaits to be »interpreted« and »incorporated« into more ambitious quantum chemical calculations.

The idea of the topological RE has led to the notion of the »acyclic polynomial,« (called by Aihara the »reference polynomial«), the polynomial which was already known in physics and mathematics as the »matching polynomial.« While the characteristic polynomial (or HMO secular equation) can be always associated with a symmetric adjacency matrix of a graph, and thus necessarily has real roots, the matching polynomial is not necessarily associated with a symmetric matrix. Nevertheless, as shown by Heilmann and Leib,[53] also the matching polynomial has always real roots. Another intriguing relationship is that between the Hosoya Z index[54,55] that can be obtained by counting all possible disjoint edges in a graph and the characteristic polynomial of acyclic structures. Trinajstić and coworkers have made numerous contributions to this overlooked domain of HMO.

Salient Features of HMO. – HMO as applied to organic compounds became a »religion« of a kind in the early days of quantum chemistry, which is reminiscent of the »gold rush« in Colorado and Alaska at the turn of the 20th century. Just as in the gold rush the gold mines were abandoned after most gold was extracted by extensive exploration, so theoretical chemists abandoned the HMO »wagon« without realizing that the »mines of HMO« offer more »riches« than a superficial traveler can see. For example, it was only in 1973 that Tomislav Živković[56] discovered the first pair of organic compounds that were »isospectral.« The notion of »isospectrality« had been unknown to chemists for over forty years of HMO! Incidentally, Živković found this by browsing through the *Dictionary of π-Electron Calculations* of Coulson and Streitwieser,[57] which listed the HMO eigenvalues and eigenvectors (molecular orbitals), where the two isospectral molecules: 2-phenylbutadiene and 1,4-divinylbenzene, were separated by two pages!

But there is much more »hidden« material in HMO that went unobserved till the rise of Chemical Graph Theory. For instance, the excessive degeneracy of HMO was mostly overlooked (except for a paper by Primas and Günthard),[32] the same was the case with the repeated occurrence of some common eigenvalues in HMO (elaborated later by Jerry R. Dias),[58] or the occurrence of coincidental coefficients in MO in symmetry non-equivalent position[59] and possibilities to use HMO for classification of conjugated hydrocarbons based on their spectral characteristics.[60]

What critics of the discussion of benzenoid and nonbenzenoid hydrocarbons by graph theory overlooked is the significance of HMO as the basic topological standard for MO calculations. This standard should be used against other, more sophisticated, MO schemes, such as PPP (Pariser-Parr-Pople)[61,62] in order to evaluate the extent to which more elaborate calculations improved upon the topological factors (embedded in HMO). This can then give some insight into the extent to which the claims of better calculations follow from the presence of additional contributions (such as electron repulsions). An illustration of such a comparative study of HMO and PPP calculations was presented by this author when comparing HMO bond orders and SCF MO bond orders of smaller benzenoid hydrocarbons.[63] The comparison has shown that the difference between the two sets of bond orders can be interpreted as giving more weight to the Fries Kekulé valence structure relative to other Kekulé resonance structures of polycyclic benzenoid hydrocarbons. Fries Kekulé valence structure[64,65] is the one that contains the maximal number of Kekulé rings with three CC single and three CC double bonds. Again, we should add that Trinajstić and his coworkers have made numerous contributions to the above field relating to the investigation of mathematical properties of HMO.

Conjugated-circuits Model. – Even today many theoretical chemists are not aware of »Conjugated Circuits«,[66–68] their role in the calculation of molecular resonance energy (RE) and characterization of aromaticity. Trinajstić was among the first to recognize the significance of this unique graph theoretical approach to characterization of benzenoid and nonbenzenoid conjugated hydrocarbons. Moreover, while Schaad and Hess[69] were the first to report on the close relationship of the Conjugated-circuit Model of this author[66–68] and the Resonance Theory of Herndon,[70,71] both of which can be shown to be mathematically equivalent under certain conditions, it was Trinajstić who was the first to point out the important differences between the two approaches that can be easily overlooked. As one can easily find, the calculation of matrix elements in the Resonance Theory requires a comparison of two Kekulé valence structures. In contrast, the corresponding quantities in the Conjugated-circuit Model can be evaluated by considering a single Kekulé valence structure at a time. At first this may not look like a big difference, but in actual applications it makes an enormous difference. Consider the case of kekulene with 200 Kekulé valence structures. Instead of considering 200 structures for enumeration of conjugated circuits in the Conjugated-circuit Model, one would have to make some 40 000 comparisons of different possible pairs of structures if using the Resonance Theory! In practice, however, both methods are much simplified by taking advantage of the symmetry of the molecule, but the difference between considering individual Kekulé structures and pairs of structures continues to persist. Moreover, in the Conjugated-circuit Model one need not consider Kekulé valence structures but rather focus on individual symmetry non-equivalent benzene rings, which allows a fast calculation of the expression for molecular RE. It is therefore no surprising that Klein and collaborators[72] were able to obtain the RE of buckminsterfullerene (with 12 500 Kekulé valence structures) by using the conjugated circuits approach rather than applying the

Resonance Theory, despite their mathematical equivalence. Trinajstić, Klein and collaborators conducted numerous theoretical studies of the quantum chemical foundations of the Conjugated-circuit Model.[73,74] They also considered the role of conjugated circuits of the same size but different shape, as is the case of 14 π-electrons conjugated circuits, which can have the shapes of the peripheries of anthracene, phenathrene or pyrene.[75]

Enumeration of Alkanes. – Several mathematicians of the past were engaged in calculating π to an ever increasing length. The value of π on seven decimals (3.141 592 6...) is easy to remember thanks to the mnemonic: Let's have a drink alcoholic of course... Here the number of letters in each word gives the corresponding digit of π (if one wants a few more digits, one can continue with after the heavy lectures involving quantum chemistry...). To some people, such efforts may appear an obsession. Similarly to some people, enumerating alkanes with increasing numbers of carbon atoms by theoretical chemists may appear to be another of such obsessions. However, neither of these activities is pursued in order to find its place in the *Guinness Book of Records*, but they have more subtle reasons: Computing π on very many digits is often used by computer scientists to check novel computer hardware and software for accuracy, while enumeration of alkanes serves to check and improve the existing algorithms for structure manipulations. If a novel program does not reproduce π to the specified length, or does not reproduce the number of isomers, then something is wrong with the algorithm (or hardware, if the algorithm is correct). Trinajstić, in a long collaboration with Jan von Knop and coworkers of the Computation Centre of the University of Düsseldorf, Germany, developed one of the most powerful computer-oriented approaches for enumeration of alkanes based on the N-tuple code.[76]

Distance Matrix. – The distance matrix was introduced into Graph Theory by Frank Harary[77] and its relevance to CGT was first brought out by Hosoya,[54] who found out that an alternative way to calculating the Wiener index,[78] W, was to add up all the entries above the main diagonal in the distance matrix of a graph. The Wiener index, seemingly an *ad hoc* quantity, was later found to be related to many other topological indices and has been the subject of numerous studies,[79,80] including those of Trinajstić and coworkers.[81] To honor Frank Harary, two groups of chemical graph theorists: Plavšić, Nikolić, Trinajstić, and Zlatko Mihalić [82] and Ivanciuc, Balaban and Balaban[83] agreed to name one of the topological indices derived from graph distances (in fact, reciprocal distances) »the Harary number.« Trinajstić *et al.*[84,85] have also generalized W to 3-D molecular structures.

The distance matrix proved to be a very useful quantity from which numerous generalizations of the Wiener number followed, starting with Balaban's J index,[86] including the reverse distance matrices,[87–89] the generalized J indices,[90] the Szeged index,[91–100] and the »corrected« Szeged index.[101] Related conceptually to the distance matrix is the detour matrix (another »invention« of F. Harary),[77] which again was the subject of several papers of Trinajstić.[102–106] Interestingly, while each graph has a unique distance matrix, we may add in passing, that different graphs may have identical detour matrices.[107] Finally, we should mention the »resistance-distance«,[108] the resistance-distance matrix[109–117] and the Kirchhoff index,[118] additional contributions to CGT in which Trinajstić played an important role.

We give a list of additional research topics to which Nenad Trinajstić significantly contributed:

(1) Graph theory, molecular orbitals and resonance structures;
(2) Graphical properties of non-bonding molecular orbitals;
(3) Graph spectral theory;
(4) Computer-aided generation of Kekulé structures;
(5) Computer identification of carcinogenic bay regions;
(6) Resonance in random polymers and π-networks;
(7) Quantum chemical aspects of conjugated circuits;
(8) Clar structures and fractal benzenoid hydrocarbons;
(9) Excitations for degenerate rearrangements;
(10) Complexity of molecular graphs;
(11) Selection of variables in multi-regressions;
(12) Nonlinear multivariate regressions;
(13) Connectivity indices and line graph connectivity indices.

Chemical Graph Theory, despite being a »popular« subject of abuse in certain circles – mostly through anonymous referees and uncritical editors who tolerated such abuse – nevertheless made a visible progress. People working in this field had numerous opportunities to exchange their views and report on their latest results at several *ad hoc* or regularly scheduled international meetings. These included numerous international meetings on Mathematical Chemistry (MATH/CHEM/COMP), Chemical Graph Theory, Gordon Conferences, and the recent Indo – USA Workshops on Mathematical Chemistry. Several initial annual MATH/CHEM/COMP meetings held in Dubrovnik were organized by Trinajstić. It is disappointing that no question concerning Chemical Graph Theory has ever been raised at any of these public gatherings, as such conferences would provide a good forum to clarify the relevant issues.

There is no doubt that the main source of confusion about Chemical Graph Theory are those who know about graphs and think that this makes them knowledgeable about Graph Theory. To settle the matter, consider the 13 Theorems of Algebra and 13 Theorems of Graph Theory listed in Table IV.

TABLE IV. Selected concepts of Algebra not necessarily known to those knowing numbers and selected theorems of Graph Theory not necessarily known to those knowing graphs

Algebra	Graph Theory
Cardano formula	Berge's theorem
Catalan numbers	Clarke's theorem
Cayley-Hamilton theorem	Euler's theorem
Chebyshev polynomials	Fary's theorem
Determinants	Hall's theorem
Fibonacci sequence	König's theorem
Karamata's theorem	Kuratowski theorem
Kronecker product	Matrix-tree theorem
Linear inequalities	Menger's theorem
Muirhead inequalities	Petersen's theorem
Polya's theorem	Ramsey's theorem
Schur's theorem	Tutte's theorem
Young diagrams	Vizing's theorem

Everybody can see that people who know numbers (that is the majority of grown-up population) generally do not know Algebra, but few can realize that the same holds for graphs, that by knowing about graphs does not make one know Graph Theory. To better illustrate the point, we have listed a selection of theorems from Graph Theory in the right column of Table IV. Those who are so eager to criticize Chemical Graph Theory should examine these theorems and see how few, if any, of these theorems they happen to know!

In the Appendix, we have listed the thirteen theorems of Table IV in order to remind readers familiar with graph theory what each of the theorems postulates. Such readers will have no difficulty to understand what each theorem states. However, those unfamiliar with Graph Theory will have to consult a textbook on Graph Theory just to find out the meaning of various technical terms, such as: characteristic polynomial, Ulam's subgraph, eulerian graph, embedding, subdivision, bipartite graph, maximal matching, minimal cover, spanning tree, incidence matrix, *k*-connectivity, clique, or chromatic number. We have listed only 13 terms, just as we have listed 13 concepts of Algebra and 13 theorems of Graph Theory, merely to remind the reader that this contribution celebrates Nenad Trinajstić, or in liberal translation »Unexpected Thirteenthson.«

Let us comment on the fact that all diatomic molecules have the same simple K_2 graph. Apparently, this fact »bothers« some critics considering that diatomic molecules are very different from one another. But, what this in fact means is that all diatomic molecules, and the same is true of any two molecules having the same graph, have the same combinatorial and topological properties. In the case of diatomic molecules, these properties are trivial, and nobody interested in the application of Graph Theory to chemistry will consider combinatorial and topological properties of diatomic molecules. If the fact that all diatomics have the same graph (which is a complete graph on two vertices K_2) makes an »argument« against the use of Graph Theory in chemistry, then if »critics« knew more about Graph Theory, they could »strengthen« their »concerns« by listing additional uses of the same K_2 graph in Graph Theory and Chemical Graph Theory. Thus, besides signifying all two-atomic molecules, K_2 in other chemical illustrations signifies totally diverse situations, like the following 13 cases show:

(1) K_2 represents degenerate isomerization of the Cope rearrangement;

(2) K_2 represents the »resonance« between the two Kekulé structures of benzene;

(3) K_2 is the dualist graph of the molecular graph of naphthalene;[119,120]

(4) K_2 is the line graph of molecular graphs of »all acyclic tri-atomic molecules«;

(5) K_2 is the only contributing subgraph in construction of a matching polynomial;

(6) Complete cover of graphs of benzenoid hydrocarbons by K_2 generates Kekulé valence structures of benzenoid hydrocarbons;

(7) K_2 is the only exception to Ulam's Graph Reconstruction Problem;[121]

(8) Counting polynomial for sets of disjoint K_2 subgraphs is Hosoya's Z-counting polynomial;[54]

(9) K_2 is one of the two ultimate components in graph dissections;[122,123]

(10) Median graphs (which are »resonance graphs« of Kekulé valence structures of benzenoid hydrocarbons)[124] consist solely of combinations of fused K_n graphs including K_2 graphs;[125,126]

(11) Caterpillar graphs have only K_2 subgraphs as branches;

(12) The pruning[127–129] method for finding the center[77,130–136] of a graph consists of repeated deleting of all terminal K_2 subgraphs;

(13) Last but not least, K_2 graph represents one of seven conjugated molecules having integral graph spectra.

As you see we continue to honor Trinajstić indirectly by listing 13 samples illustrating the use of K_2. We should add that the last item # 13 was proven already in 1974 by Cvetković, Gutman and Trinajstić.[137] We may also add that if we consider only cubic graphs, then, as Schwenk has proven,[138] there are exactly 13 regular graphs having integer spectra. Thank God that Trinajstić's surname is not Hundertwasser, since in that case I would have to continue listing the uses of K_2 graph for quite a while. Hundertwasser, the name of a well known Austrian architect and artist,[139] means »hundred waters,« and 100 instead of 13 would be the number to glorify!

TO WHOM IT MAY CONCERN

A visible fraction of the scientific output of Nenad Trinajstić involves in various ways topological indices,[140–142] which have been a subject of widespread misunderstanding and misrepresentation. There are »critics« who tend to perceive topological indices as frivolous, fraudulent, fortuitous, fiction, fabrication, foreign, fictitious, fallacious, flimsy, folly and foolish. Some are concerned with the presumed apparent »lack of interpretability« of topological indices, the »physical meaning« of which appears unclear. Before responding to such »accusations«, let us first pose a question: Why should graph theoretical quantities have a 'physical interpretation'? I am not saying that some do not have it, but merely why should they? Do various quantities of Quantum Chemistry have a »physical picture«? For instance, what is the physical picture of molecular orbitals? What is the physical picture of Kekulé valence structures? Only the total molecular wavefunction has a physical interpretation of the overall electron density, but the individual orbitals and individual Kekulé structures have no physical meaning, being non-observable quantities. Only observable quantities ought to have a »physical picture« while non-observables should have an interpretation within the model in which they are used. In that respect, molecular orbitals, Kekulé valence structures and graph theoretical indices have a proper interpretation. Note, for instance, that Kekulé valence structures have no »physical picture« even within the MO model but only within VB and GT models. Some non-observable quantities can be interpreted in different models and can even give an illusion of having a »physical interpretation.« Thus, some graph theoretical indices describe the molecular shape, chirality, molecular surface or molecular volume. However, if one closely examines the four »physical pictures« (attributes), one realizes that none of them is observable in the strict axiomatic sense of the Quantum Mechanics.

There are several papers on the interpretation of graph-theoretical indices in the literature.[140–150] Here, we will only briefly outline a structural interpretation of the connectivity index χ, which this author proposed over 25 years ago.[151–153] This indeed is the first designed structural invariant to yield a good correlation with various physicochemical molecular properties, while the Wiener index may be viewed as the first *ad hoc* non-trivial graph theoretical index used in correlation with a selection of molecular properties. Although we will here continue to discuss the connectivity index, much of what follows relating to interpretation of the connectivity index holds for other topological indices, including the »Zagreb« indices of Trinajstić and coworkers. All chemists would agree that some molecular properties are bond additive. What the connectivity index accomplished is not merely to offer a basis for the partitioning of molecular properties into bond additive components, but to show that these components have inherent weights. Thus, in the case of alkanes, the terminal CC bonds have greater weight that inner CC bonds, which agrees with the »physical picture« of terminal CC bonds having a larger molecular surface than inner CC bonds. The reason why the connectivity index is so widely used in structure-property regressions is because it so well simulates local molecular features of a molecular surface – and it does this because it has been designed to do that! It has been constructed to satisfy a set of linear inequalities that discriminate CC bonds according to their type (by differentiating primary, secondary, tertiary and quaternary carbon atoms). The inequalities themselves are based on the relative magnitude of the selected molecular property (boiling points of alkanes), which is generally believed to be a surface-dependent property. Hence, there are many »physical« ideas behind the construction of the connectivity index, which makes it in a way a »physical quantity« in the same sense in which the Pauling bond orders can be viewed as »physical quantities.« Strictly speaking, however, both quantities, the Pauling bond orders and the connectivity indices (the same of course is true of Coulson’s bond orders and the »pivotal« notion of orbitals, their overlapping, their charge populations and hybridization) are not observables. To better see that there is no conceptually essential difference between the Pauling bond orders, the validity of which nobody has ever challenged, and the connectivity index, which has been, to say the least, a »controversial« quantity, consider the use of the two molecular descriptors. Although the Pauling bond orders are non-physical quantities, by using these bond orders you can in a larger polycyclic benzenoid hydrocarbon predict which CC bond is shorter and which is longer, thus you can relate them to experimentally measurable quantities. Similarly, by using the connectivity index, a non-physical quantity, you can predict which among octane isomers or nonane isomers will have a higher boiling point and which will have a lower boiling point – boiling points, of course being measurable quantities. So what is the difference? Why should the Pauling bond orders be viewed differently from the connectivity index?

In order to remind readers of the frequent use of non-observable quantities in chemistry (this in the sense of Dirac’s well-known textbook on Quantum Mechanics),[154] we have listed a number of common non-observables of chemistry – all of the same legitimacy:

Hybridization,
Molecular orbitals,
Localized orbitals,
Natural orbitals,
HOMO,
LUMO,
Atomic charges,
Atom polarizabilities,
Pauling bond orders,
Coulson bond order,
Bond dipoles,
Bond polarizabilities,
Potential function,
Aromaticity,
Kekulé valence structure,
Clar’s structure,
Clar’s aromatic -sextet,
Fries valence structure,
Anti-Fries valence structure,
Conjugated circuits,
Resonance energy,
Rumer diagrams,
Partial ordering,
Substructure,
Graph theoretical indices,
Nucleus independent chemical shift,
Ring currents.

They are associated with General Chemistry, Structural Chemistry, Quantum Chemistry and Chemical Graph Theory and they are all on an equal footing, in other words, equally »fundamental« from the theoretical points of view. Thus, if topological indices are *ad hoc* mathematical constructions, the same can be said of Pauling's hybridization and hybrids. They are also *ad hoc* mathematical constructions. It is futile to seek distinction between different non-observables because they are all the same – *ad hoc* mathematical constructions. Hence, it is not their nature that needs to be considered but their ultimate utility that is important. Thus, just as Pauling's hybridization is of enormous use in building structural models and understanding chemical architecture, so are graph theoretical indices of enormous use in characterizing the dependence of molecular properties on molecular structure and understanding the structure-property relationship. What else is there to describe molecules and their shapes but mathematical invariants of molecules?

In my recent article *Chemical Graph Theory: Fact & Fiction*[155] I have listed a dozen recent accomplishments of chemical graph theory, so there is no need to recapitulate. However, we ought to counterbalance the concerns that some have about the »physical« interoperation of mathematical descriptors of molecules by mentioning the use of topological indices in combinatorial libraries, either for searching similar or dissimilar structures or novel lead compounds. In this respect, we would like to draw the readers' attention to the work of Professor Lahana and his group,[156] who used some 20 molecular descriptors (half of which were topological indices) and were able to screen a combinatorial library of over half a million compounds and select two dozen promising compounds for closer study. They eventually succeeded in focusing on four compounds, which were synthesized and tested for their immunosuppressive activity. One of the four compounds was found to have not two or three times, which would be quite a success, but about 100 times higher bio-activity than the lead compound! Now why should users of combinatorial libraries be concerned with physical interpretation of molecular descriptors when they use them only to filter out potentially interesting compounds from a huge pool of structures?

CONCLUDING REMARKS

To some, the outlined »tour« of the »wild« territorial waters of Chemical Graph Theory may appear less important and my responses aggressive, but we hope that enough information was presented to justify a more aggressive response to the »critics« of Chemical Graph Theory.

One may say that most of us involved in Chemical Graph Theory, Nenad Trinajstić included, have been unhappy about how Graph Theory has been treated by outsiders. We are equally sure that the »critics« must have been unhappy to see that, despite their opposition, contributions that they have rejected nevertheless appear in print. Thus, there may be plenty of unhappiness on both sides. It therefore seems appropriate to end this exposition on a positive note by indicating how to reduce this unhappiness. It appears to be no better advice for this than to list the *'Thirteen Virtues' for living a Happy Life*, that Benjamin Franklin [157] felt were the rules that would lead to a life of goodness, health, and genuine lasting happiness:

(1) Temperance,
(2) Silence,
(3) Order,
(4) Resolution,
(5) Frugality,
(6) Industry,
(7) Sincerity,
(8) Justice,
(9) Moderation,
(10) Cleanliness,
(11) Tranquility,
(12) Chastity,
(13) Humility.

I can give 13 reasons for quoting Benjamin Franklin, but I will not bore readers with them, except by mentioning just one of the 13, that dealing with silence;

Silence: Speak not but what may benefit others or yourself.

If »critics« of Chemical Graph Theory had been silent, they would spare themselves embarrassments that are becoming merciless with time. They ought to know that:

»The voice of intellect is a soft one, but it does not rest until it has gained a hearing. Ultimately, after endless rebuffs, it succeeds. This is one of the few points in which one may be optimistic about the future of mankind.« (Sigmund Freud (1856–1939)).

But I do not want to leave readers with the impression that we who have been devoted to the development of Chemical Graph Theory are an »angry lot.« We also have our pleasures such as when papers that have been rejected in reputed journals have been accepted in journals of even greater reputation!

Numerous chemists have appreciated our work and have also been supportive. A very brief list includes such chemistry dignitaries as: C. A. Coulson, F. A. Cotton, R. Hoffmann, J. Karle, A. R. Katritzky, P. O. Löwdin, R. G. Parr, O. E. Polansky, I. Ugi, and E. B. Wilson. But the circle of supporters is much wider. For example, the fact that Trinajstić has been recognized as one of the early pioneers of Chemical Graph Theory is well reflected in the review of the book of Kier and Hall: *Molecular Connectivity in Chemistry and Drug Research*[158] published in 1977 in the *Journal of Medicinal Chemistry* by J. Wright.[159] Here is the relevant passage:

»Since its inception over 100 years ago by Sylvester, the subject of molecular connectivity has attracted inordinately little concern among chemists. The past five years, however, have seen awakening of a germ of interest in the application of topological graph theory to elucidation of molecular properties. These advances are largely the issue of chemists and applied mathematicians from the Zagreb circle and their adherents in England, Germany, and the United States. Almost invariably, the work has involved predictions of thermodynamical and other properties of hydrocarbons....

In its initial three chapters, the present work does adhere to the traditional development, although the coverage is sparse and omits more significant work than it includes. Here, the authors rely principally upon calculations of the Yugoslavian theoretician, Milan Randic (now in Iowa), which are contrasted with several less successful treatments....

This book does not provide an adequate background in graph theory sufficient to establish a basic understanding of molecular connectivity. Such a review is still sorely needed to bring together a scattered and obscure literature. Rather this book is recommended as a very exciting and exotic approach to theoretical chemistry and drug design.«

From this excerpt it is clear (i) That the Zagreb circle (and this means Nenad Trinajstić) was one of the initiators in the early development of Chemical Graph Theory; (ii) That a background in Graph Theory is required to understand molecular connectivity, and (iii) That there is need for a book on Chemical Graph Theory. This last condition has been fulfilled by Trinajstić's monograph on Chemical Graph Theory published a few years after the book of Kier and Hall. Finally, I give some topics of Chemical Graph Theory in which I collaborated with Nenad Trinajstić:

(1) Symmetry of graphs of degenerate isomerizations;
(2) Conjugation and aromaticity in polycyclic conjugated hydrocarbons;
(3) Isospectral and endospectral graph;
(4) Review of solved and unsolved problems of Chemical Graph Theory;
(5) Critical examination of quantum chemical computer resonance energies;
(6) Wheland polynomial (which counts excited structures in polycyclic conjugated hydrocarbons);
(7) Statistical approach to resonance energy for large benzenoid hydrocarbons;
(8) Conjugated circuits of excited Kekulé valence structures of polycyclic conjugated hydrocarbons;
(9) Stability of nonbenzenoid hydrocarbons;
(10) Search for novel structural invariants of interest in chemistry;
(11) Historical remarks of early and less known contributions to Chemical Graph Theory;
(12) Limits of highly accurate calculations of polymers;
(13) Topological indices, including the Wiener index.

Acknowledgements. – I take this opportunity to thank Nenad Trinajstić for a long and constructive collaboration over the past 30-plus years, which resulted in over 70 joint publications.

APPENDIX

Brief outline of the selection of the Graph Theory theorems listed in Table IV

Theorem	Year	
Clarke	1972	The sum of the characteristic polynomials of Ulam subgraphs of a graph is the derivative of the characteristic polynomial of the graph.
Euler	1736	A graph is eulerian if and only if it has no vertices of odd degree.
Fary	1948	Every simple planar graph has embedding in which each edge is a straight line.
Hall	1935	The necessary and sufficient condition that a bipartite graph has a maximal matching is that for any set of vertices S holds $\lvert N(S)\rvert \geq \lvert S\rvert$, where N(S) defines the neighbor set of S.
König	1931	For bipartite graphs a maximum matching equals minimum covering.
Kuratowski	1930	A graph is planar if and only if it contains no subdivision of K_5 and $K_{3,3}$.
Matrix-tree theorem[(a)]	1940	The number of spanning trees is given by product $\boldsymbol{K} \times \boldsymbol{K}'$, where $\boldsymbol{K}$ is the matrix obtained from incidence matrix by deleting any one of its rows.
Menger	1927	A graph with $(k+1)$ vertices is k-connected if and only if two distinct vertices are connected by at least k internally-disjoint paths.
Petersen	1891	Every 3-regular graph without cut edges has a perfect matching.
Robin	1939	If a graph is 2-edge-connected then the graph has a disconnected orientation.
Turan	1941	If a graph contains no K_{m+1} (clique) then the graph is majorised by some complete m-partite graph.
Tutte	1947	A graph has a perfect matching if and only if the number of odd components in $G\text{-}S \leq \lvert S\rvert$.
Vizing	1964	The chromatic number of a graph is either equal to the maximal degree Δ or to $(\Delta + 1)$.

(a) Implicit in the work of Kirchhoff (1847).

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Russian for »hundred« (German: »Hundert«), which was sufficient for him to change his name.

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SAŽETAK

Nenad Trinajstić – Pionir kemijske teorije grafova

Milan Randić

Ukratko su prikazani brojni doprinosi Nenada Trinajstića u kemijskoj teoriji grafova, važnoj grani teorijske kemije, koja se u naše vrijeme vrlo brzo razvija. Također je prikazano djelovanje N. Trinajstića u hrvatskoj kemiji.