IRANIAN JOURNAL OF MATHEMATICAL CHEMISTRY

University of Kashan

IJMC

http://IJMC.Kashanu.ac.ir

Iranian Journal of Mathematical Chemistry

Iranian Journal of Mathematical Chemistry (IJMC) publishes quality original research papers and survey articles in Mathematical Chemistry and related areas that are of the highest possible quality.

Research papers and review articles are selected through a normal refereeing process by a member of editorial board.

It is intended that the journal may act as an interdisciplinary forum for publishing chemically important mathematical papers. Papers published in this journal must have a clear connection to chemistry with non-trivial mathematics.

Aims and Scopes: Iranian Journal of Mathematical Chemistry is a bi publication of the University of Kashan. It contains research and expository papers as well as short communications on chemically important mathematical problems.

Preparation of Manuscripts: An abstract of 150 words or less and keywords clarifying the subject of the manuscripts are required. Authors should submit the paper electronically in word file to ijmc@kashanu.ac.ir.

The language of the journal is English. Authors who are less familiar with English language are advised to seek assistance from proficient scholars to prepare manuscripts that are grammatically and linguistically free from errors. Manuscripts should be typed with double spacing and wide margins. Papers submitted for consideration for publication have to be prepared concisely and must not exceed 30 typewritten pages, (font 12, 1.15 spacing, including tables & graphs). Diagrams and figures should be submitted as original drawings. Figures and tables are to be numbered in the sequence in which they are cited in the manuscript. Every table must have a caption that explains its content. Tables and diagrams are to be prepared in separate pages and placed at the end of the manuscript. References to the literature should be numbered in square brackets in the order in which they appear in the text. A complete list of references should be presented in numerical order at the end of the manuscript. References to journals, books, proceedings and patents must be presented in accordance with the following examples:

Journals: I. Gutman, B. Zhou and B. Furtula, The Laplacian-energy like invariant is an energy like invarint MATCH Commun. Math. Comput. Chem., 64(1) (2010), 85-96.

Patents: Primack, H.S.; Method of Stabilizing Polyvalent Metal Solutions, U.S. patent No. 4, 373, 104(1983).

Indexing/ Abstracting: The Iranian Journal of Mathematoical Chemistry is indexed/abstracted in the following:

- Islamic World Science Citation Center (ISC)
- Zentralblatt für Mathematik
- Web of Science (ISI)

EditorialBoard

Past Editors

Editor-in-Chief:

Ali Reza Ashrafi
Department of Pure Mathematics, Faculty of Mathematical Sciences, University of Kashan, Kashan87317-53153, I R IRAN
mail:ashrafi@kashanu.ac.ir

Managing Director:

Behnam Bazigaran
Department of Pure Mathematics, Faculty of Mathematical Sciences, University of Kashan, Kashan87317-53153, I R IRAN
E-mail:bazigaran@kashanu.ac.ir

Language Editor:

Seyfollah Mosazadeh
Department of Pure Mathematics, Faculty of Mathematical Sciences, University of Kashan, Kashan 87317-53153, I R IRAN
E-mail: s.mosazadeh@kashanu.ac.ir

Technical Manager:

Marzieh Pourbabaee
Department of Applied Mathematics, Faculty of Mathematical Sciences, University of Kashan, Kashan 87317-53153, I R IRAN
Email:m.pourbabaee@kashanu.ac.ir

Iranian Journal of Mathematical Chemistry

Vol. 8, No. 3 September 2017

CONTENTS **pages**

Iranian J. Math. Chem. 8(3) September (2017) 231 − 257

Iranian Journal of Mathematical Chemistry

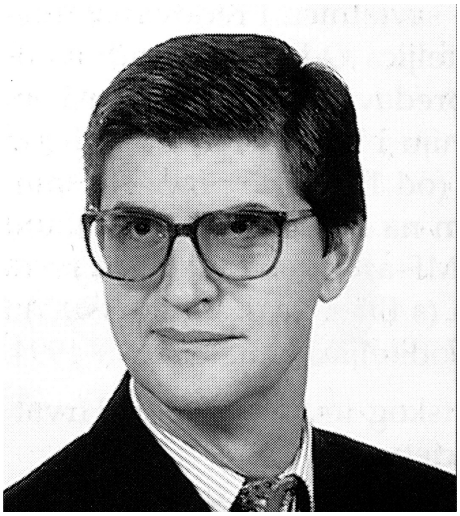
Journal homepage: ijmc.kashanu.ac.ir

Autobiographical Notes

NENAD TRINAJSTIĆ•

The Rugjer Bošković Institute and Croatian Academy of Sciences and Arts, Zagreb, Croatia

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 four 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. Our mother encouraged us 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 was until retirement 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 lives in Toronto since 1993, he is now a Canadian citizen and his daughter Emma was born in Toronto.

• Corresponding author (Email: trina@irb.hr)
DOI: 10.22052/ijmc.2017.64354.1248

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 several centuries in the place now called Trinajstići, located near Matulji) and belongs to a class of Croatian family names with numbers in their roots [2]. Šimunović [2], an in 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 (1931-2013) (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). 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 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 Pasteu (1822−1895) and Justus von Liebig (1803-1873) 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 this student left Zagreb. Then my interest suddenly focused on philosophy. I accidentally came by a book on Plato (427−347 B.C.)

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 War cup Cornforth, 1917−2013), 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 AceticAcid*. 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 (1922−2010) (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 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 Ružižka (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 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 (1930) [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 (1921−2015). In Cambridge, Randić met John Norman Murrell, FRS (1932−2016) who was working for his Ph.D. degree under Professor Hugh Christopher Longuet–Higgins, FRS (1923−2004). 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 in Murrell's Group 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 (1943)) and some even won Ph.D. degrees working with him (*e.g.*, Slobodan Danko Bosanac (1946)). 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 Walter Kroto, FRS (1939−2016), a Nobel laureate for chemistry (he shared the 1996 Prize with Robert F. Curl (1933) and Richard E. Smalley (1943–2005) for their discovery of buckminsterfullerene). Kroto was a nice friendly person. He did Ph.D. research in spectroscopy under Richard Dixon (1930). 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 (1897−1978) and Manfred Eigen (1927) 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].

Another member of Murrell's group 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 was reader in chemistry. He is now retired. 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 had already had two editions [15]. He was also senior reporter for the specialist periodical report entitled *Chemical Modeling – Applications and Theory*, published by the 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* (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 76 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* (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 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 *How I Met Michel Dewar*. 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 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 post docs was a precursor of the AM1 (Austin Model One) method – the paper introducing the AM1 was 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 (1942), who was at that time doing Ph.D. research under Professor Frederic Albert Matsen (1913−2006). 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 published over the years a number of research papers [*e.g.*, 26–28].

5. YEARS AT THE RUGJER BOŠKOVIĆ INSTITUE

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.

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* (Školska knjiga, Zagreb, 1974; this book was translated by my doctoral student Gani Jashari (1952) 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 (1937), Zvonimir Maksić (1938-2011) and I wrote a book for undergraduate

students on the use of symmetry in quantum chemistry, entitled *Symmetry of Molecules* (Školska knjiga, Zagreb, 1979). I also supervised 15 B.Sc. degree theses, 9 M.Sc. theses and 18 Ph.D. theses. Among the students who were awarded their B.Sc degrees under my supervision, Zlatko Bačić (1954) 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 (1947), who got all three degrees, B.Sc., M.Sc. and Ph.D., under my supervision, is retired, but used to be the director of the University Institute of Physics in Zagreb and a leading Croatian researcher in vacuum physics and nanotechnology. Ivan Gutman (1947) 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 used to be the 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 was 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 (1954) is a distinguished research professor in the Institute Rugjer Bošković. 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 hetero conjugated polycyclic molecules. Bono Lučić (1964) 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 (1974) got the first Croatian Ph.D. in theoretical biology

with her dissertation *Cells as Tensegrity Structures* (University of Zagreb, 2002). I suggested her this research topic. She completed the experimental part of the thesis at Harvard University working with Professor Ning Wang. Tensegrity is a contraction of terms tensional integrity. This 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 250 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 (1937) [*e.g.*, 42]. With Klasinc and his doctoral students Branko Ruščić (1952, presently a senior scientist at the Argonne National Laboratory, Argonne, Illinois) and Aleksandar Sabljić (1950, retired 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 bioactivity [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, late Albin Jurić, Dragan Amić) and

many colleagues (*e.g.*, Dragoš Cvetković, Milan Randić, Doug Klein, Tomislav Živković, Roger Blakeney Mallion, Danail Bonchev, late Ante Graovac, Dejan Plavšić, late 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 (1927−2016) [44], a distinguished mathematician from Ilmenau in the East Germany; an issue of MATCH [45] has been 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 evident 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 (1947) 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 Adrian 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 Sheard Child, FRS (1937) 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 thesis having been obtained from the University of Wales at Swansea, under Claude William 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 (1921−2005) and was a postdoctoral visitor to the

Mathematical 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 Lowell Wayne Beineke (1939) were in the same group of visitors. Another well–known graph–theoretician, Robin James Wilson (1943), 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 (1931) in Bucharest, Dennis H. Rouvray (1938) in South Africa, Haruo Hosoya (1936) in Tokyo, William C. Herndon (1932−2011) in El Paso (Texas), Roger Blakeney Mallion (1946) in Oxford and that, before them, Edgar Heilbronner (1921−2006) was very productive in this area while he was at ETH and that Coulson and Klaus Ruedenberg (1920) 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 (1918−2011), Lemont Burwell Kier (1930), William B. Purcell, Rudolf Zahradnik (1928), 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 (1908-1992) 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 (1956), 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 (1944) 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 (1934) (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 it appeared in that book as the first article.

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 structures, 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], a variable Wiener index [72] and a sum-connectivity index [72a]. 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 (1958) 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]. In 1981, in collaboration with Ovanes Mekenyan, we derived the topological super index 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, a CROMR sel procedure was introduced [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 (1953) from the University of Osijek [88], Professor Alan Roy Katritzky, FRS (1928−2014) and his group from the University of Florida (Gainesville) and Damir Nadramija and his group from PLIVA [89–91]. Our 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 (1943) and his group from the University of

Düsseldorf. We 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 Walter Kroto, FRS (1939-2016; Nobel prize in chemistry 1996) [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 [105]. 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 2627 times to the end of a year 2016.

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 (1937) 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 (1943) and Randić on zero [123] and one [124] (the computer age is based on these two numbers: 0 and 1) and alone on the number five [125], and with Iva Marija Tolić on the manifestations of the number five in biology [126]. We also published an article on the number 13 [127]. Later Pogliani published book entitled *Numbers Zero, One, Two, and Three in Science and Humanities* (Kragujevac, 2006, pp. 250).

I was also interested in the uses of graph-theoretical matrices in chemistry. My research in this area resulted in a number of publications and two editions of the book entitled *Graph−Theoretical Matrices in Chemistry* (the first edition University of Kragujevac, Kragujevac, 2007; the second edition CRC press/Taylor and Francis Group, Boca Raton, 2015). As I already mentioned I was interested in history of chemistry in Croatia. My studies in this direction already resulted in two monographs: N. Trinajstić, *100 Croatian Chemists*, Školska knjiga, Zagreb, 2002 and S. Paušek-Baždar and N. Trinajstić,

Croatian Chemistry in the 20th Century, Školska knjiga, Zagreb, 2014. Croatian Academy of Sciences and Arts published my book on my *Life in Science* (Zagreb, 2016).

Citations of my various contributions are rather modest. My h index is 59, the most cited paper is I. Gutman, M. Milun, N. Trinajstić, Graph theory and molecular orbitals. Nonparametric resonance energies of arbitrary conjugated systems, *J. Am. Chem. Soc*. 1977, 99, 1692−1704 (SCI=561), citations of my papers is 13760, of my books is 4937 and the total citations were 20176 (these numbers provided Bono Lučić).

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, the Mid–America State Universities Association Distinguished Foreign Scholar Award in 1987 and Croatian State Award for Life Achivements in Science (2004). 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). Two MATH/CHEM/COMP meetings (in 2002 and 2016) had a day-symposia in my honour.

Several journals published issues in my honour, such as *Internet Electronic Journal of Molecular Design* (2003, issues 7 to 12; 2004, issues 1 to 6), *Croatica Chemica Acta* (2004, 77, 1−414), *Journal of Chemical Information and Modeling* (2007, 47, 705−951), *International Journal of Chemical Modeling* (2015, 6, 1941−3955). It is interesting to note that *Journal of Chemical Information and Modeling* in 2010 has celebrated the 50th anniversary. In the anniversary issue were listed 50 most cited papers published in this journal and 50 authors with the highest numbers of papers published in this journal. In the 50 years, this journal published about 10.000 papers. Among the 50 most cited papers are 5 papers from Croatian authors: 3 of Randić, one of Gutman and one of Mihalić, Nikolić and myself. Among the 50 most productive authors are tri Croatian authors: Randić the second, I am listed as the ninth and Gutman as 12th most productive author in this journal.

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* (1999−2002), *Gazophylacium* (since 2000) and *Computational Biology and Chemistry* (2003−2006). 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 editor–in–chief since 1993),

the editor–in chief of *Croatica Chemica Acta* (1994−2005) and of *Prirodoslovlje* (2001−2008). 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 who became a member of the Academy and the first theoretical chemist ever. I am also a member of the International Academy of Mathematical Chemists since 2006.

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 (1929) 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 (1938) in the Department of Chemistry), the University of Düsseldorf (staying in the Computing Center with Professor Jan von Knop at least once a year from 1973 to 2003. I probably spent 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 (1938)), the Chemical Research Center of the Hungarian Academy of Sciences in Budapest (visiting Dr István Lukovits (1944−2007)), 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.

ACKNOWLEDGMENT

I sincerely thank my family for their continuous support and all my teachers, former students, my colleagues and friends all over the world for their kindness, patience and help shown to me throughout my life. Of course, without my dear wife Judita nothing listed above would happen; her support since the day we met was decisive.

REFERENCES

1. M. Moguš, *A History of Croatian Language*: *Toward a Common Standard*, Globus, Zagreb, 1995.
2. P. Šimunović, *Naša prezimena* (*Our Family Names*), Nakladni zavod Matice Hrvatske, Zagreb, 1985.
3. S. J. Cyvin, J. Brunvoll and B. N. Cyvin, Di–4–Catafusenes: A New Class of Polygonal Systems Representing Polycyclic Conjugated Hydrocarbons, *Croat. Chem. Acta* **1996**, *69*, 177–190.
4. N. Trinajstić, *100 hrvatskih kemičara* (*100 Croatian Chemists*), Školska knjiga, Zagreb, 2003, pp. 50–51.
5. N. Trinajstić, Obituary – Krešimir Humski (1939–1997), *Croat. Chem. Acta* **1998**, *71*, A9–A16.
6. N. Trinajstić, Obituary – Krešimir Balenović (1914–2003), *Croat. Chem. Acta* **2003**, *76*, A3–A4.
7. N. Trinajstić, *Ogledi o znanosti i znanstvenicima* (*Essays on Science and Scientists*), Matica hrvatska, Zagreb, 1998, pp. 50–80.
8. S. Nikolić and N. Trinajstić, Milan Randić – Life and Work, *Croat. Chem. Acta* **2002**, *75*, 319–327.
9. N. Trinajstić, Quantum Chemistry in Croatia – Beginnings, *Kem. ind.* (Zagreb) **2001**, *50*, 427–429.
10. C. A. Coulson and W. E. Moffitt, I. Properties of Certain Strained Hydrocarbons, *Phil. Mag.* **1949**, *40* (ser. 7), 1–35.
11. D. Phillips, Obituary – George Porter (1920–2002), Nature **2002**, *419*, 578.
12. S. Carter, N. Trinajstić and S. Nikolić, On the Use of ID Numbers in Drug Research: A QSAR of Neuroleptic Pharmacophores, *Med. Sci. Res.* **1988**, *16*, 185–186; S. Carter, S. Nikolić and N. Trinajstić, A Novel Algorithm for QSAR, *Int. J. Quantum Chem.*: *Quantum Biol. Symp.* **1989**, *16*, 323–330; N. Trinajstić, S. Nikolić and S.Carter, QSAR: Theory and Application, *Kem. ind.* (Zagreb) **1989**, *38*, 469–484; S. Nikolić, N. Trinajstić, Z. Mihalić and S. Carter, On the Geometric–Distance Matrix and the Corresponding Structural Invariants of Molecular Systems, *Chem. Phys. Lett.* **1991**, *179*, 21–28.
13. A. Hinchliffe and N. Trinajstić, Calculation of Proton Coupling Constants for Dibenzothiophene Radical Anion, *Theoret. Chim. Acta* **1968**, *10*, 458–460.
14. A. Hinchliffe and N. Trinajstić, Electronic Properties of Conjugated Ions, *Theoret. Chim. Acta* **1968**, *11*, 271–273.

15. A. Hinchliffe, Chemical Modeling – From Atoms to Liquids, Wiley, Chichester, 1999.
16. S. Carter, J. N. Murrell, E. J. Rosch, N. Trinajstić and P. A. H. Wyatt, The Kinetics of Unsymmetrical Quinone–Hydroquinone Redox Reactions, *J. Chem. Soc. B* **1967**, 477–484.
17. A. Hinchliffe, J. N. Murrell and N. Trinajstić, Calculation on the Energy Levels of Alternant Hydrocarbon Anions, *Trans. Faraday Soc.* **1966**, *62*, 1362–1369; N. Trinajstić, Molecular Orbital Calculations for Tetracene Monopositive Ion, *Croat. Chem. Acta* **1966**, *38*, 283–286.
18. J. N. Murrell, J. G. Stamper and N. Trinajstić, Localized Orbitals of Water, *J. Chem. Soc. A* **1966**, 1624–1627; J. G. Stamper and N. Trinajstić, Localized Orbitals for Some Simple Molecules, *J. Chem. Soc. A* **1967**, 782–784.
19. N. Trinajstić and M. Randić, Maximum Overlap Hybridisation in Methyl Substituted Cyclopropanes, *J. Chem. Soc.* **1965**, 5621–5624.
20. J. N. Murrell, Michael James Steuart Dewar (24 September 1918–11 October 1997), *Biog. Mems. Fell. R. Soc. Lond.* **1998**, *44*, 127–140.
21. M. J. S. Dewar, A. J. Harget and N. Trinajstić, Ground States of Conjugated Molecules. XV. Bond Localization and Resonance Energies in Compounds Containing Nitrogen or Oxygen, *J. Am. Chem. Soc.* **1969**, *91*, 6321–6325.
22. M. J. S. Dewar and N. Trinajstić, Ground States of Conjugated Molecules. XX. SCF MO Treatment of Compounds Containing Bivalent Sulfur, *J. Am. Chem. Soc.* **1970**, *92*, 1453–1459.
23. M. J. S. Dewar, D. H. Lo, D. B. Patterson, N. Trinajstić and G. E. Peterson, MINDO/2 Calculations of Nuclear Quadrupole Coupling Constants of Chlorobenzenes, *J. C. S. Chem. Comm.* **1971**, 238–239.
24. M. J. S. Dewar, M. C. Kohn and N. Trinajstić, Cyclobutadiene and Diphenylcyclobutadiene, *J. Am. Chem. Soc.* **1971**, *93*, 3437–3440.
25. M. J. S. Dewar, E. G. Zoebisch, E. F. Healy and J. J. P. Stewart, AM1: A New General Purpose Quantum Mechanical Molecular Model, *J. Am. Chem. Soc.* **1985**, *107*, 3902–3909.
26. D. J. Klein and N. Trinajstić, Hückel Rules and Electron Correlation, *J. Am. Chem. Soc.* **1984**, *106*, 8050–8056.
27. D. J. Klein, T. Živković and N. Trinajstić, Resonance in Random π–Electron Polymers, *J. Math. Chem.* **1987**, *1*, 309–334
28. N. Trinajstić, T. G. Schmalz, T. P. Živković, S. Nikolić, G. E. Hite, D. J. Klein and W. A. Seitz, [N]phenylenes: A Theoretical Study, *New J. Chem.* **1991**, *15*, 27–31.
29. I. Lukovits, S. Nikolić and N. Trinajstić, On Relationship Between Vertex–Degrees, Path–Numbers and GraphValence–Shells in Trees, *Chem. Phys. Lett.* **2002**, *354*, 417–422; I. Lukovits and N. Trinajstić, Atomic Walk Counts of Negative Order, *J.*

Chem. Inf. Comput. Sci. in press; D. Amić, D. Davidović–Amić, D. Bešlo and N. Trinajstić, Structure–Radical Scavenging Activity Relationship of Flavonoids, *Croat. Chem. Acta* **2003**, *76*, 55–61.

30. A. T. Balaban, A. S. Dreiding and A. Kerber, Oskar E. Polansky (1919–1989) and MATCH, *MATCH – Commun. Math. Computer Chem.* **1989**, *24*, I–V.
31. H. W. Kroto, J.R. Heath, S. C. O'Brien, R. F. Curl and R. E. Smalley, C_{60}: Buckminsterfullerene, *Nature* **1985**, 318, 162–163.
32. N. Trinajstić, Calculation of Carbon–Sulphur Bond Lengths, *Tetrahedron Lett.* **1968**, 1529–1532.
33. J. N. Herak and N. Trinajstić, Free Valence Indices of Carbon in Heterocyclic Compounds, *Theoret. Chim. Acta* **1968**, *9*, 333–335.
34. M. Randić. Conjugated Circuits and Resonance Energies of Benzenoid Hydrocarbons, *Chem. Phys Lett.* **1976**, *38*, 68–70. It appears that José A.N.F. Gomes discovered independently conjugated–circuit model in 1976 while he was in Oxford doing Ph.D. research (private information by R. B. Mallion in his letter of March 24, 2003). See also J. A. N. F. Gomes, Why are the Properties of Polycyclic Hydrocarbons Additive over Conjugated Circuits?, *Croat. Chem. Acta* **1980**, *53*, 561–569.
35. M. Randić and N. Trinajstić, Conjugation and Aromaticity of Corannulenes, *J. Am. Chem. Soc.* **1984**, *106*, 4428–4434.
36. M. Randić, N. Trinajstić, J. von Knop, and Ž. Jeričević, Aromatic Stability of Heterocyclic Conjugated Systems, *J. Am. Chem. Soc.* **1985**, *107*, 849–859.
37. M. Randić and N. Trinajstić, On the Relative Stabilities of Conjugated Heterocycles Containing Divalent, Sulfur, *Reports* **1986**, *6*, 379–429.
38. M. Randić, S. Nikolić and N. Trinajstić, On the Aromatic Stability of a Conjugated C_{60} Cluster, *Croat. Chem. Acta* **1987**, *60*, 595–604.
39. D. J. Klein and N. Trinajstić, Foundations of Conjugated–Circuits Models, *Pure Appl. Chem.* **1989**, *61*, 2107–2115.
40. S. Nikolić, N. Trinajstić and D. J. Klein, The Conjugated–Circuit Model, *Comput. Chem.* **1990**, *14*, 313–322.
41. J. Koller, A. Ažman and N. Trinajstić, *Ab Initio* Molecular Orbital Studies in Quantum Biology. Electronic Characteristics of Indole and Benzofuran, in: *Quantitative Structure–Activity Relationships*, M. Tichy, Ed., Akademiai Kiado, Budapest, **1976**, pp. 205–209.
42. H. Güsten, L. Klasinc, J. von Knop, and N. Trinajstić, Application of Photoelectron Spectrometry to Biologically Active Molecules and Their Constituent Parts. I. Indoles, in: *Excited States of Biological Molecules*, J. B. Birks, Ed., Wiley, Chichester, Sussex, **1975**, pp. 45–49.

43. L. Klasinc, B. Ruščić, A. Sabljić and N. Trinajstić, Application of Photoelectron Spectroscopy to Biologically Active Molecules and Their Constituent Parts. VI. Opiate Narcotics, *J. Am. Chem. Soc.* **1979**, *101*, 7477–7482.
44. H. Sachs, Beziehungen zwischen den in einem Graphen enthaltenen Kreisen und seinem charakterischen Polynom, *Publ. Math.* (Debrecen) **1964**, *11*, 119–134.
45. *MATCH – Commun. Math. Computer Chem.* **2003**, *48*, 1–223.
46. A. Graovac, I. Gutman, N. Trinajstić and T. Živković, Graph Theory and Molecular Orbitals. Application of Sachs Theorem, *Theoret. Chim. Acta* **1972**, *26*, 67–78.
47. I. Gutman, Impact of the Sachs Theorem on Theoretical Chemistry: A Participant's Testimony, *MATCH –Commun. Math. Computer Chem.* **2003**, *48*, 17–34.
48. R. B. Mallion, A. J. Schwenk and N. Trinajstić, A Graphical Study of Heteroconjugated Molecules, *Croat. Chem. Acta* **1974**, *46*, 171–182.
49. R. B. Mallion, A. J.Schwenk and N. Trinajstić, On the Characteristic Polynomial of a Rooted Graph, in: Recent Advances in Graph Theory, M. Fiedler, Ed., Academia, Prague, 1975, pp. 345–350.
50. N. Trinajstić, Charles Alfred Coulson (1910–1974), *Croat. Chem. Acta* **1974**, *46*, A5–A6.
51. H. Hosoya, The Topological Index Z Before and After 1971, *Internet Electron. J. Mol. Des.* **2002**, *1*, 428–442,
52. H. Hosoya, Topological Index. A Newly Proposed Quantity Characterizing the Topological Nature of Structural Isomers of Saturated Hydrocarbons, *Bull. Chem. Soc. Jpn.* **1971**, *44*, 2332–2339.
53. M. Randić, private communication.
54. I. Gutman, M. Milun and N. Trinajstić, Topological Definition of Resonance Energy, *MATCH – Commun. Math. Computer Chem.* **1975**, *1*, 171–175.
55. I. Gutman, M. Milun N. Trinajstić, Graph Theory and Molecular Orbitals. XIX. Non–Parametric Resonance Energies of Arbitrary Conjugated Systems, *J. Am.* Chem. Soc. 1977, 99, 1692–1704.
56. P. Ilić and N. Trinajstić, Topological Resonance Energies of Conjugated Ions, Radicals and Ion–Radicals, *J. Org. Chem.* **1980**, *45*, 1738–1748; P. Ilić, B. Sinković and N. Trinajstić, Topological Resonance Energies ofConjugated Structures, *Israel J. Chem.* **1980**, *20*, 258–269.
57. A. Sabljić and N. Trinajstić, Aromatic Stability of Bridged Annulenes, *J. Org. Chem.* **1981**, *46*, 3457–3461.
58. B. Mohar and N. Trinajstić, On Computation of the Topological Resonance Energy, *J. Comput. Chem.* **1982**, *3*, 28–36.
59. J. Aihara, A New Definition of Dewar–Type Resonance Energies, *J. Am. Chem. Soc.* **1976**, *98*, 2750–2758.

60. C. D. Godsil and I. Gutman, On the Theory of the Matching Polynomial, *J. Graph Theory* **1981**, *5*, 137–144.
61. V. I. Minkin, M. N. Glukhovtsev and B. Y. Simkin, *Aromaticity and Antiaromaticity*, Wiley–Interscience, New York, 1994, pp. 14–19.
62. N. Trinajstić, Hückel Theory and Topology, in: Semiempirical Methods of Electronic Structure Calculation. Part A: Techniques, G. A. Segal, Ed., *Modern Theoretical Chemistry*, Vol. 7, Plenum, New York, 1977, pp. 1–27 .
63. A. Sabljić and N. Trinajstić, Quantitative Structure–Activity Relationships: The Role of Topological Indices, *Acta Pharm. Jugosl.* **1981**, *31*, 189–214.
64. D. Plavšić, S. Nikolić, N. Trinajstić and Z. Mihalić, On the Harary Index for the Characterization of Chemical Graphs, *J. Math. Chem.* **1993**, *12*, 235–250; K. Xu, K.Ch. Das and N. Trinajstić, *The Harary Index of a Graph*, Springer, JHeidelberg, pp, 74.
65. B. Lučić, A. Miličević, S. Nikolić and N. Trinajstić, Harary Index – Twelve Years Later, *Croat. Chem. Acta* **2002**, *75*, 847–868.
66. D. Amić and N. Trinajstić, On the Detour Matrix, *Croat. Chem. Acta* **1995**, *68*, 53–62.
67. N. Trinajstić, S. Nikolić, B. Lučić. D. Amić and Z. Mihalić, The Detour Matrix in Chemistry, *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 631–638.
68. S. Nikolić, N. Trinajstić and Z. Mihalić, The Detour Matrix and the Detour Index, in: *Topological Indices and Related Descriptors in QSAR and QSPR*, J. Devillers and A.T. Balaban, Eds., Gordon and Breach Science Publishers, The Netherlands, 1999, pp. 279–306.
69. B. Bogdanov, S. Nikolić and N. Trinajstić, On the Three–Dimensional Wiener Number, J. Math. Chem. **1989**, *3*,299–309; *J. Math. Chem.* **1990**, *5*, 305–306. However, the earliest effort to use the 3–D Wiener index in QSPR/QSAR has been described in O. Mekenyan, D. Peitchev, D. Bonchev, N. Trinajstić and I. Bangov, Modelling the Interaction of Small Organic Molecules with Biomacromolecules. I. Interaction of Substituted Pyridines with Anti–3–azopyridine Antibody, *Drug Res.* **1986**, *36*, 176–183.
70. D. Amić, D. Bešlo, B. Lučić, S. Nikolić and N. Trinajstić, The Vertex–Connectivity Index Revisited, *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 819–822.
71. S. Nikolić, N. Trinajstić and M. Randić, Wiener Index Revisited, *Chem. Phys. Lett.* **2001**, *333*, 319–321.
72. B. Lučić, A. Miličević, S. Nikolić and N. Trinajstić, On Variable Wiener Index, *Indian J. Chem. A* **2003**, 42A, 1279−1282. [72a] B. Zhou and N. Trinajstić, On a novel connectivity index, *J. Math. Chem.* **2009**, 46, 1252−1270; B. Lučić, N. Trinajstić and B. Zhou, Comparison between the sum-connectivity and product-

connectivity indices for benzenoid hydrocarbons, *Chem. Phys. Lett.* **2009**, 475, 146−148,

73. O. Ivanciuc, T.–S. Balaban and A. T. Balaban, Design of Topological Indices. Part 4. Reciprocal Distance Matrix, Related Local Vertex Invariants and Topological Indices, *J. Math. Chem.* **1993**, *12*, 309–318.
74. A. T. Balaban and O. Ivanciuc, Historical Development of Topological Indices, in: *Topological Indices and Related Descriptors in QSAR and QSPR*, J. Devillers and A. T. Balaban, Eds., Gordon and Breach Science Publishers, The Netherlands, 1999, pp. 21–57.
75. M. Randić, P. J. Hansen and P. C. Jurs, Search for Useful Graph Theoretical Invariants of Molecular Structure, *J. Chem. Inf. Comput. Sci.* **1988**, *28*, 60–68.
76. I. Gutman and J. Žerovnik, Corroborating a Modification of the Wiener Number, *Croat. Chem. Acta* **2002**, *75*, 603–612.
77. J. Devillers and A. T. Balaban, Eds., *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon & Breach, Amsterdam, 1999.
78. R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000; R. Todeschini and V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley−VCH, Weinheim, 2000.
79. I. Gutman and N. Trinajstić, Graph Theory and Molecular Orbitals. Total π–Electron Energy of Alternant Hydrocarbons, *Chem. Phys. Lett.* **1972**, *17*, 535–538.
80. I. Gutman, B. Ruščić, N. Trinajstić and C. F. Wilcox, Jr., Graph Theory and Molecular Orbitals. XII. Acyclic Polyenes, *J. Chem. Phys.* **1975**, *62*, 3399–3405.
81. M. Randić, On Characterization of Molecular Branching, *J. Am. Chem. Soc.* **1975**, *97*, 6609–6615; this paper is the 94th on the list of the 125 most cited JACS publications in the last 125 years.
82. B. Lučić, A. Miličević, S. Nikolić and N. Trinajstić, The Zagreb Indices Thirty Years After, *Croat. Chem. Acta* **2003**, *76*, 113−124.
83. A. Miličević and S. Nikolić, On Variable Zagreb Indices, *Croat. Chem. Acta* **2004**, *77*, 89−95.
84. D. Bonchev and N. Trinajstić, Information Theory, Distance Matrix, and Molecular Branching, *J. Chem. Phys.* **1977**, *67*, 4517–4533.
85. D. Bonchev, Ov. Mekenyan and N. Trinajstić, Isomer Discrimination by Topological Information Approach, *J. Comput. Chem.* **1981**, *2*, 127–148.
86. D. Bonchev, Information Theoretic Indices for Characterization of Chemical Structures, Research Studies Press/Wiley, Chichester, 1983.
87. B. Lučić and N. Trinajstić, Multivariate Regression Outperforms Several Robust Architectures of Neural Networks in QSAR Modeling, *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 121–132.

88. B. Lučić, D. Amić and N. Trinajstić, Nonlinear Multivariate Regression Outperforms Several Concisely Designed Neural Networks on Three QSPR Data Sets, *J. Chem. Inf. Comput. Sci*. **2000**, *40*, 403–413.
89. B. Lučić, N. Trinajstić, S. Sild, M. Karelson and A. R. Katritzky, A New Efficient Approach for Variable Selection Based on Multiregression: Prediction of Gas Chromatographic Retention Times and Response Factors, *J. Chem. Inf. Comput. Sci*. **1999**, *39*, 610–621.
90. A. R. Katritzky, K. Chen, Y. Wang, M. Karelson, B. Lučić, N. Trinajstić, T. Suzuki and G. Schüürmann, Prediction of Liquid Viscosity for Organic Compounds by a Quantitative Structure–Property Relationship, *J. Phys. Org. Chem*. **2000**, *13*, 80–86.
91. B. Lučić, I. Bašic, D. Nadramija, A. Miličević, N. Trinajstić, T. Suzuki, R. Petrukhin, M. Karelson and A. R. Katritzky, Correlation of Liquid Viscosity with Molecular Structure Using Different Variable Selection Methods, *Arkivoc* **2002**, *IV*, 45–49, http://www.arkat–usa.org/
92. Z. Mihalić and N. Trinajstić, A Graph–Theoretical Approach to Structure–Property Relationships, *J. Chem. Educ*. **1992**, *69*, 701–712.
93. J. von Knop, W. R. Müller, K. Szymanski, and N. Trinajstić, *Computer Generation of Certain Classes of Molecules*, SKTH/Kemija u industriji, Zagreb, 1985.
94. N. Trinajstić, S. Nikolić, J. von Knop, W. R. Müller, and K. Szymanski, *Computational Chemical Graph Theory*: *Characterization, Enumeration and Generation of Chemical Structures by Computer Methods*, Simon & Schuster/Horwood, Chichester, 1991.
95. J. von Knop, W. R. Müller, Ž. Jeričević and N. Trinajstić, Computer Enumeration and Generation of Trees and Rooted Trees, *J. Chem. Inf. Comput. Sci*. **1981**, *21*, 91–99.
96. W. R. Müller, K. Szymanski, J. von Knop, S. Nikolić and N. Trinajstić, On the Enumeration and Generation of Polyhex Hydrocarbons, *J. Comput. Chem*. **1990**, *11*, 223–235.
97. M. Randić, Compact Molecular Codes, *J. Chem. Inf. Comput. Sci*. **1986**, *26*, 136–148.
98. M. Randić, Compact Codes. 2. Bicyclic Saturated Hydrocarbons, *Croat. Chem. Acta* **1986**, *59*, 327–343.
99. M. Randić, S. Nikolić and N. Trinajstić, Compact Molecular Codes for Polycyclic Systems, *J. Mol. Struct*. (*Theochem*) **1988**, *165*, 213–228.
100. S. Nikolić and N. Trinajstić, Compact Molecular Codes for Annulenes, Aza–annulenes, Annulenoannulenes, Aza–annulenoannulenes, Cyclazines and Aza–cyclazines, *Croat. Chem. Acta* **1990**, *63*, 155–170.

101. J. von Knop, W.R. Müller, K. Szymanski, S. Nikolić and N. Trinajstić, Computer–Oriented Molecular Codes, in: *Computational Chemical Graph Theory*, ed. D. H. Rouvray, Nova Sci. Publ., Commack, N.Y., 1990, pp. 9–32.
102. M. Randić, S. Nikolić and N. Trinajstić, Compact Codes: On Nomenclature of Acyclic Chemical Compounds, *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 357–365.
103. M. L. Contreras, J. Alvarez, M. Riveros, G. Arias and R. Rozas, Exhaustive Generation of Organic Isomers. 6. Stereoisomers Having Isolated and Spiro Cycles and New Extended N–tuples, *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 964–977.
104. S. Davidson, Fast Generation of an Alkane–Series Dictionary Ordered by Side–Chain Complexity, *J. Chem. Inf. Comput. Sci.* **2002**, *42*, 147–156.
105. J. August, H. W. Kroto, and N. Trinajstić, Interstellar Polyynes and Related Species, *Astrophys. Space Sci.* **1986**, *128*, 411–419.
106. J. von Knop, K. Szymanski, W.R. Müller, H.W. Kroto and N. Trinajstić, Computer Enumeration and Generation of Physical Trees, *J. Comput. Chem.* **1987**, *8*, 549–554.
107. I. Lukovits, Isomer Generation: Syntactic Rules for Detection of Isomorphism, *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 563–568.
108. I. Lukovits and I. Gutman, On Morgan–Trees, Croat. Chem. Acta **2002**, *75*, 563–576; T. Došlić, Morgan Tress and Dyck Paths, *Croat.Chem. Acta* **2002**, *75*, 881–889.
109. D. J. Klein, D. Babić and N. Trinajstić, Enumeration in Chemistry, in: *Chemical Modelling*: *Applications and Theory*, A. Hinchliffe, Ed., The Royal Society of Chemistry, London, 2002, Vol. 2, pp. 56–95; D. Babić, D.J. Klein, J. von Knop and N. Trinajstić, Combinatorial Enumeration in Chemistry, in: *Chemical Modeling*: *Applications and Theory*, A. Hinchliffe, Ed., The Royal Society of Chemistry, London, 2004, Vol. 3, pp. 126-170; A. Miličević and N. Trinajstić , Combinatorial Enumeration in Chemistry, in: *Chemical Modeling*: *Applications and Theory*, A. Hinchliffe, Ed., The Royal Society of Chemistry, London, The Royal Society of Chemistry, London, 2006, Vol. 4, pp. 405-469.
110. M. Randić and N. Trinajstić, Semiempirical Calculation of Bond Lengths in Cyclopentadienyl Ligands, *J. Chem. Phys.* **1967**, *46*, 1469–1474.
111. D. Bonchev and W. A. Seitz, The Concept of Complexity in Chemistry, in: *Concepts in Chemistry – A Contemporary Challenge*, D. H. Rouvray, Ed., Wiley, New York, 1997, 353–381.
112. R. B. Mallion and N. Trinajstić, Reciprocal Spanning–Tree Density: A New Index Characterising the Intricacy of (Poly)cyclic Molecular–Graph, *MATCH – Commun. Math. Computer Chem.* **2003**, *48*, 97–116.
113. S. Nikolić, I. M. Tolić, N. Trinajstić and I. Baučić, On the Zagreb Indices as Complexity Indices, *Croat. Chem. Acta* **2000**, *73*, 909–921.

114. S. Nikolić, N. Trinajstić and I. M. Tolić, Complexity of Molecules, *J. Chem. Inf. Comput. Sci.* **2000**, *40*, 920–926.
115. S. Nikolić, N. Trinajstić, I.M. Tolić, G. Rücker and C. Rücker, On Molecular Complexity Indices, in: *Complexity– Introduction and Fundamentals*, D. Bonchev and D.H. Rouvray, Eds., Taylor & Francis, London, 2003, pp. 29–89.
116. N. Trinajstić, The 70th Anniversary of CROATICA CHEMICA ACTA 1927–1997, *Croat. Chem. Acta* **1997**, *59*, I–IV.
117. N. Trinajstić, Quantum Theory in Chemistry – Early Developments, *Kem. ind.* (*Zagreb*) **2001**, *50*, 427–429.
118. N. Trinajstić, Quantum Theory in Chemistry, in: *Hundred Years of Quantum Theory*, D. Tadić, Ed., Croatian Academy of Sciences and Arts, Zagreb, 2002, pp. 55–65.
119. N. Trinajstić, Hoffmann, Roald (1937) – Primijenjena teorijska kemija (Applied Theoretical Chemistry), in:*Velikani naše Epohe* (*Great Men of Our Time*), R. Vince, Ed., Hrvatski radio, Zagreb 1994, 317–322.
120. N. Trinajstić, Roald Hoffmann – Scientist and Poet, Ref. 7, pp. 94–109.
121. N. Trinajstić, Dopisivanje s profesorom Vladimirom Prelogom (Correspondence with Professor Vladimir Prelog), *Kem. ind.* (*Zagreb*) **1999**, *48*, 151–157.
122. M. Randić and N. Trinajstić, Notes on Some Less Known Early Contributions to Chemical Graph Theory, *Croat. Chem. Acta* **1994**,*67*, 1–35.
123. L. Pogliani, M. Randić and N. Trinajstić, Much Ado about Nothing – An Introductory Inquiry about Zero, *Int. J. Math. Educ. Sci. Technol.* **1998**, *29*, 729–744.
124. L. Pogliani, M. Randić and N. Trinajstić, About One – An Inquiry About the Meaning and Uses of the Number One, *Int. J. Math. Educ. Sci. Technol.* **2000**, *31*, 811–824.
125. N. Trinajstić, The Magic of the Number Five, *Croat. Chem. Acta* **1993**, *66*, 227–254.
126. I. M. Tolić and N. Trinajstić, The Number Five in Biology, *Period. Biol.* **1998**, *100*, 259–265.
127. L. Pogliani, M. Randić and N. Trinajstić, What Can Be Said About Number 13 Beyond the Fact That It Is a Prime Number?, *Croat. Chem. Acta* **2004**, 77, 447−456.

Iranian J. Math. Chem. 8(3) September (2017) 259 − 273

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

Graphs with Smallest Forgotten Index

I. GUTMAN[1], A. GHALAVAND[2], T. DEHGHAN–ZADEH[2] AND A. R. ASHRAFI[2,•]

[1]Faculty of Science, University of Kragujevac, 34000 Kragujevac, Serbia
[2]Department of Pure Mathematics, Faculty of Mathematical Science, University of Kashan, Kashan 87317−53153, I. R. Iran

ARTICLE INFO

Article History:

Received: 22 April 2016
Accepted: 28 July 2016
Published online 11 February 2017
Academic Editor: Hassan Yousefi-Azari

Keywords:

Forgotten topological index
unicyclic graphs
bicyclic graphs
tricyclic graphs
tetracyclic graphs
pentacyclic graphs

ABSTRACT

The forgotten topological index of a molecular graph G is defined as $F(G) = \sum_{v \in V(G)} d(v)^3$, where $d(v)$ denotes the degree of vertex v in G. The first through the sixth smallest forgotten indices among all trees, the first through the third smallest forgotten indices among all connected graph with cyclomatic number $\gamma = 1, 2$, the first through the fourth for $\gamma = 3$, and the first and the second for $\gamma = 4, 5$ are determined. These results are compared with those obtained for the first Zagreb index.

1. INTRODUCTION

All graphs considered are assumed to be simple and finite. The sets of vertices and edges of a graph G are denoted by $V(G)$ and $E(G)$, respectively. By n and m we denote the number of vertices and edges of G, i.e., $n = |V(G)|$ and $m = |E(G)|$. If G has p components, then $\gamma = \gamma(G) = m - n + p$ is called the *cyclomatic number* of G. In this work we shall be mainly concerned with connected graphs, for which $p = 1$. A connected graph with $\gamma = 0$ is said to be a tree. Graphs with $\gamma = 1, 2, 3, 4, 5$ are then called *unicyclic*, *bicyclic*, *tricyclic*, *tetracyclic* and *pentacyclic*, respectively.

•Corresponding Author (Email address: ashrafi@kashanu.ac.ir)
DOI: 10.22052/ijmc.2017.43258

The set of all connected graphs with exactly n vertices and cyclomatic number γ is denoted by $C^{\gamma}(n)$. In particular, $C^{0}(n)$ is the set of all n-vertex trees.

The number of the first neighbors of a vertex $u \in V(G)$ is said to be its *degree*, and will be denoted by $d(u) = d_G(u)$. As well known,

$$\sum_{u \in V(G)} d(u) = 2m.$$

Consequently, for all graphs belonging to a set $\boldsymbol{C^{\gamma}(n)}$, the sum of the vertex degrees is the same.

Let $V(G) = \{v_1, v_1, \ldots, v_n\}$, and let the vertices of G be labeled so that $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$. Then the *degree sequence* of G is $[d(v_1), d(v_2), \ldots, d(v_n)]$. As customary, we shall write this degree sequence in an abbreviated manner, as the below two self–explanatory examples show:

$$[4,3,3,3,3,2,2,2,2,2,2,2,1,1,1,1] \equiv [4,3^4,2^7,1^4]$$
$$[4,4,4,1,1,1,1,1,1,1,1] \equiv [4^3,1^8].$$

The greatest vertex degree of the graph G will be denoted by $\Delta = \Delta(G)$. The number of vertices of degree i in G will be denoted by $n_i = n_i(G)$. If we assume that the graph G has no isolated vertices (= vertices of degree zero), which is a necessary condition for being connected, then $n_0 = 0$. For such graphs,

$$\sum_{i=1}^{\Delta(G)} n_i = n \quad \text{and} \quad \sum_{i=1}^{\Delta(G)} i n_i = 2m.$$

For a subset W of $V(G)$, let $G - W$ be the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, for a subset E' of $E(G)$, $G - E'$ denotes the subgraph of G obtained by removing the edges of E'. If $W = \{v\}$ and $E' = \{xy\}$, then the subgraphs $G - W$ and $G - E'$ will be shorter written as $G - v$ and $G - xy$, respectively. Finally, if x and y are non-adjacent vertices of G, then $G + xy$ is the graph obtained from G by adding an edge xy. Our other notations are standard and can be taken from the most of textbooks on graph theory. The *first Zagreb index*, $M_1(G)$, of the graph G is defined as

$$M_1 = M_1(G) = \sum_{u \in V(G)} d(u)^2. \qquad (1)$$

The theory of this degree–based topological index, introduced in the 1970s [9], is nowadays well elaborated [6–8,11].

Furtula and one of the present authors [4], recalled that in the formulas for total π −electron energy, reported in [9], in addition to M_1, also the sum of cubes of vertex degrees was encountered. This latter degree–based graph invariant did not attract any

attention in mathematical chemistry literature for more than 40 years. In view of this, it was named *forgotten topological index*, and defined as

$$F = F(G) = \sum_{u \in V(G)} d(u)^3. \quad (2)$$

It can be shown that the F-index satisfies the identity

$$F(G) = \sum_{e=uv \in E(G)} [d(u)^2 + d(v)^2].$$

At this point, it needs to be mentioned that Zhang and Zhang [14] introduced the *first general Zagreb index* of a graph G as

$$M_1^\alpha = M_1^\alpha(G) = \sum_{u \in V(G)} d(u)^\alpha,$$

where α is an arbitrary real number. Evidently, the forgotten index is just the special case of the first general Zagreb index for $\alpha = 3$. In [14], all unicyclic graphs with the first three smallest and greatest values of M_1^α were characterized. Zhang et al. [13], determined all n-vertex bicyclic graphs, $n \geq 5$, with the first three smallest and greatest M_1^α when $\alpha > 1$. They also characterized the greatest and the first three smallest values of the first general Zagreb index when $0 < \alpha < 1$. Tong et al. [12], characterized all tricyclic graphs with the greatest, the second and third greatest values of M_1^α, and the tricyclic graphs with the smallest, the second and third smallest values of this index. These results are automatically applicable to the F-index. The aim of the present work is to extend the considerations to graphs with cyclomatic number $\gamma > 3$.

Until now, there are very few researches concerned solely with the F-index. Furtula et al. [5], among other results, proved that for triangle–free graphs $2F \leq M_1^2$. Abdo et al. [1] studied *n*-vertex trees with maximal values of the forgotten index. They proved that if $n - 2$ is divisible by 3, then the maximum value of the forgotten index is $22n - 42$ and when $3 \nmid n - 2$, then the maximum forgotten index will be $22(n-1) - 21x + x3$, where x is uniquely determined by $2 \leq x \leq 3$ and $n - 1 - x \equiv 0 \,(mod\, 3)$. Anyway, because of the close analogy between the first Zagreb index and the forgotten index, one may expect that in the majority of cases, the graphs extremal with respect to M_1 will also be extremal with respect to F. The truly interesting results would then be the specification of cases in which these two indices have a (significantly) different behavior. We also refer to [2,3] for more information on this topic.

From Eqs. (1) and (2) it is evident that two graphs with equal degree sequence necessarily have equal first Zagreb indices and equal forgotten indices. Bearing this in mind, it is purposeful to partition each set $C^\gamma(n)$ into equivalence classes, each class pertaining to a particular degree sequence. All elements of such an equivalence class have equal M_1 and equal F indices. Because we are aiming at finding graphs (i.e., the respective

equivalence classes) with smallest F-values, we will consider only a few selected such classes, those in which many vertex degrees are equal to two. These equivalence classes are listed in Tables 1–10 in the subsequent section.

In Tables 1–10 are listed the equivalence classes (Eq.Cl.) of the sets $C^{\gamma}(n)$ that are of interest for the present considerations. The value of n is assumed to be sufficiently large, so that each equivalence class is non-empty. In order to facilitate the analysis, in the last column of each table, expression for the F-index of the elements of the respective equivalence class is given.

2. MAIN RESULTS

The aim of this section is to characterize the graphs (i.e., the respective equivalence classes) in which the F-index assumes the first few smallest values. We do this for the sets $C^{i}(n)$ for $0 \leq i \leq 5$.

In order to achieve this goal, we first introduce a graph transformation that decreases the forgotten index.

Transformation A. Let G_1 be a graph with vertices v_1 and v_2, such that $d_{G_1}(v_1) \geq 2$ and $d_{G_1}(v_2) = 1$. Let G_2 be another graph and w its vertex. Construct the graph G from G_1 and G_2 by connecting the vertices w and v_1. Construct the graph G' so that $G' = G - wv_1 + wv_2$.

Lemma 2.1. $F(G') < F(G)$.

Proof. $F(G) - F(G') = [(d_{G_1}(v_1) + 1)^3 + 1^3] - [d_{G_1}(v_1)^3 + 2^3] > 0$, as $d_{G_1}(v_1) \geq 2$. □

Remark 2.2. *Note that in the exactly same manner we get $M_1(G') < M_1(G)$. This implies that whichever result is deduced for the F-index using Lemma 2.1, an analogous result will also hold for the first Zagreb index.*

We now focus our attention to the case $\gamma = 0$, namely to trees, i.e., to the equivalence classes of the set $C^{0}(n)$, listed in Table 1. First we state an auxiliary result:

Lemma 2.3. *If T is a tree with n vertices, then*

$$n_1 = 2 + \sum_{i=3}^{\Delta(G)} (i-2)n_i \quad \text{and} \quad n_2 = n - 2 - \sum_{i=3}^{\Delta(G)} (i-1)n_i.$$

Proof. The proof follows from $\sum_{i=1}^{\Delta(G)} n_i = n$ and $\sum_{i=1}^{\Delta(G)} in_i = 2(n-1)$. □

Corollary 2.4. *There exists a tree T of order n with $2 \leq n_1(T) \leq 6$, if and only if T belongs to one of the equivalence classes given in Table 1.*

Proof. We distinguish the following five cases:

(1) $n_1(T) = 2$,
(2) $n_1(T) = 3$,
(3) $n_1(T) = 4$,
(4) $n_1(T) = 5$,
(5) $n_1(T) = 6$.

We present a proof for the case (1) whereas other cases are treated in a similar manner. Assume that $n_1(T) = 2$. Then by Lemma 2.3, there is a tree T with $n_1(T) = 2$ if and only if $\sum_{i=3}^{\Delta(G)}(i-2)n_i = 0$ if and only if $n_2(T) = n-2$ and $n_i(T) = 0$, for each $i \geq 3$. This leads to the proof. □

Theorem 2.5. *Let $T_1 \in N_1$, $T_2 \in N_2$, $T_3 \in N_4$, $T_4 \in N_7$, $T_5 \in N_3$, and $T_6 \in N_{12}$. If $n \geq 10$ and $\in C^0(n) \setminus \{T_1, T_2, \ldots, T_6\}$, then $F(T_1) < F(T_2) < F(T_3) < F(T_4) < F(T_5) < F(T_6) < F(T)$.*

Proof. From Table 1, one can see that $F(T_1) < F(T_2) < F(T_3) < F(T_4) < F(T_5) < F(T_6)$. If $n_1(T) = 5$ or 6, then the proof follows from the data in Table 1. If $n_1(T) \geq 7$, then by a repeated application of Transformation A, we obtain a tree T_s such that $n_1(T_s) = 6$. By Lemma 2.1, $F(T_s) < F(T)$ and by Table 1, $F(T_6) \leq F(T_s)$, which yields the result. □

Lemma 2.6. *If G is a connected unicyclic graph with n vertices, then*

$$n_1 = \sum_{i=3}^{\Delta(G)} (i-2)n_i \text{ and } n_2 = n - \sum_{i=3}^{\Delta(G)} (i-1)n_i.$$

Proof. The proof follows from $\sum_{i=1}^{\Delta(G)} n_i = n$ *and* $\sum_{i=1}^{\Delta(G)} in_i = 2n$. □

Corollary 2.7. *There is a connected unicyclic graph G of order n with $n_1(G) \leq 2$ if and only if G belongs to one of equivalence classes given in Table 2.*

Proof. We distinguish the following three cases:

(1) $n_1(G) = 0$,
(2) $n_1(G) = 1$,
(3) $n_1(G) = 2$.

In order to prove (1), assume that $n_1(G) = 0$. Then by Lemma 2.6, there exists a connected unicyclic graph G with $n_1(G) = 0$ if and only if $\sum_{i=3}^{\Delta(G)}(i-2)n_i = 0$. But, this is equivalent to the fact that if and only if $n_2(T) = n$ and $n_i(T) = 0$, for each $i \geq 3$. The proofs of the remaining cases are similar and are omitted. □

Theorem 2.8. *Let* $G_1 \in A_1$, $G_2 \in A_2$ *and* $G_3 \in A_4$. *If* $G \in C^1(n) \setminus \{G_1, G_2, G_3\}$ *and* $n \geq 5$, *then* $F(G_1) < F(G_2) < F(G_3) < F(G)$.

Proof. From Table 2, one can see that $F(G_1) < F(G_2) < F(G_3)$. If $n_1(G) = 2$, then Table 2 leads us to the proof. If $n_1(G) \geq 3$, then by a repeated application of Transformation A, we obtain a connected unicyclic graphs Q such that $n_1(Q) = 2$. By Lemma 2.1, we have $F(Q) < F(G)$. On the other hand, by the data given in Table 2, $F(G_3) \leq F(Q)$, which yields the result. □

Lemma 2.9. *If* G *is a connected bicyclic graph with n vertices, then*

$$n_1 = \sum_{i=3}^{\Delta(G)}(i-2)n_i - 2 \quad \text{and} \quad n_2 = n + 2 - \sum_{i=3}^{\Delta(G)}(i-1)n_i.$$

Proof. The proof follows from $\sum_{i=1}^{\Delta(G)} n_i = n$ and $\sum_{i=1}^{\Delta(G)} in_i = 2n + 2$. □

Corollary 2.10. *There exists a connected bicyclic graph* G *of order n with* $n_1(G) \leq 1$ *if and only if* G *belongs to one of the equivalence classes given in Table* 3.

Proof. We distinguish the following two cases:

(1) $n_1(G) = 0$,

(2) $n_1(G) = 1$.

In order to prove (1), assume that $n_1(G) = 0$. Then by Lemma 2.9, there exists a connected bicyclic graph G with $n_1(G) = 0$ if and only if $\sum_{i=3}^{\Delta(G)}(i-2)n_i = 2$. But the latter requirement is equivalent to one of the following two conditions:

1. $n_2(G) = n - 1$, $n_3(G) = 0$, $n_4(G) = 1$, and $n_i(G) = 0$, for each $i \geq 5$,
2. $n_2(G) = n - 2$, $n_3(G) = 2$, and $n_i(G) = 0$, for each $i \geq 4$.

The proof of case (2) is analogous, and we omit it. □

Theorem 2.11. *Let* $G_1 \in B_2$, $G_2 \in B_1$, *and* $G_3 \in B_5$. *If* $G \in C^2(n) \setminus \{G_1, G_2, G_3\}$ *and* $n \geq 7$, *Then* $F(G_1) < F(G_2) < F(G_3) < F(G)$.

Proof. From Table 3, we have $F(G_1) < F(G_2) < F(G_3)$. If $n_1(G) = 1$, then the theorem can be proven by Table 3. If $n_1(G) \geq 2$, then by repeated application of Transformation

A, we obtain a connected bicyclic graph, say Q, such that $n_1(Q) = 1$. By applying Lemma 2.1 we conclude that $F(Q) < F(G)$. On the other hand, by the data in Table 3, $F(G_3) \leq F(Q)$, which yields the result. □

Lemma 2.12. *If G is a connected tricyclic graph with n vertices, then*

$$n_1 = \sum_{i=3}^{\Delta(G)} (i-2)n_i - 4 \text{ and } n_2 = n + 4 - \sum_{i=3}^{\Delta(G)} (i-1)n_i.$$

Corollary 2.13. *There is a connected tricyclic graph G of order n with $n_1(G) \leq 2$ if and only if G belongs to one of the equivalence classes given in Tables 4, 5, or 6.*

Theorem 2.14. *Let $G_1 \in D_5$, $G_2 \in E_7$, $G_3 \in D_4$ and $G_4 \in F_{11}$. If $n \geq 11$ and $G \in C^3(n) \setminus \{G_1, G_2, G_3, G_4\}$. Then $F(G_1) < F(G_2) < F(G_3) < F(G_4) < F(G)$.*

Proof. From Tables 4, 5, and 6, one can see that $F(G_1) < F(G_2) < F(G_3) < F(G_4)$. The case of $n_1(G) \leq 2$ is a direct consequence of the data given Tables 4, 5, and 6. If $n_1(G) \geq 3$, then by repeated applications of Transformation A, we obtain a connected tricyclic graphs, for example Q, such that $n_1(Q) = 2$. By applying Lemma 2.1 we get that $F(Q) < F(G)$. Then the data given in Table 6 imply that $F(G_4) \leq F(Q)$, which yields the result. □

Lemma 2.15. *If G is a connected tetracyclic graph with n vertices, then*

$$n_1 = \sum_{i=3}^{\Delta(G)} (i-2)n_i - 6 \text{ and } n_2 = n + 6 - \sum_{i=3}^{\Delta(G)} (i-1)n_i.$$

Corollary 2.16. *There exists a connected tetracyclic graph G of order n with $n_1(G) \leq 1$ if and only if G belongs to one of the equivalence classes given in Tables 7 and 8.*

Theorem 2.17. *Let $G_1 \in H_{11}$ and $G_2 \in I_{15}$. If $n \geq 12$ and $G \in C^4(n) \setminus \{G_1, G_2\}$. Then $F(G_1) < F(G_2) < F(G)$.*

Proof. From Tables 7 and 8 one can see that $F(G_1) < F(G_2)$. If $n_1(G) = 0$ or $n_1(G) = 1$, then the data given in Tables *7* and *8* completes the proof.

If $n_1(G) \geq 2$, then by repeated applications of Transformation A, a connected tetracyclic graph Q is obtained for which $n_1(Q) = 1$. By Lemma 2.1, $F(Q) < F(G)$ and by Table *8*, $F(G_2) \leq F(Q)$, which yields the result. □

Lemma 2.18. *If G is a connected pentacyclic graph with n vertices, then*

$$n_1 = \sum_{i=3}^{\Delta(G)} (i-2)n_i - 8 \quad \text{and} \quad n_2 = n + 8 - \sum_{i=3}^{\Delta(G)} (i-1)n_i.$$

Corollary 2.19. *There exists a connected pentacyclic graph G of order n with $n_1(G) \leq 1$ if and only if G belongs to one of the equivalence classes given in Tables 9 and 10.*

Theorem 2.20. *Let $G_1 \in K_{22}$ and $G_2 \in L_{29}$. If $n \geq 16$ and $G \in C^5(n) \setminus \{G_1, G_2\}$. Then $F(G_1) < F(G_2) < F(G)$.*

Proof. From Tables 9 and 10, it can be seen that $F(G_1) < F(G_2)$. If $n_1(G) = 0$ or $n_1(G) = 1$, then Tables 9 and 10 lead us to the proof. If $n_1(G) \geq 2$, then by repeated applications of Transformation A, a connected pentacyclic graph Q can be constructed, such $that\, n_1(Q) = 1$. By Lemma 2.1, $F(Q) < F(G)$ and by the data in Table 10, $F(G_2) \leq F(Q)$, which proves the result. □

3. CONCLUDING REMARKS

In this paper the connected graphs with fixed number of vertices and cyclomatic number (i.e., the respective equivalence classes of such graphs) are determined, whose $F-$indices assume the smallest possible value. Since the $F-$index is defined in a similar manner as the first Zagreb index, cf. Eqs. (1) and (2), their properties are expected also very similar. In view of this, it is purposeful to compare the result for these two graph invariants. For the sake of completeness, we first state three relevant results as follows:

Theorem 3.1. *The characterization of n-vertex trees, n-vertex unicyclic, and n-vertex bicyclic graphs with the smallest, the second smallest and the third smallest first Zagreb index are as follows:*

1. *Li and Zhao* [10]: *Trees with degree sequence* $[2^{n-2}, 1^2], [3, 2^{n-4}, 1^3]$, *and* $[3^2, 2^{n-6}, 1^4]$ *have the smallest, second smallest, and third smallest values of the first Zagreb index among all n-vertex trees.*
2. *Zhang and Zhang* [14, Theorem 1]: *Let G be an $n-$vertex unicyclic graph, $n \geq 7$. Then $M_1(G)$ attains the smallest, the second smallest, and the third smallest value if and only if the degree sequence of G is* $[2^n], [3, 2^{n-2}, 1]$, *and* $[3^2, 2^{n-4}, 1^2]$, *respectively.*
3. *Zhang et al.* [13, Theorems 1 and 4]: *Suppose that G is a bicyclic graph on $n \geq 5$ vertices, L_1 denotes the set of such graphs with degree sequence* $[4, 2^{n-1}]$ *or* $[3^3, 2^{n-4}, 1]$ *and L_2 is the set of all n-vertex bicyclic graphs with degree sequence* $[4, 3, 2^{n-3}, 1]$ *or* $[3^4, 2^{n-6}, 1^2]$. *Then the first Zagreb index $M_1(G)$ attains the smallest, the second smallest and the third smallest value if and only if the degree sequence of G is* $[3^2, 2^{n-2}]$, *$G \in L_1$, and $G \in L_2$, respectively.*

By Theorem 2.8, the n-vertex unicyclic graphs with degree sequences $[2^n]$, $[3, 2^{n-2}, 1]$ and $[3^2, 2^{n-4}, 1^2]$ have the smallest, second smallest and third smallest values of forgotten index which are the same as the case of the first Zagreb index. On the other hand, by Theorem 2.11, n-vertex bicyclic graphs with degree sequences $[3^2, 2^{n-2}]$, $[4, 2^{n-1}]$ and $[3^3, 2^{n-4}, 1]$ have the smallest, second smallest, and third smallest values of the forgotten index. Thus, the bicyclic graphs with smallest value of the forgotten and first Zagreb index are the same, but these graph invariants attain their second and third smallest value in different classes of bicyclic graphs.

Table 1. Degree distributions of trees with $2 \leq n_1 \leq 6$.

Eq.Cl.	n_6	n_5	n_4	n_3	n_2	n_1	$n_i\ (i \geq 7)$	F
N_1	0	0	0	0	$n-2$	2	0	$8n-14$
N_2	0	0	0	1	$n-4$	3	0	$8n-2$
N_3	0	0	1	0	$n-5$	4	0	$8n+28$
N_4	0	0	0	2	$n-6$	4	0	$8n+10$
N_5	0	1	0	0	$n-6$	5	0	$8n+82$
N_6	0	0	1	1	$n-7$	5	0	$8n+40$
N_7	0	0	0	3	$n-8$	5	0	$8n+22$
N_8	1	0	0	0	$n-7$	6	0	$8n+166$
N_9	0	1	0	1	$n-8$	6	0	$8n+94$
N_{10}	0	0	2	0	$n-8$	6	0	$8n+70$
N_{11}	0	0	1	2	$n-9$	6	0	$8n+52$
N_{12}	0	0	0	4	$n-10$	6	0	$8n+34$

Table 2. Degree distributions of connected unicyclic graphs with $n_1 \leq 2$.

Eq.Cl.	n_4	n_3	n_2	n_1	$n_i\ (i \geq 5)$	F
A_1	0	0	n	0	0	$8n$
A_2	0	1	$n-2$	1	0	$8n+12$
A_3	1	0	$n-3$	2	0	$8n+42$
A_4	0	2	$n-4$	2	0	$8n+24$

Table 3. Degree distributions of connected bicyclic graphs with $n_1 \leq 1$.

Eq.Cl.	n_5	n_4	n_3	n_2	n_1	$n_i\ (i \geq 6)$	F
B_1	0	1	0	$n-1$	0	0	$8n + 56$
B_2	0	0	2	$n-2$	0	0	$8n + 38$
B_3	1	0	0	$n-2$	1	0	$8n + 110$
B_4	0	1	1	$n-3$	1	0	$8n + 68$
B_5	0	0	3	$n-4$	1	0	$8n + 58$

Table 4. Degree distributions of connected tricyclic graphs with $n_1 = 0$.

Eq.Cl.	n_6	n_5	n_4	n_3	n_2	n_1	$n_i\ (i \geq 7)$	F
D_1	1	0	0	0	$n-1$	0	0	$8n + 208$
D_2	0	1	0	1	$n-2$	0	0	$8n + 136$
D_3	0	0	2	0	$n-2$	0	0	$8n + 112$
D_4	0	0	1	2	$n-3$	0	0	$8n + 94$
D_5	0	0	0	4	$n-4$	0	0	$8n + 76$

Table 5. Degree distributions of connected tricyclic graphs with $n_1 = 1$.

Eq.Cl.	n_7	n_6	n_5	n_4	n_3	n_2	n_1	$n_i\ (i \geq 8)$	F
E_1	1	0	0	0	0	$n-2$	1	0	$8n + 328$
E_2	0	1	0	0	1	$n-3$	1	0	$8n + 220$
E_3	0	0	1	1	0	$n-3$	1	0	$8n + 166$
E_4	0	0	1	0	2	$n-4$	1	0	$8n + 148$
E_5	0	0	0	2	1	$n-4$	1	0	$8n + 124$
E_6	0	0	0	1	3	$n-5$	1	0	$8n + 106$
E_7	0	0	0	0	5	$n-6$	1	0	$8n + 88$

Table 6. Degree distributions of connected tricyclic graphs with $n_1 = 2$.

Eq.Cl.	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	$n_i\ (i \geq 9)$	F
F_1	1	0	0	0	0	0	$n-3$	2	0	$8n + 490$
F_2	0	1	0	0	0	1	$n-4$	2	0	$8n + 340$
F_3	0	0	1	0	1	0	$n-4$	2	0	$8n + 250$
F_4	0	0	1	0	0	2	$n-5$	2	0	$8n + 232$
F_5	0	0	0	2	0	0	$n-4$	2	0	$8n + 220$
F_6	0	0	0	1	1	1	$n-5$	2	0	$8n + 178$
F_7	0	0	0	1	0	3	$n-6$	2	0	$8n + 160$
F_8	0	0	0	0	3	0	$n-5$	2	0	$8n + 154$
F_9	0	0	0	0	2	2	$n-6$	2	0	$8n + 136$
F_{10}	0	0	0	0	1	4	$n-7$	2	0	$8n + 118$
F_{11}	0	0	0	0	0	6	$n-8$	2	0	$8n + 100$

Table 7. Degree distributions of connected tetracyclic graphs with $n_1 = 0$.

Eq.Cl.	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	$n_i\ (i \geq 9)$	F
H_1	1	0	0	0	0	0	$n-1$	0	0	$8n + 504$
H_2	0	1	0	0	0	1	$n-2$	0	0	$8n + 354$
H_3	0	0	1	0	1	0	$n-2$	0	0	$8n + 264$
H_4	0	0	1	0	0	2	$n-3$	0	0	$8n + 246$
H_5	0	0	0	2	0	0	$n-2$	0	0	$8n + 234$
H_6	0	0	0	1	1	1	$n-3$	0	0	$8n + 192$
H_7	0	0	0	1	0	3	$n-4$	0	0	$8n + 174$
H_8	0	0	0	0	3	0	$n-3$	0	0	$8n + 168$
H_9	0	0	0	0	2	2	$n-4$	0	0	$8n + 150$
H_{10}	0	0	0	0	1	4	$n-5$	0	0	$8n + 132$
H_{11}	0	0	0	0	0	6	$n-6$	0	0	$8n + 114$

Table 8. Degree distributions of connected tetracyclic graphs with $n_1 = 1$.

Eq.Cl.	n_9	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	n_i $(i \geq 10)$	F
I_1	1	0	0	0	0	0	0	$n-2$	1	0	$8n + 714$
I_2	0	1	0	0	0	0	1	$n-3$	1	0	$8n + 516$
I_3	0	0	1	0	0	1	0	$n-3$	1	0	$8n + 384$
I_4	0	0	1	0	0	0	2	$n-4$	1	0	$8n + 366$
I_5	0	0	0	1	1	0	0	$n-3$	1	0	$8n + 318$
I_6	0	0	0	1	0	1	1	$n-4$	1	0	$8n + 276$
I_7	0	0	0	1	0	0	3	$n-5$	1	0	$8n + 258$
I_8	0	0	0	0	2	0	1	$n-4$	1	0	$8n + 246$
I_9	0	0	0	0	1	2	0	$n-4$	1	0	$8n + 222$
I_{10}	0	0	0	0	1	1	2	$n-5$	1	0	$8n + 204$
I_{11}	0	0	0	0	1	0	4	$n-6$	1	0	$8n + 186$
I_{12}	0	0	0	0	0	3	1	$n-5$	1	0	$8n + 180$
I_{13}	0	0	0	0	0	2	3	$n-6$	1	0	$8n + 162$
I_{14}	0	0	0	0	0	1	5	$n-7$	1	0	$8n + 144$
I_{15}	0	0	0	0	0	0	7	$n-8$	1	0	$8n + 125$

Table 9. Degree distributions of connected pentacyclic graphs with $n_1 = 0$.

Eq.Cl.	n_{10}	n_9	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	$n_i\ (i \geq 11)$	F
K_1	1	0	0	0	0	0	0	0	$n-1$	0	0	$8n + 992$
K_2	0	1	0	0	0	0	0	1	$n-2$	0	0	$8n + 740$
K_3	0	0	1	0	0	0	1	0	$n-2$	0	0	$8n + 560$
K_4	0	0	1	0	0	0	0	2	$n-3$	0	0	$8n + 542$
K_5	0	0	0	1	0	1	0	0	$n-2$	0	0	$8n + 452$
K_6	0	0	0	1	0	0	1	1	$n-3$	0	0	$8n + 410$
K_7	0	0	0	1	0	0	0	3	$n-4$	0	0	$8n + 392$
K_8	0	0	0	0	2	0	0	0	$n-2$	0	0	$8n + 416$
K_9	0	0	0	0	1	1	0	1	$n-3$	0	0	$8n + 344$
K_{10}	0	0	0	0	1	0	2	0	$n-3$	0	0	$8n + 320$
K_{11}	0	0	0	0	1	0	1	2	$n-4$	0	0	$8n + 302$
K_{12}	0	0	0	0	1	0	0	4	$n-5$	0	0	$8n + 284$
K_{13}	0	0	0	0	0	2	1	0	$n-3$	0	0	$8n + 290$
K_{14}	0	0	0	0	0	2	0	2	$n-4$	0	0	$8n + 272$
K_{15}	0	0	0	0	0	1	2	1	$n-4$	0	0	$8n + 248$
K_{16}	0	0	0	0	0	1	1	3	$n-5$	0	0	$8n + 230$
K_{17}	0	0	0	0	0	1	0	5	$n-6$	0	0	$8n + 212$
K_{18}	0	0	0	0	0	0	4	0	$n-4$	0	0	$8n + 224$
K_{19}	0	0	0	0	0	0	3	2	$n-5$	0	0	$8n + 206$
K_{20}	0	0	0	0	0	0	2	4	$n-6$	0	0	$8n + 188$
K_{21}	0	0	0	0	0	0	1	6	$n-7$	0	0	$8n + 170$
K_{22}	0	0	0	0	0	0	0	8	$n-8$	0	0	$8n + 152$

Table 10. Degree distributions of connected pentacyclic graphs with $n_1 = 1$

Eq.Cl.	n_{11}	n_{10}	n_9	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	n_i $(i \geq 12)$	F
L_1	1	0	0	0	0	0	0	0	0	$n-2$	1	0	$8n + 1316$
L_2	0	1	0	0	0	0	0	0	1	$n-3$	1	0	$8n + 1004$
L_3	0	0	1	0	0	0	0	1	0	$n-3$	1	0	$8n + 770$
L_4	0	0	1	0	0	0	0	0	2	$n-4$	1	0	$8n + 752$
L_5	0	0	0	1	0	0	1	0	0	$n-3$	1	0	$8n + 614$
L_6	0	0	0	1	0	0	0	1	1	$n-4$	1	0	$8n + 572$
L_7	0	0	0	1	0	0	0	0	3	$n-5$	1	0	$8n + 554$
L_8	0	0	0	0	1	1	0	0	0	$n-3$	1	0	$8n + 536$
L_9	0	0	0	0	1	0	1	0	1	$n-4$	1	0	$8n + 464$
L_{10}	0	0	0	0	1	0	0	2	0	$n-4$	1	0	$8n + 440$
L_{11}	0	0	0	0	1	0	0	1	2	$n-5$	1	0	$8n + 422$
L_{12}	0	0	0	0	1	0	0	0	4	$n-6$	1	0	$8n + 404$
L_{13}	0	0	0	0	0	2	0	0	1	$n-4$	1	0	$8n + 428$
L_{14}	0	0	0	0	0	1	1	1	0	$n-4$	1	0	$8n + 374$
L_{15}	0	0	0	0	0	1	0	2	1	$n-5$	1	0	$8n + 332$
L_{16}	0	0	0	0	0	1	0	1	3	$n-6$	1	0	$8n + 314$
L_{17}	0	0	0	0	0	1	0	0	5	$n-7$	1	0	$8n + 296$
L_{18}	0	0	0	0	0	0	3	0	0	$n-4$	1	0	$8n + 344$
L_{19}	0	0	0	0	0	0	2	1	1	$n-5$	1	0	$8n + 302$
L_{20}	0	0	0	0	0	0	2	0	3	$n-6$	1	0	$8n + 284$
L_{21}	0	0	0	0	0	0	1	3	0	$n-5$	1	0	$8n + 278$
L_{22}	0	0	0	0	0	0	1	2	2	$n-6$	1	0	$8n + 260$
L_{23}	0	0	0	0	0	0	1	1	4	$n-7$	1	0	$8n + 242$
L_{24}	0	0	0	0	0	0	1	0	7	$n-8$	1	0	$8n + 243$
L_{25}	0	0	0	0	0	0	0	4	1	$n-6$	1	0	$8n + 236$
L_{26}	0	0	0	0	0	0	0	3	3	$n-7$	1	0	$8n + 218$
L_{27}	0	0	0	0	0	0	0	2	5	$n-8$	1	0	$8n + 200$
L_{28}	0	0	0	0	0	0	0	1	7	$n-9$	1	0	$8n + 182$
L_{29}	0	0	0	0	0	0	0	0	9	$n-10$	1	0	$8n + 164$

REFERENCES

1. H. Abdo, D. Dimitrov, I. Gutman, On extremal trees with respect to the *F*-index, *Kuwait J. Sci.*, in press.
2. B. Basavanagoud, V. R. Desai, Forgotten topological index and hyper-Zagreb index of generalized transformation graphs, *Bull. Math. Sci. Appl.* **14** (2016) 1–6.
3. N. De, S. M. A. Nayeem, A. Pal, F-index of some graph operations, *Discrete Math. Algorithm Appl.* **8**(2) (2016) 1650025.
4. B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190.
5. B. Furtula, I. Gutman, Z. Kovijanić Vukićević, G. Lekishvili, G. Popivoda, On an old/new degree–based topological index, *Bull. Acad. Serbe Sci. Arts* (*Cl. Math. Natur.*) **40** (2015) 19–31.
6. I. Gutman, Degree–based topological indices, *Croat. Chem. Acta* **86** (2013) 351–361.
7. I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.
8. I. Gutman, B. Furtula, Z. Kovijanić Vukićević, G. Popivoda, On Zagreb indices and coindices, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 5–16.
9. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.
10. X. Li, H. Zhao, Trees with the first three smallest and largest general topological indices, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 57–62.
11. S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003) 113–124.
12. Y. M. Tong, J. B. Liu, Z. Z. Jiang, N. N. Lv, Extreme values of the first general Zagreb index in tricyclic graphs, *J. Hefei Univ. Nat. Sci.* **1** (2010) 4–7.
13. S. Zhang, W. Wang, T. C. E. Cheng, Bicyclic graphs with the first three smallest and largest values of the first general Zagreb index, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 579–592.
14. S. Zhang, H. Zhang, Unicyclic graphs with the first three smallest and largest first general Zagreb index, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 427–438.

Iranian J. Math. Chem. 8 (3) September (2017) 275 − 283

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

On the First Variable Zagreb Index

KHOSRO MORADIAN[1], RAMIN KAZEMI[2,•] AND MOHAMMAD HASAN BEHZADI[3]

[1,3]Department of Statistics, Science and Research Branch, Islamic Azad University, Tehran, Iran

[2]Department of Statistics, Imam Khomeini International University, Qazvin, Iran

ARTICLE INFO

Article History:

Received 29 December 2016
Accepted 8 April 2016
Published online 21 April 2017
Academic Editor: Sandi Klavžar

Keywords:

First variable Zagreb index
Random increasing trees
Distribution function
Expected value

ABSTRACT

The first variable Zagreb index of graph G is defined as $M_1^{\lambda}(G) = \sum_{x \in V(G)} d(v)^{2\lambda}$, where λ is a real number and $d(v)$ is the degree of vertex v. In this paper, some lower and upper bounds for the expected value and distribution function of this index in random increasing trees (recursive trees, plane-oriented recursive trees and binary increasing trees) are given.

1. INTRODUCTION

The concept of the variable molecular descriptors was proposed as an alternative way of characterizing heteroatoms in molecules, but also to assess the structural differences, such as, for example, the relative role of carbon atoms of acyclic and cyclic parts in alkyl cycloalkanes. The idea behind the variable molecular descriptors is that the variables are determined during the regression so that the standard error of estimate for a studied property is as small as possible. Several molecular descriptors, have already been generalized in their variable forms, but here we will only pay attention to first Zagreb index. This index has been used to study molecular complexity, chirality, ZE-isomerism and hetero-systems. Overall, Zagreb indices exhibit a potential applicability for deriving multi-linear regression models [2].

The first variable Zagreb index of graph G is defined by

•Corresponding author (Email: r.kazemi@sci.ikiu.ac.ir)
DOI: 10.22052/ijmc.2017.71544.1262

$$M_1^{\lambda} = M_1^{\lambda}(G) = \sum_{v \in V(G)} d(v)^{2\lambda}, \tag{1}$$

where λ is a real number and $d(v)$ is the degree of vertex v (for example, see [1] for the case $\lambda \in [0,1/2]$).

There are several tree models, namely so called recursive trees, plane-oriented recursive trees (also known as non-uniform recursive trees or heap ordered trees) and binary increasing trees, which turned out to be appropriate in order to describe the behaviour of a lot of quantities in various applications. All the tree families mentioned above can be considered as so called increasing trees, i.e. labelled trees, where the nodes of a tree of size n are labelled by distinct integers of the set $\{1,2,...,n\}$ in such a way that each sequence of labels along any path starting at the root is increasing. E. g., plane-oriented recursive trees are increasingly labelled ordered trees (= planted plane trees) and binary increasing trees are obtained from (unlabelled) d-ary trees via increasing labellings [2]. We can describe the tree evolution process which generates random trees (of arbitrary size n) of grown trees. This description is a consequence of the considerations made in:

Step 1: The process starts with the root labelled by 1.

Step $i+1$*:* At step $i+1$ the node with label $i+1$ is attached to any previous node v (with out-degree $d^+(v)$) of the already grown tree of size i with probabilities

$$p(v) := \begin{cases} \dfrac{1}{i}, & \textit{for recursive trees} \\ \dfrac{2-d^+(v)}{i+1}, & \textit{for binary increasing trees} \\ \dfrac{d^+(v)+1}{2i-1}, & \textit{for plane-oriented recursive trees.} \end{cases} \tag{2}$$

Since the structures of many molecules are tree like, our interest here is to study the first variable Zagreb index of increasing trees. Several other topological indices of random trees have been studied by many authors. We refer the reader to Kazemi [3, 4, 5] for the first Zagreb, eccentric connectivity index and second Zagreb indices, Kazemi and Meimondari for degree distance and Gutman index [6] and references therein. Our aim in this paper is to consider the expected value and distribution function of the first variable Zagreb index in random trees. In the following, we use the notation R_n^{α} to denote the first variable Zagreb index of an increasing tree of size n with $a \in R$.

2. CASE $\alpha = 2\lambda \in \mathbb{N} \setminus \{1\}$

Let $\alpha = 2\lambda \in \mathbb{N} \setminus \{1\}$ and R_n^{α} be the first variable Zagreb index of an increasing tree of size n. For $\alpha = 1$ (or $\lambda = 1/2$),

$$R_n^1 = \sum_{v \in V(G)} d(v) = 2(n-1).$$

Let $d_{k,n}$ denote the degree of node labeled k in the random tree of size n. Considering the insertion of label n at the nth stage, we obtain

$$\begin{aligned} R_n^\alpha &= R_{n-1}^\alpha + (d_{U_n,n-1}+1)^\alpha - d_{U_n,n-1}^\alpha + 1 \\ &= R_{n-1}^\alpha + \sum_{j=0}^{\alpha-1} \binom{\alpha}{j} d_{U_n,n-1}^j + 1, \end{aligned} \tag{3}$$

where

$$U_n = \sum_{k=1}^{n-1} k\, \mathrm{I}(\textit{node } k \textit{ is the parent of node } n)$$

is uniformly distributed on the set $\{1,2,...,n-1\}$.

Now, let F_n be the sigma-field generated by the first n stages of the increasing trees. By stochastic growth rule of the random increasing trees and definition of conditional expectation,

$$\begin{aligned} \mathbf{E}(R_n^\alpha \mid \mathsf{F}_{n-1}) &= \mathbf{E}(R_n^\alpha \mid d_{k,n-1}, k = 1,...,n-1) \\ &= R_{n-1}^\alpha + p(v) \sum_{k=1}^{n-1} \sum_{j=0}^{\alpha-1} \binom{\alpha}{j} d_{k,n-1}^j + 1. \end{aligned} \tag{4}$$

As our first result, we prove the following theorem.

Theorem 1 *We have*

$$\mathbf{E}(R_n^\alpha) \le \begin{cases} n + \sum_{j=3}^{n} \dfrac{(2j-3)^\alpha}{j-1}, & \textit{for recursive trees} \\ n + 2\sum_{j=2}^{n} \dfrac{(2j-3)^\alpha}{j} - 1, & \textit{for binary increasing trees} \\ n + \sum_{j=2}^{n} (2j-3)^{\alpha-1}(j-1) - 1, & \textit{for plane-oriented recursive trees.} \end{cases}$$

Also

$$\mathbf{E}(R_n^\alpha) \ge \begin{cases} n + 2(2^\alpha - 1)\sum_{j=2}^{n} \dfrac{j-2}{j-1}, & \textit{for recursive trees} \\ n + 4(2^\alpha - 1)\sum_{j=2}^{n} \dfrac{j-2}{j} - 1, & \textit{for binary increasing trees} \\ n + 2(2^\alpha - 1)\sum_{j=2}^{n-1} \dfrac{j-2}{2j-3} - 1, & \textit{for plane-oriented recursive trees.} \end{cases}$$

Proof. We have

$$\begin{aligned}\mathbf{E}(R_n^\alpha \mid \mathsf{F}_{n-1}) &= R_{n-1}^\alpha + p(v)\sum_{k=1}^{n-1}\sum_{j=0}^{\alpha-1}\binom{\alpha}{j} d_{k,n-1}^j + 1 \\ &= R_{n-1}^\alpha + p(v)\sum_{j=0}^{\alpha-1}\binom{\alpha}{j}\Big(\sum_{k=1}^{n-1} d_{k,n-1}^j\Big) + 1 \\ &\le R_{n-1}^\alpha + p(v)\sum_{j=0}^{\alpha}\binom{\alpha}{j}(R_{n-1}^1)^j + 1 \\ &= R_{n-1}^\alpha + p(v)(2n-3)^\alpha + 1\end{aligned}$$

and then

$$\mathbf{E}(R_n^\alpha) \le \mathbf{E}(R_{n-1}^\alpha) + p(v)(2n-3)^\alpha + 1.$$

Also,

$$\begin{aligned}\mathbf{E}(R_n^\alpha \mid \mathsf{F}_{n-1}) &\ge R_{n-1}^\alpha + p(v)\sum_{j=0}^{\alpha-1}\binom{\alpha}{j} R_{n-1}^1 + 1 \\ &= R_{n-1}^\alpha + p(v)(2(n-2))(2^\alpha - 1) + 1.\end{aligned}$$

Now proof is completed by (2) since $R_1^\alpha = 0$ and $R_2^\alpha = 2$.

For a path P_n, $P_n^\alpha := R_n^\alpha(P_n) = 2 + 2^\alpha(n-2)$ and for a star S_n,

$$S_n^\alpha := R_n^\alpha(S_n) = (n-1) + (n-1)^\alpha.$$

We use the notation $\xrightarrow{D}$ to denote convergence in distribution. If $d_{U_n,n}$ is the degree of a random node in a randomly chosen tree of size n, $d_{U_n,n} \xrightarrow{D} X$ with [7]

$$P(X = k) = \begin{cases} \dfrac{1}{2^k}, & \textit{for recursive trees}: k \ge 1 \\ \dfrac{1}{3}, & \textit{for binary increasing trees}: 1 \le k \le 3 \\ \dfrac{2}{3\binom{k+2}{3}}, & \textit{for plane-oriented recursive trees}: k \ge 1. \end{cases} \tag{5}$$

Thus

$$M(j) := \mathbf{E}(X^j) = \begin{cases} Li_{-j}(\frac{1}{2}), & \textit{for recursive trees} \\ \frac{1}{3}H(j;3), & \textit{for binary increasing trees} \\ 4F(j), & \textit{for plane-oriented recursive trees} \end{cases}$$

where $Li_s(z)$ is the polylogarithm function, $H(p;n) = \sum_{k=1}^{n} k^p$ is the $(p+1)$-th-degree polynomial of n and

$$F(j) = \sum_{k=1}^{\infty} \frac{k^j}{(k+2)(k+1)k}, \quad j \le \alpha - 1.$$

Theorem 2 *For n large enough,*

$$\mathbf{E}(R_n^{\alpha}) = n + (n-1)\sum_{j=0}^{\alpha-1} \binom{\alpha}{j} M(j) - 1.$$

Proof. If we denote by $X_1 \overset{D}{=} X_2$ the equality in distribution of random variables X_1 and X_2, then from (3),

$$R_{n-1}^{\alpha} + \sum_{j=0}^{\alpha-1} \binom{\alpha}{j} d_{U_n,n-1}^{j} + 1 \overset{D}{=} R_{n-1}^{\alpha} + \sum_{j=0}^{\alpha-1} \binom{\alpha}{j} X^j + 1.$$

Thus

$$\begin{aligned} \mathbf{E}(R_n^{\alpha}) &= \mathbf{E}(R_{n-1}^{\alpha}) + \sum_{j=0}^{\alpha-1} \binom{\alpha}{j} \mathbf{E}(X^j) + 1 \\ &= \cdots = n - 1 + (n-1)\sum_{j=0}^{\alpha-1} \binom{\alpha}{j} M(j), \end{aligned}$$

since $R_1^{\alpha} = 0$.

Corollary 1 *For $\alpha = 2$ in random recursive trees that reduce to the first Zagreb index, we have*

$$\begin{aligned} \mathbf{E}(R_n^2) &= n + (n-1)\sum_{j=0}^{1} \binom{2}{j} \mathrm{Li}_{-j}(\frac{1}{2}) - 1 \\ &= n + (n-1)\left(\mathrm{Li}_0(\frac{1}{2}) + 2\mathrm{Li}_{-1}(\frac{1}{2}) \right) - 1 \\ &= n - 1 + (n-1)(1+4) \\ &= 6n - 6, \end{aligned}$$

since

$$\mathrm{Li}_0(z) = \frac{z}{1-z}, \quad \mathrm{Li}_{-1}(z) = \frac{z}{(1-z)^2}.$$

Let Δ_n be the maximum degree of any node in a random recursive tree. Szyma n′ski [8] proved that

$$\Delta_n \le \log_2 n,$$

for all but $o((n-1)!)$ recursive trees on n nodes. For a binary increasing trees, $\Delta_n \le 3$.

Theorem 3 *i*) *For all but* $o((n-1)!)$ *recursive trees on* n *nodes,*

$$\mathbf{E}(R_n^\alpha) \le n + (2^\alpha - 1)(\log_2 (n-1)!)^{\alpha-1} - 1.$$

ii) For binary increasing trees,

$$\mathbf{E}(R_n^\alpha) \le n + (n-1)4^\alpha - 1.$$

Proof. i) We have:

$$\begin{aligned}
\mathbf{E}(R_n^\alpha) &= \mathbf{E}(R_{n-1}^\alpha) + \mathbf{E}\left(\sum_{j=0}^{\alpha-1}\binom{\alpha}{j} d_{U_n,n-1}^j\right) + 1 \\
&\le \mathbf{E}(R_{n-1}^\alpha) + \sum_{j=0}^{\alpha-1}\binom{\alpha}{j}\mathbf{E}(\Delta_{n-1}^j) + 1 \\
&\le \mathbf{E}(R_{n-1}^\alpha) + (2^\alpha - 1)(\log_2 (n-1))^{\alpha-1} + 1 \\
&\le \cdots \le n + (2^\alpha - 1)(\log_2 (n-1)!)^{\alpha-1} - 1.
\end{aligned}$$

Similarly, we can prove Part (*ii*).

Theorem 4 *For all increasing trees,*

$$\mathbf{E}(R_n^\alpha) \ge P_{n+1}^\alpha - 2.$$

Proof. From (3),

$$\begin{aligned}
\mathbf{E}(R_n^\alpha) &= \mathbf{E}(R_{n-1}^\alpha) + \mathbf{E}\left(\sum_{j=0}^{\alpha-1}\binom{\alpha}{j} d_{U_n,n-1}^j\right) + 1 \\
&= \mathbf{E}(R_{n-1}^\alpha) + \sum_{j=0}^{\alpha-1}\binom{\alpha}{j}\mathbf{E}(d_{U_n,n-1}^j) + 1 \\
&\ge \mathbf{E}(R_{n-1}^\alpha) + \sum_{j=0}^{\alpha-1}\binom{\alpha}{j} + 1, \quad j \ge 0 \\
&= \cdots = 2^\alpha (n-1).
\end{aligned}$$

Theorem 5 *Let* $F_n^\alpha(r) = P(R_n^\alpha \le r)$ *be the distribution function of* R_n^α, $r > 2(n-1)$ *and* n *be large enough.*

i) For recursive trees,

$$2\left(1-\frac{1}{2^{\sqrt[\alpha]{\frac{r-n}{n-2}}}}\right) < F_n^{\alpha}(r) < 2\left(1-\frac{1}{2^{\sqrt[\alpha-1]{\frac{r-n}{n-2}}}}\right).$$

ii) For binary increasing trees,

$$\frac{\sqrt[\alpha]{\frac{r-n}{n-2}}-1}{3} < F_n^{\alpha}(r) < \frac{\sqrt[\alpha-1]{\frac{r-n}{n-2}}-1}{3}.$$

iii) For plane-oriented recursive trees,

$$\sum_{k=1}^{\sqrt[\alpha]{\frac{r-n}{n-2}}-1} \frac{4}{k(k+1)(k+2)} < F_n^{\alpha}(r) < \sum_{k=1}^{\sqrt[\alpha-1]{\frac{r-n}{n-2}}-1} \frac{4}{k(k+1)(k+2)}.$$

Proof. Suppose $T_\alpha = \sum_{j=0}^{\alpha-1}\binom{\alpha}{j}X^j$. Thus from (3),

$$\begin{aligned} F_n^{\alpha}(r) &= P(R_n^{\alpha} \le r) \\ &= P(R_{n-1}^{\alpha} + T_\alpha + 1 \le r) \\ &= P(T_\alpha \le r - R_{n-1}^{\alpha} - 1) \\ &= \cdots = P((n-2)T_\alpha \le r-n) \\ &= P(T_\alpha \le \frac{r-n}{n-2}). \end{aligned}$$

Also,

$$Z = (1+X)^{\alpha-1} < T_\alpha < W = (1+X)^{\alpha}$$

and

$$F_W(\frac{r-n}{n-2}) < P(T_\alpha \le \frac{r-n}{n-2}) < F_Z(\frac{r-n}{n-2}),$$

where F_Z and F_W are the distribution functions of Z and W, respectively. Now the proof is completed by (5).

3. GENERAL CASE $\alpha \in \mathbb{R}$

Lemma 1 *Let $f(x) = (x+1)^{\alpha} - x^{\alpha}$, where $x > 1$. Then $f(x)$ is decreasing (respectively increasing) for $0 < \alpha < 1$ (respectively for $\alpha < 0$ or $\alpha > 1$).*

Proof. It is enough to note that $f'(x)$ is negative (respectively positive) for $0 < \alpha < 1$ (respectively for $\alpha < 0$ or $\alpha > 1$).

Theorem 6 *Let* $f(n) = (n+1)^{\alpha} - n^{\alpha}$.

i) For $0 < \alpha < 1$,

$$\mathbf{E}(R_n^{\alpha}) \le \begin{cases} P_n^{\alpha}, & \textit{for recursive trees} \\ n + 2(2^{\alpha} - 1)\sum_{j=2}^{n} \frac{j-1}{j} - 1, & \textit{for binary increasing trees} \\ n + (2^{\alpha} - 1)\sum_{j=3}^{n} \frac{(j-1)(j-2)}{2j-3} - 1, & \textit{for plane-oriented recursive trees} \end{cases}$$

and

$$\mathbf{E}(R_n^{\alpha}) \ge \begin{cases} S_n^{\alpha} + 1, & \textit{for recursive trees} \\ n + 2\sum_{j=2}^{n} \frac{j-1}{j} f(j-2) - 1, & \textit{for binary increasing trees} \\ n + 2\sum_{j=2}^{n} \frac{j-1}{2j-3} f(j-2) - 1, & \textit{for plane-oriented recursive trees} \end{cases}$$

ii) For $\alpha < 0$ or $\alpha > 1$, the presented bounds in Part (i) should be changed by other.

Proof. We have

$$\mathbf{E}(R_n^{\alpha} \mid \mathsf{F}_{n-1}) = R_{n-1}^{\alpha} + p(v)\sum_{k=1}^{n-1} f(d_{k,n-1}) + 1,$$

where $f(1) = 2^{\alpha} - 1$ and $f(n-2) = (n-1)^{\alpha} - (n-2)^{\alpha}$. For Part (i), $f(n-2) < f(1)$ and for Part (ii), $f(1) < f(n-2)$. Now, proof is completed by Lemma 1.

ACKNOWLEDGEMENT. We would like to express our deepest gratitude to the referees for their invaluable comments and suggestions which improve the quality of this paper.

REFERENCES

1. V. Andova and M. Petrusevski, Variable Zagreb indices and Karamata's inequality, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 685–690.
2. M. Drmota, *Random Trees, An Interplay Between Combinatorics and Probability*, Springer, Wien-New York, 2009.
3. R. Kazemi, Probabilistic analysis of the first Zagreb index, *Trans. Comb.* **2** (2) (2013) 35–40.
4. R. Kazemi, The eccentric connectivity index of bucket recursive trees, *Iranian J. Math. Chem.* **5** (2) (2014) 77–83.

5. R. Kazemi, The second Zagreb index of molecular graphs with tree structure, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 753–760.
6. R. Kazemi and L. K. Meimondari, Degree distance and Gutman index of increasing trees, *Trans. Comb.* **5** (2) (2016) 23–31.
7. M. Kuba and A. Panholzer, On the degree distribution of the nodes in increasing trees, *J. Combin. Theory Ser. A* **114** (4) (2007) 597–618.
8. J. Szymanski, On the maximum degree and height of a random recursive tree, Wiley, New York, 1990.

Iranian J. Math. Chem. 8 (3) September (2017) 285 − 290

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

Computing the Additive Degree–Kirchhoff Index with the Laplacian Matrix

JOSÉ LUIS PALACIOS•

Electrical and Computer Engineering Department, The University of New Mexico, Albuquerque, NM 87131, USA

ARTICLE INFO

Article History:

Received: 2 November 2016
Accepted: 4 December 2016
Published online 7 July 2017
Academic Editor: Tomislav Došlić

Keywords:

Degree-Kirchhoff index
Laplacian matrix

ABSTRACT

For any simple connected undirected graph, it is well known that the Kirchhoff and multiplicative degree–Kirchhoff indices can be computed using the Laplacian matrix. We show that the same is true for the additive degree–Kirchhoff index and give a compact Matlab program that computes all three Kirchhoffian indices with the Laplacian matrix as the only input.

1. INTRODUCTION

Let $G = (V, E)$ be a finite simple connected graph with vertex set $V = \{1,2,\cdots,n\}$ and degrees d_i for $1 \leq i \leq n$. The general formula

$$R^f(G) = \sum_{\{i<j\}} f(i,j) R_{\{ij\}}, \quad (1)$$

where $R_{\{ij\}}$ is the effective resistance between vertices i and j and $f(i,j)$ is some real function of the vertices, identifies a family of descriptors widely studied in Mathematical Chemistry. Among these, the ones that have undergone a more intense scrutiny are the Kirchhoff index R(G), the multiplicative degree–Kirchhoff index $R^*(G)$ and the additive degree–Kirchhoff index $R^+(G)$ defined by (1) when taking $f(i,j) = 1$, $f(i,j) = d_i d_j$ and $f(i,j) = d_i + d_j$, respectively, and introduced in [10], [3] and [6] respectively. The references [9, 12, 17–20] are a recent sample of works where some interesting relationships between these three indices are highlighted.

•Corresponding Author (Email address: jpalacios@unm.edu)
DOI: 10.22052/ijmc.2017.64656.1249

A possible approach to compute these indices is to find first the individual values $R_{\{ij\}}$ and then compute the sums in (1). It is well known (see [2]), for instance, that

$$R_{\{ij\}} = L^{\#}{}_{\{ii\}} + L^{\#}{}_{\{jj\}} - L^{\#}{}_{\{ij\}} - L^{\#}{}_{\{ji\}}, \tag{2}$$

where $\boldsymbol{L}^{\#}$ is the Moore–Penrose inverse of the Laplacian matrix **L** = **D** − **A**, **D** is the diagonal matrix with the degrees of the vertices in the diagonal, and **A** is the adjacency matrix of G. It is also known (see [2]) that the resistances can be expressed in terms of the Laplacian matrix:

$$R_{\{ij\}} = \frac{\det \mathbf{L}(i,j)}{\det \mathbf{L}(i)}, \tag{3}$$

where **L**(i,j) and **L**(i) are obtained from **L** by deleting its $i-th$ row and $j-th$ column, and by deleting its $i-th$ row and column, respectively.

This approach, though amenable to being programmed, does not seem to be computationally efficient, because it entails computing $n^2 + n$ determinants just to get the values of the effective resistances. If in addition we want to compute the additive degree–Kirchhoff index, besides storing the matrix **L** we need to store the matrix of resistances **R** = $R_{\{ij\}}$ in order to compute $\sum_{\{i,j\}} d_i d_j R_{\{ij\}}$ with an additional set of additions and multiplications.

A major breakthrough in the computation of these indices is the fact that two of them have a simple expression in terms of certain eigenvalues, namely (see [7, 21]), and also [8] and [15] for alternative proofs)

$$R(G) = n \sum_{i=1}^{n-1} \frac{1}{\lambda_i} \tag{4}$$

for $\lambda_1 \geq \cdots \geq \lambda_{n-1} > \lambda_n = 0$ the eigenvalues of the Laplacian matrix. Likewise (see [3])

$$R^*(G) = 2|E| \sum_{i=1}^{n-1} \frac{1}{\beta_i}, \tag{5}$$

for $2 \geq \beta_1 \geq \cdots \geq \beta_{n-1} > \beta_n = 0$ the eigenvalues of the normalized Laplacian matrix $\boldsymbol{\mathcal{L}} = \mathbf{D}^{\frac{-1}{2}}\mathbf{L}\mathbf{D}^{\frac{-1}{2}}$, and also (see [16])

$$R^*(G) = 2|E| \sum_{i=2}^{n} \frac{1}{1-\alpha_i} \tag{6}$$

for $1 = \alpha_1 > \alpha_2 \geq \cdots \geq \alpha_n \geq -1$ the eigenvalues of the transition probability matrix **P** = $\mathbf{D}^{-1}\mathbf{A}$ of the random walk on *G*.

There is a probabilistic connection between effective resistances and random walks on graphs that allow us to express $R(G)$ in terms of the fundamental matrix **Z** of the random walk on *G* (see [14]), $R^*(G)$ in terms of the eigenvalues of **P**, as in(6), and $R^+(G)$ as a more involved expression

$$R^+(G) = \frac{1}{d_G} R^*(G) + \sum_j \sum_i \pi_i E_i T_j, \tag{7}$$

where $\pi = (\pi_i)_{1 \le i \le n}$ is the stationary distribution of the random walk on G, which can be given explicitly as $\pi_i = \frac{d_i}{2|E|}$, and where $E_i T_j$ denotes the expected hitting time of the vertex j by the walk on G started at the vertex i (see [1] for all matters regarding random walks on graphs). In principle, one could use the expression (7) to compute $R^+(G)$, but in addition to working with **L** for the calculation of $R^*(G)$, we need to store **Z,** then compute the hitting times and store them in an additional matrix from which the sum $\sum_j \sum_i \pi_i E_i T_j$ can be computed with additional operations.

In [20] and [9] they came up, almost simultaneously, with the same idea of expressing

$$R^+(G) = d_G R(G) + n \,\text{trace}\,(\mathbf{DL}^{\#}). \tag{8}$$

Calculating $R^+(G)$ with (8) is perfectly feasible. A possible concern is the complexity in the calculation of the Moore Penrose inverse. More on this below.

Also recently (see [18]), we found that

$$R^+(G) = \frac{1}{d_G} R^*(G) + 2|E| \sum_{i=1}^{n} \frac{1}{\upsilon_i} - n, \tag{9}$$

where the $\upsilon_i s$ are the eigenvalues of the modified Laplacian matrix $\mathbf{L} + \mathbf{DW}$, and **W** is the matrix all of whose rows are copies of the stationary distribution π^T defined above.

The interesting point now is to realize that the new modified Laplacian matrix can be written exclusively in terms of the Laplacian matrix: indeed, the matrix **D** is the diagonal matrix whose elements are those in the diagonal of **L** (see below the simple Matlab command to get **D** from **L**) and

$$\boldsymbol{W} = \frac{1}{2|E|} \mathbf{OD}$$

where **O** is the $n \times n$ matrix of all whose entries are ones. In what follows we will use for the computation of the Kirchhoffian indices only the formulas (4),(5) and (9) where in the last equation, the $\upsilon_i s$ are the eigenvalues of the invertible matrix $\mathbf{L} + \frac{1}{2|E|} \mathbf{DOD}$.

2. THE COMPUTATIONS

Clearly (4), (5) and (9) depend exclusively on **L**. Perhaps this is more evident if we write 2|E| trace **L**=trace **D**.

Also, the sums of inverses of eigenvalues in (4),(5) and (9) can be written as

$$\sum_{i=1}^{n-1} \frac{1}{\lambda_i} = -\frac{a_2}{a_1} \tag{10}$$

$$\sum_{i=1}^{n-1} \frac{1}{\beta_i} = -\frac{b_2}{b_1} \tag{11}$$

and

$$\sum_{i=1}^{n} \frac{1}{\nu_i} = -\frac{c_1}{c_0} \tag{12}$$

where a_i, i = 1, 2 (resp. b_i, i=1, 2 and c_i, i = 0, 1) are the coefficients of x^i in the characteristic polynomial of **L** (resp. $\mathcal{L}$ and $\mathbf{L} + \frac{1}{2|E|}\mathbf{DOD}$).

To see for instance that (10) holds, we notice that:

$$\sum_{i=1}^{n-1} \frac{1}{\lambda_i} = \frac{\sum \lambda_{i_1}\lambda_{i_2}\cdots\lambda_{i_{n-2}}}{\lambda_1\lambda_2\cdots\lambda_{n-1}}$$

where the sum in the numerator runs over all (n–2)–long products of distinct nonzero eigenvalues. We then apply Vieta's formulas (see [13]) for the sums of products of the roots of a polynomial in terms of its coefficients. Formulas (11) and (12) follow similarly.

We will now write the Matlab commands to obtain the three indices when the only input is the Laplacian matrix of the graph. Matlab is a registered trademark of the Mathworks [11].

Once **L** has been entered, no other matrix needs to be manipulated, and these are the commands used (with a brief comment of their purpose in the parentheses):

>>[n,n]=size(L) (recovers the number of vertices of the graph)

>>a=flip(charpoly(L)) (finds the vector of coefficients $a(i)$ of x^{i-1},$1 \le i \le n+1$ for the characteristic polynomial of L)

>>R1 = $-n * \frac{a(3)}{a(2)}$ (finds the Kirchhoff index)

>>D = diag(diag(L)) (finds the diagonal matrix D)

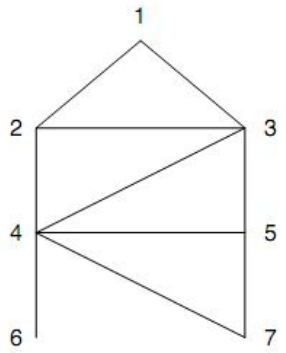
>>b = flip(charpoly($D \wedge (\frac{-1}{2}) * L * D \wedge (\frac{-1}{2})$)) (finds the vector of coefficients b(i) of x^{i-1},$1 \le i \le n+1$ for the characteristic polynomial of $\mathcal{L}$

>>R2 = $-\mathrm{trace}(L) * \frac{b(3)}{b(2)}$ (finds the multiplicative degree–Kirchhoff index)

>> c = flip(charpoly(L+1/trace(D)*D*ones(n)*D)) (finds the vector of coefficients $c(i)$ of x^{i-1}, $1 \le i \le n+1$, for the characteristic polynomial of $\mathbf{L} + \frac{1}{2|E|}\mathbf{DOD}$

>>R3 = $n * R2/trace(D) - trace(D) * c(2)/c(1) - n$ (finds the additive degree–Kirchhoff index)

For illustration purposes we will use the graph in the following figure.



Once the matrix **L** has been entered, Matlab returns the vectors

a:

0 385 −1106 1181 −600 156 −20 1

b:

0 1.5278 −9.4944 23.3194 −29.2417 19.8917 −7.0000 1.0000

c:

1.0e+03*

−1.1000 3.6284 −4.6636 3.0416 −1.0985 0.2219 −0.0234 0.0010

and the indices R1 = 20.1091, R2 = 124.2909, R3 = 102.4727.

Final remarks. A question may arise as to the advantages of using formula (9) instead of (8) when computing $R^+(G)$. We can point to the fact that the computation of the characteristic polynomial of the matrix $\mathbf{L} + \frac{1}{2|E|}\mathbf{DOD}$ is done in Matlab using the well studied Hessenberg's algorithm (see [4]) with the command "charpoly", and the computation of the Moore–Penrose inverse with the command "pinv" of Matlab, and other algorithms, is cause for concern as to the time and space requirements. Indeed, both "charpoly" and "pinv" are of order $O(n^3)$, but the constant of the n^3 term seems to be much larger in the case of the "pinv" command (see [5]).

REFERENCES

1. D. Aldous, J. Fill, Reversible Markov chains and random walks on graphs, unfinished monograph, 2014, available at http://www.stat.berkeley.edu/~aldous/RWG/book.html.
2. R. B. Bapat, I. Gutman and W. Xiao, A simple method for computing the effective resistance, *Z. Naturforsch. A* **58** (2003) 494–498.
3. H. Chen and F. Zhang, Resistance distance and the normalized Laplacian spectrum, *Discrete Appl. Math.* **155** (2007) 654–661.

4. H. Coen, *A Course in Computational Algebraic Number Theory*, Graduate texts in Mathematics, **138**, Springer–Verlag, 1993.
5. P. Courrieu, Fast computation of Moore–Penrose inverse matrices, *Neural Inform. Process. Lett. Rev* **8** (2005) 25–29.
6. I. Gutman, L. Feng and G. Yu, Degree resistance distance of unicyclic graphs, *Trans. Comb.* **1** (2012) 27–40.
7. I. Gutman and B. Mohar, The quasi–Wiener and the Kirchhoff indices coincide, *J. Chem. Inf. Comput. Sci.* **36** (1996) 982–985.
8. I. Gutman, D. Vidović and B. Furtula, Chemical applications of the Laplacian spectrum VII. Studies of the Wiener and Kirchhoff indices, *Indian J. Chem*. **42A** (2003) 1272–1278.
9. S. Huang, J. Zhou and C. Bu, Some results on Kirchhoff index and degree–Kirchhoff index, *MATCH Commun. Math. Comput. Chem*. **75** (2016) 207–222.
10. D. J. Klein and M. Randi'c, Resistance distance, *J. Math. Chem*. **12** (1993) 81–95.
11. Matlab. The Mathworks. http://www.mathworks.com/products/matlab/
12. I. Milovanović, I. Gutman and E. Milovanović, On Kirchhoff and degree Kirchhoff indices, *Filomat* **29** (2015) 1869–1877.
13. A. Mostowski and M. Stark, *Introduction to Higher Algebra*, The Macmillan Company, New York, 1964.
14. J. L. Palacios, Resistance distance in graphs and random walks, *Int. J. Quantum Chem* **81** (2001) 29–33.
15. J. L. Palacios and J. M. Renom, Sum rules for hitting times of Markov chains, *Linear Algebra Appl.* **433** (2010) 491–497.
16. J. L. Palacios and J. M. Renom, Broder and Karlin's formula for hitting times and the Kirchhoff index, *Int. J. Quantum Chem.* **111** (2011) 35–39.
17. J. L. Palacios, Some interplay of the three Kirchhoffian indices, *MATCH Commun. Math. Comput. Chem.* **75** (2016) 199–206.
18. J. L. Palacios, Some more interplay of the three Kirchhoffian indices, *Linear Algebra Appl.* **511** (2016) 421–429.
19. M. Somodi, On the Ihara zeta function and resistance distance-based indices, *Linear Algebra Appl.* 513 (2017) 201–209
20. Y. Yang and D. J. Klein, A note on the Kirchhoff and additive degree–Kirchhoff indices of graphs, *Z. Naturforsch. A* **70** (2015) 459–463.
21. H. Y. Zhu, D. J. Klein and I. Lukovits, Extensions of the Wiener number, *J. Chem. Inf. Comput. Sci.* **36** (1996) 420–428.

Iranian J. Math. Chem. 8(3) September (2017) 291 – 298

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

On the Spectra of Reduced Distance Matrix of the Generalized Bethe Trees

ABBAS HEYDARI•

Department of Science, Arak University of Technology, Arak, Iran

ARTICLE INFO

Article History:

Received: 8 June 2015
Accepted:8 June 2017
Published online14 July 2017
Academic Editor: Bijan Taeri

Keywords:

Reduced distance matrix
Generalized Bethe tree
Spectrum

ABSTRACT

Let G be a simple connected graph and $\{v_1, v_2, v_3, \dots, v_k\}$ be the set of pendant (vertices of degree one) vertices of G. The reduced distance matrix of G is a square matrix of order k whose (i,j)-entry is the topological distance between v_i and v_j of G. A rooted tree is called a generalized Bethe tree if its vertices at the same level have equal degree. In this paper, we compute the spectrum of the reduced distance matrix of the generalized Bethe trees.

1. INTRODUCTION

Let G be a simple connected graph with vertex set $V(G) = \{v_1, v_2, v_3, \dots, v_n\}$. The distance between the vertices v_i and v_j of G, is equal to the length (= number of edges) of each shortest path starting at v_i and ending at v_j (or vice versa) [2], and will be denoted by $d_G(v_i, v_j)$. The distance matrix of G is defined as the $n \times n$ matrix $D(G) = [d_{ij}]$, where d_{ij} is the distance between vertices v_i and v_j in G. While the problem of computing the characteristic polynomial of adjacency matrix and its spectrum appears to be solved for many large graphs, the related distance polynomials have received much less attention. The distance matrix is more complex than the ordinary adjacency matrix of a graph since the distance matrix is a complete matrix while in the adjacency matrix most of entries are zero. Thus the computation of the characteristic polynomial of the distance matrix is computationally a much more intense problem and, in general, there are no simple analytical solutions except for a few trees [6]. For this reason, distance polynomials of only trees have been studied extensively in the mathematical literature [6, 7]. The distance

•Corresponding Author (Email address: heydari@arakut.ac.ir)
DOI: 10.22052/ijmc.2017.30051.1116

matrix of a graph and its spectrum has numerous applications to chemistry and other branches of science. The distance matrix, contains information on various walks and self-avoiding walks of chemical graphs, is immensely useful in the computation of topological indices such as the Wiener index, is useful in the computation of thermodynamic properties such as pressure and temperature coefficients and it contains more structural information compared to a simple adjacency matrix [1].

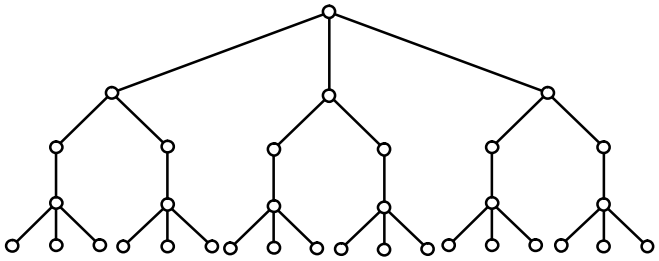


Figure 1: A Generalized Bethe Tree with 5 Levels.

In a number of recently published articles, the so-called reduced distance matrix [10] or terminal distance matrix [5, 8] of trees was considered. If an n-vertex graph G has n' pendant vertices (= vertices of degree one), labeled by $\{v_1, v_2, v_3, \dots, v_{n'}\}$, then its reduced distance matrix is the square matrix of order n' whose (i,j)-entry is $d_G(v_i, v_j)$ and will be denoted by $RD(G)$. Reduced distance matrices were used for modeling of amino acid sequences of proteins and of the genetic code, and were proposed to serve as a source of novel molecular structure descriptors [5, 8].

Recall that a tree is a connected acyclic graph. In a tree, any vertex can be chosen as the root vertex. The level of a vertex on a tree is one more than its distance from the root vertex. Suppose T is an unweighted rooted tree such that its vertices at the same level have equal degrees. We agree that the root vertex is at level 1 and that T has k levels. In [9], Rojo and Robbiano, called such a tree with, generalized Bethe tree and denoted by β_k (see Figure 1). This class of trees has been much studied by mathematical chemists, for details see [3, 9].

In this paper we will compute the spectrum of the reduced distance matrix of the generalized Bethe trees by using methods of computation of eigenvalues of the tensor product of matrices. Recall that if A is a $m \times n$ matrix and B is a $p \times q$ matrix, then the tensor product $A \otimes B$ is the $mp \times nq$ block matrix as follows:

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \dots & a_{1n}B \\ a_{21}B & a_{22}B & \dots & a_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \dots & a_{mn}B \end{bmatrix}.$$

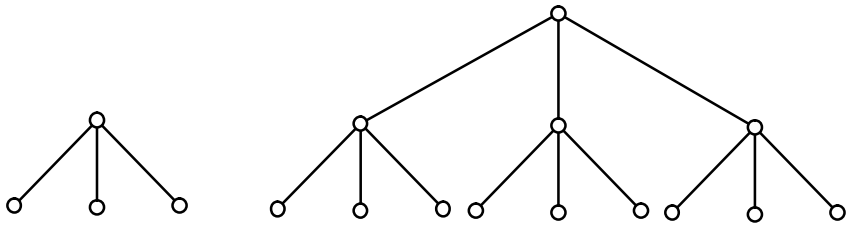


Figure 2: Simple Examples of β_2 and β_3.

Acyclic connected graphs or trees are wildly used in application of graph theory such as molecular graphs, telecommunication networks and the intellectual data analysis. Thus computation of numerical descriptors of trees has been studied in many recent papers [4−9]. The spectrum of the generalized Bethe trees can be used to obtain sharp bound for spectrum and some distance based topological indices of trees [9]. In this paper we will compute the spectrum of the reduced distance matrix of the generalized Bethe trees by exact formula in terms of its vertex degrees and the number of its levels.

2. RESULTS AND DISCUSSION

As we mentioned the computation of the characteristic polynomial and spectrum of the distance based matrices of a graph is computationally a much more intense problem and, in general, there are no simple analytical solutions except for graphs with simple structure. We will compute the spectrum of the reduced distance matrix of β_k by rewrite this matrix as a special type of block matrices, which can be described by the tensor product of some simple matrices. For this purpose, we assume that d_{k-j+1} denotes the degree of vertices on the j–th level of β_k , for $j = 1,2,\dots,k$. Put

$$e_j = \begin{cases} d_j, & j = k, 1 \\ d_j - 1, & 1 < j < k. \end{cases}$$

Thus e_j denotes the number of vertices on the (j+1)-th level which are adjacent with a vertex on the j-th level of β_k, for $j = 1,2,\dots,k-1$. If n_k denotes the number of the pendant vertices of β_k, then $n_k = \prod_{j=1}^{k} e_j$. Suppose that I_n denotes the identity matrix of order n and $J = [J_{ij}]$ denotes a square matrix of order n, where

$$J_{ij} = \begin{cases} 0 & if\ j = i \\ 1 & if\ j \neq i. \end{cases}$$

Put $B_n = I_n + J_n$. So B_n is asquare matrix of order n with all elements equal exactly 1. To obtain the reduced distance matrix of β_k we note that β_2, is a star of order $e_2 + 1$, see Figure 2. This is because that degree of the non-pendant vertices of β_2 must be e_2. Thus the reduced distance matrix of β_2 is given as $RD(\beta_2) = 2J_{e_2}$. In what follows, we

will describe the reduced distance matrix of β_3, which is obtained by making a new vertex adjacent to all central vertices of e_3 copy of β_2, see Figure 2. For this purpose we shall use the tensor product of real matrices as follows:

$$RD(\beta_3) = \begin{bmatrix} 2J_{e_2} & 4B_{e_2} & 4B_{e_2} & \dots & 4B_{e_2} \\ 4B_{e_2} & 2J_{e_2} & 4B_{e_2} & \dots & 4B_{e_2} \\ 4B_{e_2} & 4B_{e_2} & 2J_{e_2} & \dots & 4B_{e_2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 4B_{e_2} & 4B_{e_2} & 4B_{e_2} & \dots & 2J_{e_2} \end{bmatrix}_{e_3 \times e_3} = I_{e_3} \otimes RD(\beta_2) + J_{e_3} \otimes 4B_{e_2}.$$

Thus for j $\geq$ 2, the reduced distance matrix of β_{j+1} can be obtained by a recursive formula in terms of the reduced distance matrix of β_j by using the inductive method. Let $n_1 = 1$ and $n_j = \sum_{i=1}^{j} e_i$ denote the number of the pendant vertices of β_j, for $j = 2,3,\dots,k-1$. Since β_{j+1}, is obtained by making a new vertex adjacent to all central vertices of e_{j+1} copy of β_j, put $D_2 = 2J_{e_2}$ (the reduced distance matrix of β_2) and

$$D_{j+1} = I_{e_{j+1}} \otimes D_j + J_{e_{j+1}} \otimes 2jB_{n_j},$$

for $j = 2,3,\dots,k-1$. Then the reduced distance matrix of the generalized Bethe trees with k levels is given by $RD(\beta_k) = D_k$. Therefore to compute the spectrum of $RD(\beta_k)$ we must introduce a method to calculate the eigenvalues of the block matrix which is defined in (1). First we recall a classical theorem related to the tensor product of two square matrices [11].

Theorem A. Let $\{\lambda_i\}$ and $\{x_i\}, 1 \leq i \leq n$, denote the eigenvalues and the corresponding eigenvectors for n-square matrix A, respectively and $\{\mu_j\}$ and $\{y_j\}, 1 \leq j \leq m$, denote the eigenvalues and the corresponding eigenvectors for m-square matrix B, respectively. Then the eigenvalues of $A \otimes B$ are $\{\lambda_i \otimes \mu_j\}$ with corresponding eigenvectors $\{x_i \otimes y_j\}$, where $1 \leq i \leq n$ and $1 \leq j \leq m$.

In what follows, we introduce a method for computation the spectrum of the block matrices, which are defined in (1). Recall that the spectrum of an n-square matrix with all entries equal 1, contains n and 0 with multiplicity $n-1$.

Lemma 1. Let B_{n_j} denote an n_j-square matrix with all entries equal 1. If x denotes an eigenvector of $D_j, j \geq 2$, then $B_{n_j}x = 0$ for all eigenvector of D_j except x_0, one of the eigenvectors of D_j such that $B_{n_j}x_0 = n_j x_0$.

Proof. We proceed by induction on j. For $j = 2$, let λ be an eigenvalue of $D_2 = 2J_{e_2}$ with corresponding eigenvector x, then

$$B_{n_2}\mathrm{x} = \left(I_{n_2} + J_{n_2}\right)\mathrm{x} = \mathrm{x} + \frac{\lambda}{2}x,$$

since $n_2 = e_2$. Obviously, $\lambda = -2$ or $\lambda = 2(e_2 - 1)$, so $B_{n_2}\mathrm{x} = 0$ or $B_{n_2}\mathrm{x} = n_2\mathrm{x}$. Thus the result is true for $j = 2$. Now suppose that the lemma is true for all positive integers less than j. Since $n_j = e_j n_{j-1}$, if μ is an eigenvalue of B_{e_j} with associated eigenvector y, then

$$B_{n_j}(x \otimes y) = \left(B_{n_{j-1}} \otimes B_{e_j}\right)(x \otimes y) = B_{n_{j-1}}x \otimes \mu y.$$

By induction hypothesis, we have $B_{n_{j-1}}x = 0$ or $B_{n_{j-1}}x = n_{j-1}x$. Since $\mu = 0$ or $\mu = e_j$, $B_{n_j}x = 0$ or $B_{n_j}x = n_j x$. This completes the proof. □

Now by using Lemma 1, the spectrum of square matrix D_{j+1}, which is defined in equation (1), can be computed in terms of the eigenvalues of D_j for $j \geq 2$.

Lemma 2. Let as above, x_0 be an eigenvector of D_j associated to the eigenvalue λ_0 which $B_{n_j}x_0 = n_j x_0$ for $j \geq 2$. If $\lambda_1 \neq \lambda_0$ is an eigenvalue of D_j with multiplicity k, then the spectrum of D_{j+1} contains λ_1 with multiplicity $e_{j+1}k$, $\lambda_0 - 2jn_j$ with multiplicity $e_{j+1} - 1$ and $\lambda_0 + 2jn_j(e_{j+1} - 1)$ with multiplicity 1.

Proof. Let x be an eigenvector of D_j associated to λ and y be an eigenvector of $J_{e_{j+1}}$ associated to μ, then by use of (1) we have

$$D_{j+1}(y \otimes x) = (I_{e_{j+1}} \otimes D_j + J_{e_{j+1}} \otimes 2jB_{n_j})(y \otimes x) = y \otimes \lambda x + \mu y \otimes 2jB_{n_j}x.$$

If $x \neq x_0$, then by Lemma 1 we get $B_{n_j}x = 0$, thus $D_{j+1}(y \otimes x) = y \otimes \lambda x$. Since λ_1 is an eigenvalue of D_j with multiplicity k and $J_{e_{j+1}}$ is a square matrix of order e_{j+1}, so λ_1 is an eigenvalue of D_{j+1} with multiplicity ke_{j+1}. Now suppose that $x \neq x_0$, by Lemma 1 we have $B_{n_j}x = n_j x$. Note that $\mu = -1$ with multiplicity $e_{j+1} - 1$ or $\mu = e_{j+1} - 1$ with multiplicity 1. If $\mu = -1$, then $D_{j+1}(y \otimes x) = \left(\lambda_0 - 2jn_j\right)(y \otimes x)$. Hence $\lambda_0 - 2jn_j$ is an eigenvalue of D_{j+1} with multiplicity $e_{j+1} - 1$. Otherwise if $\mu = e_{j+1} - 1$, then

$$D_{j+1}(y \otimes x) = \left(\lambda_0 + 2jn_j(e_{j+1} - 1)\right)(y \otimes x).$$

Hence $\lambda_0 + 2jn_j(e_{j+1} - 1)$ is an eigenvalue of D_{j+1} with multiplicity 1. Therefore the proof is complete. □

Now we can compute the spectrum of the square block matrix D_{j+1} which is given in equation (1), using Lemma 2 and determine the elements of the spectrum of β_k.

Theorem 1. The spectrum of the reduced distance matrix of β_k, the generalized Bethe tree

of level k, contains -2 with multiplicity $(e_2-1)\prod_{i=3}^{k} e_i$, $\sum_{i=1}^{m-1} 2i(e_{i+1}-1)n_i - 2mn_m$ with multiplicity $(e_{m+1}-1)\prod_{j=m+2}^{k} e_j$ for $m = 2,3,\dots,k-1$ and $\sum_{i=1}^{k-1} 2i(e_{i+1}-1)n_i$ with multiplicity 1.

Proof. We proceed by induction on k. If $k = 2$, then the reduced distance matrix of β_2 is given by$D_2 = 2J_{e_2}$. Hence the spectrum of D_2 contains -2 with multiplicity $e_2 - 1$ and $2(e_2 - 1)$ with multiplicity 1. Thus the argument is true for $k = 2$. We now assume that the theorem is true for all positive integers less than k. By using the assumption of induction, the spectrum of $RD(\beta_{k-1})$ contains -2 with multiplicity $(e_2-1)\prod_{i=3}^{k-1} e_i$, $\sum_{i=1}^{m-1} 2i(e_{i+1}-1)n_i - 2mn_m$ with multiplicity$(e_{m+1}-1)\prod_{j=m+2}^{k-1} e_j$ for $m = 2,3,\dots,k-2$ and $\sum_{i=1}^{k-2} 2i(e_{i+1}-1)n_i$ with multiplicity 1. By using Lemma 2, the spectrum of $RD(\beta_k)$ contains -2 with multiplicity

$$e_k(e_2-1)\prod_{i=3}^{k-1} e_i = (e_2-1)\prod_{i=3}^{k} e_i.$$

On the other hand, the spectrum of $RD(\beta_k)$ should contain the elements $\sum_{i=1}^{m-1} 2i(e_{i+1}-1)n_i - 2mn_m$ of the spectrum of $RD(\beta_{k-1})$ for $m = 2,3,\dots,k-2$, with multiplicity

$$e_k(e_{m+1}-1)\prod_{j=m+2}^{k-1} e_j = (e_{m+1}-1)\prod_{j=m+2}^{k} e_j.$$

Also corresponding to the elements $\sum_{i=1}^{k-2} 2i(e_{i+1}-1)n_i$ of the spectrum of $RD(\beta_{k-1})$, by using Lemma 2, $\sum_{i=1}^{k-2} 2i(e_{i+1}-1)n_i - 2(k-1)n_{k-1}$ is an element of the spectrum of $RD(\beta_k)$. Hence the spectrum of $RD(\beta_k)$ contains $\sum_{i=1}^{m-1} 2i(e_{i+1}-1)n_i - 2mn_m$ with multiplicity $e_{m+1}-1$ for $m = k-1$. Finally, by using Lemma 2, the spectrum of $RD(\beta_k)$ should contain the following values with multiplicity 1:

$$\sum_{i=1}^{k-2} 2i(e_{i+1}-1)n_i + 2(k-1)n_{k-1}(e_k-1) = \sum_{i=1}^{k-1} 2i(e_{i+1}-1)n_i.$$

Therefore the proof is completed. □

By using Theorem 1, the spectrum of the reduced distance matrix of trees such that vertices on same level have equal degree can be computed. For example the reduced distance spectrum of the dendrimer trees, the caterpillar trees and the B-trees will be computed by using this method.

Example 1. As an application of Theorem 1, we compute the spectrum of the reduced distance matrix of T, a generalized Bethe tree of order 63 which is shown in Figure 3. Notice that T is a tree with 5 levels and $e_2 = 2$, $e_3 = 3$, $e_4 = 3$ and $e_5 = 2$. By using Theorem 1, the spectrum of $RD(T)$ contains -2 with multiplicity $(e_2-1)\prod_{i=3}^{5} e_i = 18$.

Also the reduced distance matrix of T contains the following integer numbers with

multiplicity $(e_3 - 1)\prod_{i=4}^{m+1} e_i$ for $m = 2,3,4$,

$$\sum_{i=1}^{m-1} 2i(e_{i+1} - 1)n_i - 2mn_m.$$

If $m = 2$, then $\sum_{i=1}^{m-1} 2i(e_{i+1} - 1)n_i - 2mn_m = 2(1) - 2(2)(2) = -6$. If $m = 3$, then $\sum_{i=1}^{m-1} 2i(e_{i+1} - 1)n_i - 2mn_m = 2(1) + 4(2)(2) - 6(6) = -18$ and if $m = 4$, then $\sum_{i=1}^{m-1} 2i(e_{i+1} - 1)n_i - 2mn_m = 2(1) + 4(2)(2) + 6(2)(3)(2) - 8(18) = -54$. Hence, the spectrum of $RD(T)$ contains -6 with multiplicity 12, -18 with multiplicity 4 and 54 with multiplicity 1. Finally, the last element of the spectrum of $RD(T)$ with multiplicity 1 is computed as $\sum_{i=1}^{k-1} 2i(e_{i+1} - 1)n_i = 2(1)(1) + 4(2)(2) + 6(2)(6) + 8(1)(18) = 234$.

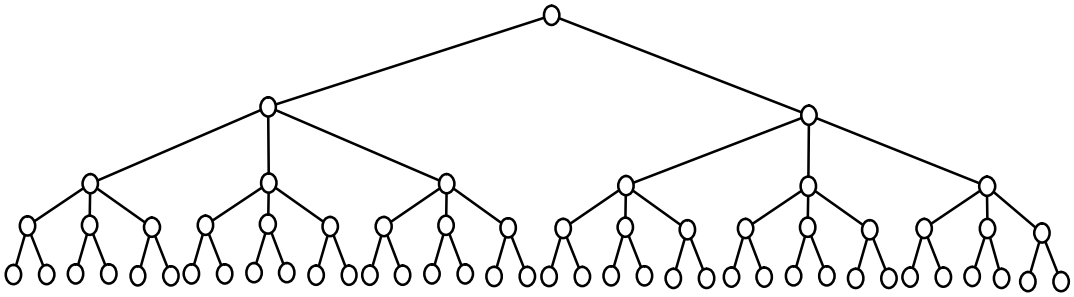


Figure 3: A Generalized Bethe Tree of Order 63.

REFERENCES

1. K. Balasubramanian, Computer generation of distance polynomials of graphs, *J. Comput. Chem.* **11** (1990) 829–836.
2. F. Buckley, F. Harary, Distance in Graphs, Addison-Wesley, Redwood, 1990.
3. A. Heydari, On the Wiener and terminal Wiener index of generalized Bethe trees, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 141–150.
4. A. Heydari, On the spectrum of reduced distance matrix of dendrimers, *Trans. Comb.* **2** (2) (2013) 41–46.
5. B. Horvat, T. Pisanski, M. Randić, Terminal polynomials and star-like graphs, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 493–512.
6. R. L. Graham, L. Lovasz, Distance matrix polynomials of trees, *Adv. Math.* **29** (1978) 60–88.
7. B. D. McKay, On the spectral characterization of trees, *Ars Combin.* **3** (1977) 219–232.
8. M. Randić, J. Zupan, D. Vikić-Topić, On representation of proteins by starlike graphs, *J. Mol. Graph. Model.* **26** (2007) 290–305.

9. O. Rojo, M. Robbiano, An explicit formula for eigenvalues of Bethe trees and upper bounds on the largest eigenvalue of any tree, *Linear Algebra Appl.* **427** (2007) 138−150.

10. E. A. Smolenskii, E. V. Shuvalova, L. K. Maslova, I. V.Chuvaeva, M. S. Molchanova, Reduced matrix of topological distances with a minimum number of independent parameters: distance vectors and molecular codes, *J. Math. Chem.* **45** (2009) 1004−1020.

11. F. Zhang, Matrix Theory, Basic Results and Techniques, Springer-Verlag New York Inc, 1991.

Iranian J. Math. Chem. 8(3) September (2017) 299 − 311

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

On the Second Order First Zagreb Index

B. BASAVANAGOUD[1], S. PATIL[1] AND H. DENG[2,•]

[1]Department of Mathematics, Karnatak University, Dharwad − 580 003, Karnataka, India

[2]Key Laboratoryof High Performance Computing and Stochastic Information Processing, College of Mathematics and Computer Science, Hunan Normal University, Changsha, Hunan, 410081, P. R. China

ARTICLE INFO

Article History:

Received: 24 April 2017
Accepted: 28 August 2017
Published online 31 August 2017
Academic Editor: Bo Zhou

Keywords:

Topological index
Line graph
Subdivision graph
Nanostructure
Tadpole graph

ABSTRACT

Inspired by the chemical applications of higher-order connectivity index (or Randic′ index), we consider here the higher-order first Zagreb index of a molecular graph. In this paper, we study the linear regression analysis of the second order first Zagreb index with the entropy and acentric factor of an octane isomers. The linear model, based on the second order first Zagreb index, is better than models corresponding to the first Zagreb index and F-index. Further, we compute the second order first Zagreb index of line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$, tadpole graphs, wheel graphs and ladder graphs.

1. INTRODUCTION

Let $G = (V, E)$ be a simple (molecular) graph. The number of vertices and edges of G are denoted by n and m, respectively. As usual n is said to be the order and m the size of G. The degree of a vertex $v \in V(G)$, denoted by $d_G(v)$, is the number of vertices adjacent to v in G, and $s_G(v) = \sum_{u \in N_G(v)} d_G(u)$, where $N_G(v) = \{u | uv \in E(G)\}$ is the set of neighbor vertices of v in G. Let $E_\alpha(G)$ be the set of all paths of length α in G and clearly $E_1(G) = E(G)$. If all the vertices of G have same degree equal to r, then G is called a r-regular graph. The tadpole graph $T_{n,k}$ is a graph of order $n + k$ obtained by joining an end of a path of length k to a vertex of a cycle graph C_n [34].

•Corresponding Author (Email address: hydeng@hunnu.edu.cn)
DOI: 10.22052/ijmc.2017.83138.1284

The join $G + H$ of graphs G and H is a graph with the vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H) \cup \{uv | u \in V(G)$ and $v \in V(H)\}$. The join $C_n + K_1$ of a cycle C_n and a single vertex is referred to as a wheel graph W_{n+1} of order $n + 1$. The Cartesian product $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a, x)(b, y)$ is an edge of $G \times H$ if and only if $[a = b$ and $xy \in E(H)]$ or $[x = y$ and $ab \in E(G)]$. The ladder graph L_n is given by $L_n = K_2 \times P_n$, where P_n is a path of order n. The subdivision graph $S(G)$ [14] of a graph G is the graph obtained from G by replacing each of its edges by a path of length 2. The line graph $L(G)$ of a graph G [14] is the graph whose vertex set is $E(G)$ in which two vertices are adjacent if and only if they share a common vertex in G. We refer to [14] for unexplained graph theoretic terminology and notation.

Chemical graph theory is a branch of mathematics which combines graph theory and chemistry. Graph theory is used to mathematically model molecules in order to gain insight into the physical properties of these chemical compounds. The basic idea of chemical graph theory is that physico-chemical properties of molecules can be studied by using the information encoded in their corresponding chemical graphs. A graph invariant is any function on a graph that does not depend on a labeling of its vertices. Such quantities are called topological indices. The Zagreb indices have been introduced in 1972 in the report of Gutman and Trinajstić on the topological basis of the π-electron energy-two terms appeared in the topological formula for the total π-energy of alternate hydrocarbons, which were in 1975 used by Gutman et al. as branching indices, and later employed as molecular descriptors in QSAR and QSPR. The first Zagreb index M_1 and second Zagreb index M_2 of a graph G are defined as

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2 \text{ and } M_2(G) = \sum_{uv \in E_1(G)} d_G(u) d_G(v).$$

The first Zagreb index can be written also as

$$M_1(G) = \sum_{uv \in E_1(G)} [d_G(u) + d_G(v)]. \quad (1.1)$$

Another vertex-degree-based graph invariant

$$F(G) = \sum_{v \in V(G)} d_G(v)^3$$

was encountered in [13] and also called F-index [12].

The connectivity index (or Randić index) of a graph G, denoted by $\chi(G)$, was introduced by Randić [31] in the study of branching properties of alkanes. It is defined as

$$\chi(G) = \sum_{uv \in E_1(G)} \frac{1}{\sqrt{d_G(u) d_G(v)}} \quad (1.2)$$

In [16, 17], with the intention of extending the applicability of the connectivity index, Kier, Hall, Murray and Randic′ considered the higher-order connectivity index of a graph G as

$${}^{\alpha}\chi(G) = \sum_{u_1 u_2 \cdots u_{\alpha+1} \in E_\alpha(G)} \frac{1}{\sqrt{d_G(u_1) d_G(u_2) \cdots d_G(u_{\alpha+1})}} \quad (1.3)$$

It has found numerous applications [6, 18, 19, 22, 23, 24, 25, 26, 35, 36]. Results related to the mathematical properties of this index have been reported in [27, 28].

Bearing in mind Eqs. (1.2) and (1.3), we can consider the higher-order first Zagreb index of Eq. (1.1) as

$$ {}^{\alpha}M_1(G) = \sum_{u_1u_2\cdots u_{\alpha+1}\in E_\alpha(G)} [d_G(u_1) + d_G(u_2) + \cdots + d_G(u_{\alpha+1})] \quad (1.4)$$

By Eq. (1.4), it is consistent to define the second order first Zagreb index as

$$ {}^{2}M_1(G) = \sum_{u_1u_2u_3\in E_2(G)} [d_G(u_1) + d_G(u_2) + d_G(u_3)]. \quad (1.5)$$

The present paper is organized as follows: In Section 2, we study the chemical applicability of the second order first Zagreb index. In Section 3, we establish some basic results on ${}^{2}M_1$ which are useful in later sections. In Sections 4, we obtain explicit formula for computing the second order first Zagreb index of line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$, tadpole graphs, wheel graphs and ladder graphs.

2. On the Chemical Applicability of the Second Order First Zagreb Index

In this section, we will discuss the regression analysis of entropy (S) and acentric factor (AcentFac) of an octane isomers on the degree based topological indices of the corresponding molecular graph. The productivity of the second order first Zagreb index was tested by using a data set of octane isomers, that can be found at http://www.moleculardiscriptors.eu/dataset.htm, it is shown that the second order first Zagreb index is highly correlated with the entropy (R = 0.961093128) and also with acentric factor (R = 0.990202) of octane isomers. The data set of octane isomers (columns 1-3 and 5 of Table 1) are taken from above web link whereas last column taken form [5], and the fourth column of Table 1 is computed by Eq. (1.5).

The linear regression models for the entropy and acentric factor of Table 1 are obtained by using the least squares fitting procedure as implemented in R software [2]. More details about the linear regression can be found in [33]. The fitted models are:

$$S = 123.14880(\pm 1.30984) - 0.31608(\pm 0.02271)^2M_1 \quad (2.1)$$

$$S = 150.8878(\pm 3.5756) - 1.4722(\pm 0.1153)M_1 \quad (2.2)$$

$$S = 122.31091(\pm 1.38791) - 0.20607(\pm 0.01643)F \quad (2.3)$$

$$AcentFac = 0.4792(\pm 0.005195) - 0.002555(\pm 0.00009006)^2M_1 \quad (2.4)$$

$$AcentFac = 0.6996325(\pm 0.0216422) - 0.0117797(\pm 0.0006977)M_1 \quad (2.5)$$

$$AcentFac = 0.4700828(\pm 0.0093940) - 0.0016380(\pm 0.0001112)F \quad (2.6)$$

where the values in the brackets of Eqs. (2.1) to (2.6) are the corresponding standard errors of the regression coefficients (intercept and slope).

Tables 2 and 3 show that, the correlation coefficient (R = 0.961093128 and R = 0.990202) of the experimental entropy and acentric factor of an octane isomers with

second order first Zagreb index in the models (2.1) and (2.4) are better than in the models (2.2), (2.3) and (2.5), (2.6), respectively, also the model (2.1) is better than the model related to entropy of octane isomers on Sanskruti index ($R = 0.829$ and residual standard error is 17.837) [15].

Table 1: Experimental values of the entropy, acentric factor and the corresponding values of degree based topological indices of octane isomers.

Alkane	S	AcentFac	$^2M_1$	M_1	F
n-octane	111.67	0.397898	34	26	50
2-methyl-heptane	109.84	0.377916	41	28	62
3-methyl-heptane	111.26	0.371002	43	28	62
4-methyl-heptane	109.32	0.371504	43	28	62
3-ethyl-hexane	109.43	0.362472	45	28	62
2,2-dimethyl-hexane	103.42	0.339426	58	32	92
2,3-dimethyl-hexane	108.02	0.348247	52	30	74
2,4-dimethyl-hexane	106.98	0.344223	50	30	74
2,5-dimethyl-hexane	105.72	0.35683	48	30	74
3,3-dimethyl-hexane	104.74	0.322596	62	32	92
3,4-dimethyl-hexane	106.59	0.340345	54	30	74
2-methyl-3-ethyl-pentane	106.06	0.332433	54	30	74
3-methyl-3-ethyl-pentane	101.48	0.306899	66	32	92
2,2,3-trimethyl-pentane	101.31	0.300816	71	34	104
2,2,4-trimethyl-pentane	104.09	0.30537	65	34	104
2,3,3-trimethyl-pentane	102.06	0.293177	73	34	104
2,3,4-trimethyl-pentane	102.39	0.317422	61	32	86
2,2,3,3-tetramethylbutane	93.06	0.255294	90	38	134

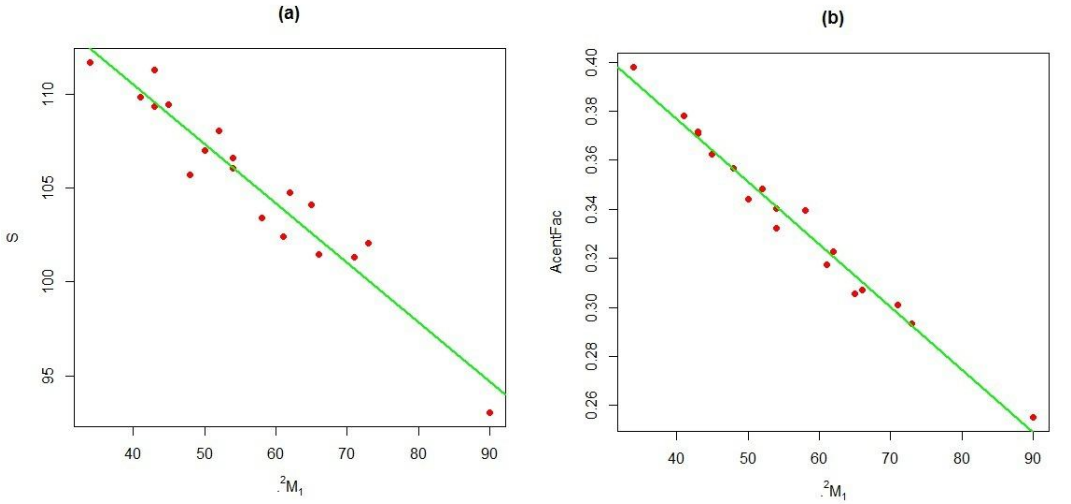


Figure 1: Scatter diagram of (a) S on $^2M_1$; (b) $AcentFac$ on $^2M_1$, superimposed by the fitted regression line.

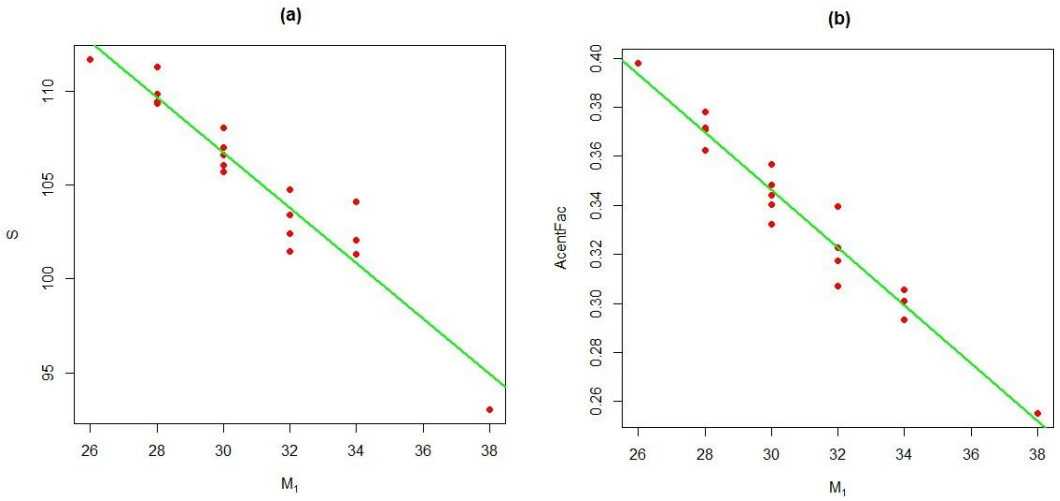


Figure 2: Scatter diagram of (a) S on M_1; (b) $AcentFac$ on M_1, superimposed by the fitted regression line.

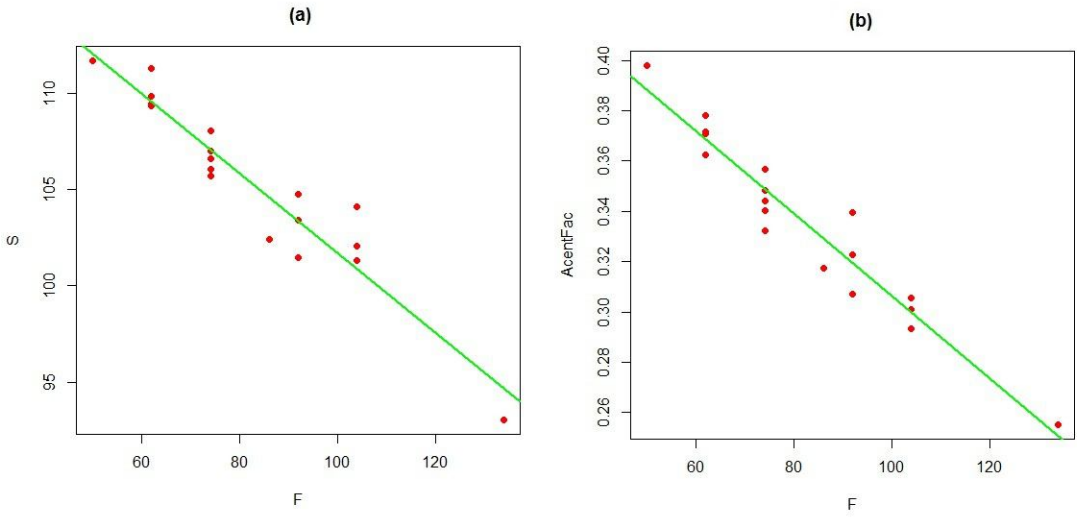


Figure 3: Scatter diagram of (a) S on F; (b) $AcentFac$ on F, superimposed by the fitted regression line.

Table 2: Correlation coefficient and residual standard error of regression model.

Index	Correlation coefficient (R) with entropy	Residual standard error
${}^2M_1$	0.961093128	1.286
M_1	0.954306031	1.392
F	0.952732911	1.415

Table 3: Correlation coefficient and residual standard error of regression model

Index	Correlation coefficient (R) with acentric fac	Residual standard error
${}^2M_1$	0.990202	0.005101
M_1	0.973087869	0.008424
F	0.965038859	0.009577

3. MATHEMATICAL PROPERTIES FOR THE SECOND ORDER FIRST ZAGREB INDEX OF A GRAPH

In this section, we will establish some basic results on ${}^2M_1$ which are useful in later sections.

Theorem 3.1 *For a graph* $G = (V, E)$,

$$ {}^2M_1(G) = 2M_2(G) + \frac{1}{2}F(G) - \frac{3}{2}M_1(G). \tag{3.1}$$

Proof. By Eq. (1.5), we have

$$\begin{aligned} {}^2M_1(G) &= \sum_{uvw \in E_2(G)} (d_G(u) + d_G(v) + d_G(w)) \\ &= \sum_{v \in V(G)} \sum_{u \neq w \in N_G(v)} (d_G(u) + d_G(v) + d_G(w)). \end{aligned}$$

In $\sum_{u \neq w \in N_G(v)} (d_G(u) + d_G(v) + d_G(w))$, the quantity $d_G(v)$ appears $\binom{d_G(v)}{2} = \frac{d_G(v)(d_G(v)-1)}{2}$ times, and each quantity $d_G(u)$ of $\{d_G(u) | u \in N_G(v)\}$ appears $(d_G(v) - 1)$ times, i.e., the quantity $s_G(v) = \sum_{u \in N_G(v)} d_G(u)$ appears $(d_G(v) - 1)$ times. So,

$$\begin{aligned} {}^2M_1(G) &= \sum_{v \in V(G)} \sum_{u \neq w \in N_G(v)} (d_G(u) + d_G(v) + d_G(w)) \\ &= \sum_{v \in V(G)} \left[\frac{d_G(v)(d_G(v)-1)}{2} d_G(v) + (d_G(v) - 1)s_G(v)\right] \\ &= \frac{1}{2}\left[\sum_{v \in V(G)} d_G^3(v) - \sum_v d_G^2(v)\right] + \sum_v d_G(v)s_G(v) - \sum_v s_G(v) \\ &= \frac{1}{2}[F(G) - M_1(G)] + 2\sum_{uv \in E(G)} d(u)d(v) - \sum_{v \in V(G)} d^2(v) \\ &= \frac{1}{2}F(G) - \frac{1}{2}M_1(G) + 2M_2(G) - M_1(G) \\ &= 2M_2(G) + \frac{1}{2}F(G) - \frac{3}{2}M_1(G). \end{aligned}$$

Theorem 3.1 shows that the second order first Zagreb index ${}^2M_1$ is a linear combination of the first Zagreb index M_1, the second Zagreb index M_2 and the F-index F. For the path P_n, the wheel W_{n+1} $(n \geq 3)$ and the complete bipartite graph $K_{r,s}$, we have

$$\begin{gathered} F(P_n) = 8n - 14, M_1(P_n) = 4n - 6, M_2(P_n) = 4n - 8; \\ F(W_{n+1}) = n^3 + 27n, M_1(W_{n+1}) = n^2 + 9n, M_2(W_{n+1}) = 3n^2 + 9n; \\ F(K_{r,s}) = rs(r^2 + s^2), M_1(K_{r,s}) = rs(r + s), M_2(K_{r,s}) = r^2s^2. \end{gathered}$$

By Eq. (3.1) in Theorem 3.1, we can get the following result.

Corollary 3.2 *For* $n \geq 3$, $^2M_1(P_n) = 6n - 14$.

Corollary 3.3 *For* $n \geq 3$, $^2M_1(W_{n+1}) = \frac{1}{2}[n^3 + 9n^2 + 36n]$.

Corollary 3.4 $^2M_1(K_{r,s}) = \frac{rs}{2}[r^2 + s^2 + 4rs - 3r - 3s]$.

Theorem 3.5 *Let* G *be a* r*-regular graph on* n *vertices. Then* $^2M_1(G) = \frac{3n}{2}[r^3 - r^2]$.

Proof. Since G is a r-regular graph, $M_1(G) = nr^2$, $F(G) = nr^3$ and $M_2(G) = \frac{r^3n}{2}$. Hence, by Theorem 3.1, we get the desired result.

Corollary 3.6 *For the cycle* C_n *on* $n \geq 3$ *vertices,* $^2M_1(C_n) = 6n$.

Corollary 3.7 *For the complete graph* K_n *on* $n \geq 3$ *vertices,* $^2M_1(K_n) = \frac{3n(n-2)(n-1)^2}{2}$.

Lemma 3.8 [3] *Let* G *be a graph with* n *vertices and* m *edges. Then*

$$M_1(G) \leq m(\frac{2m}{n-1} + n - 2). \tag{3.2}$$

Lemma 3.9 [4] *Let* G *be a graph with* n *vertices and* m *edges,* $m > 0$. *Then the equality*

$$M_1(G) = m\left(\frac{2m}{n-1} + n - 2\right)$$

holds if and only if G is isomorphic to the star graph S_n or K_n or $K_{n-1} \cup K_1$.

Theorem 3.10 *Let* G *be a graph with* n *vertices and* m *edges. Then*

$$^2M_1(G) \leq 3m(n-1)(\frac{m}{n-1} + \frac{n-4}{2}) \tag{3.3}$$

with equality if and only if G is isomorphic to K_n.

Proof.

$$\begin{aligned} ^2M_1(G) &= \sum_{uvw \in E_2(G)} [d_G(u) + d_G(v) + d_G(w)] \\ &\leq \sum_{uvw \in E_2(G)} 3(n-1) \qquad (3.4) \\ &= 3(n-1)\sum_{v \in V(G)} \binom{d_G(v)}{2} = 3(n-1)(-m + \frac{1}{2}M_1(G)) \\ &\leq 3(n-1)(-m + \frac{1}{2}m(\frac{2m}{n-1} + n - 2)) \qquad (3.5) \\ &= 3m(n-1)\left(\frac{m}{n-1} + \frac{n-4}{2}\right). \end{aligned}$$

The relations (3.4) and (3.5) were obtained by taking into account $d_G(v) \leq n-1$ for each vertex $v \in V(G)$ and Eq. (3.2), respectively. The equality in (3.3) holds if and only if the equalities in (3.4) and (3.5) hold, if and only if $d_G(v) \leq n-1$ for each vertex $v \in V(G)$, i.e., G is a complete graph from Lemma 3.9.

Lemma 3.11 [4] *Let G be a graph with n vertices and m edges. Then*

$$M_1(G) \geq 2m(2p+1) - pn(1+p), \text{ where } p = \left\lfloor \frac{2m}{n} \right\rfloor,$$

and the equality holds if and only if the difference of the degrees of any two vertices of graph G is at most one.

Theorem 3.12 *Let G be a graph with n vertices, m edges and the minimum vertex degree δ. Then*

$$^2M_1(G) \geq \frac{3\delta}{2}(4mp - pn(p+1)), \text{ where} p = \left\lfloor \frac{2m}{n} \right\rfloor, \tag{3.6}$$

and the equality holds if and only if G is a regular graph.

Proof.

$$\begin{aligned} ^2M_1(G) &= \sum_{uvw \in E_2(G)} [d_G(u) + d_G(v) + d_G(w)] \\ &\geq \sum_{uvw \in E_2(G)} 3\delta \qquad (3.7) \\ &= 3\delta(-m + \tfrac{1}{2}M_1(G)) \\ &\geq 3\delta(-m + \tfrac{1}{2}(2m(2p+1) - pn(1+p))) \qquad (3.8) \\ &= \tfrac{3\delta}{2}(4mp - pn(p+1)). \end{aligned}$$

The relations (3.7) and (3.8) were obtained by taking into account $d_G(v) \geq \delta$ for each vertex $v \in V(G)$ and Lemma 3.11, respectively. The equality in (3.6) holds if and only if the equalities (3.7) and (3.8) hold, i.e., $d_G(v) \geq \delta$ for each vertex $v \in V(G)$ and G is a regular graph from Lemma 3.11.

4. THE SECOND ORDER FIRST ZAGREB INDICES OF SPECIAL FAMILIES OF GRAPH

Let p and q denote the number of squares in a row and the number of rows of squares, respectively in the $2D$-lattice, nanotube and nanotours of $TUC_4C_8[p,q]$, see Figure 3 (a), (b) and (c), where $p = 4$ and $q = 3$. In [29, 30], Ranjini et al. presented explicit formulas for computing the Shultz index and Zagreb indices of the subdivision graphs of the tadpole $T_{n,k}$, the wheel W_n and the ladder graph L_n. In 2015, Su and Xu [32] calculated the general sum-connectivity index and co-index of the $L(S(T_{n,k}))$, $L(S(W_n))$ and $L(S(L_n))$. In [20], Nadeem et al. derived some exact formulas for computing ABC_4 and GA_5 indices of the

line graphs of the tadpole $T_{n,k}$, the wheel W_n and the ladder graph L_n by using the notion of subdivision. Recently, authors in [1, 15, 21] obtained the expressions for certain topological indices of line graphs of subdivision graphs of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p, q]$. For more information on nanostructures, we refer the articles [7, 8, 9, 10, 11].

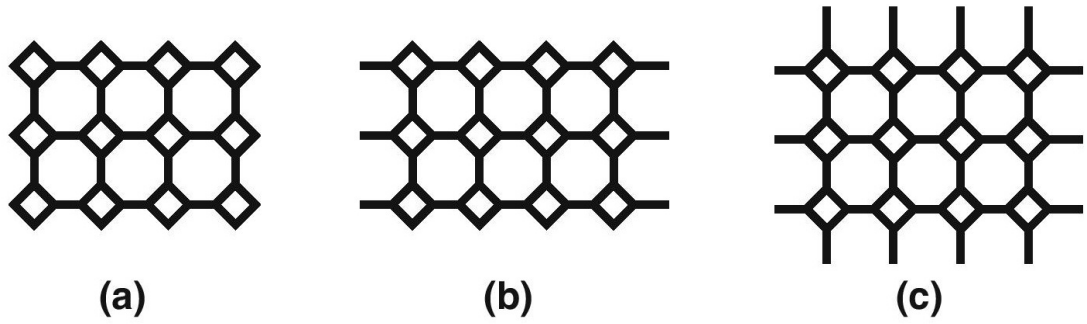


Figure 4: (a) 2D-lattice of $TUC_4C_8[4,3]$; (b) $TUC_4C_8[4,3]$ nanotube; (c) $TUC_4C_8[4,3]$ nanotorus.

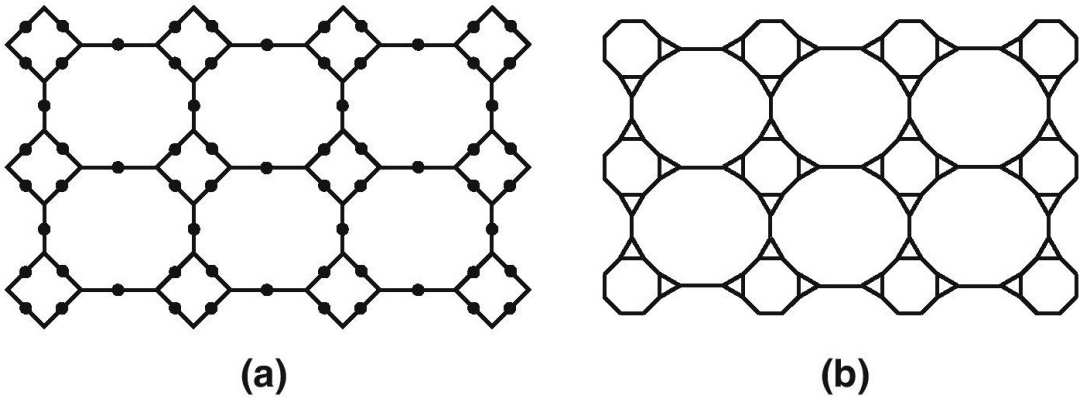


Figure 5: (a) Subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$; (b) line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$.

Lemma 4.1 [21] *Let A be the line graph of the subdivision graph of $2D$-lattice of $TUC_4C_8[p, q]$. Then $M_1(A) = 108pq - 38p - 38q$, $F(A) = 324pq - 130p - 130q$ and $M_2(A) = 162pq - 67(p + q) + 4$.*

From Lemma 4.1 and Theorem 3.1, we can immediately get the following result.

Theorem 4.2 *Let A be the line graph of the subdivision graph of $2D$-lattice of $TUC_4C_8[p, q]$. Then* $^2M_1(A) = 324pq - 142p - 142q + 8$.

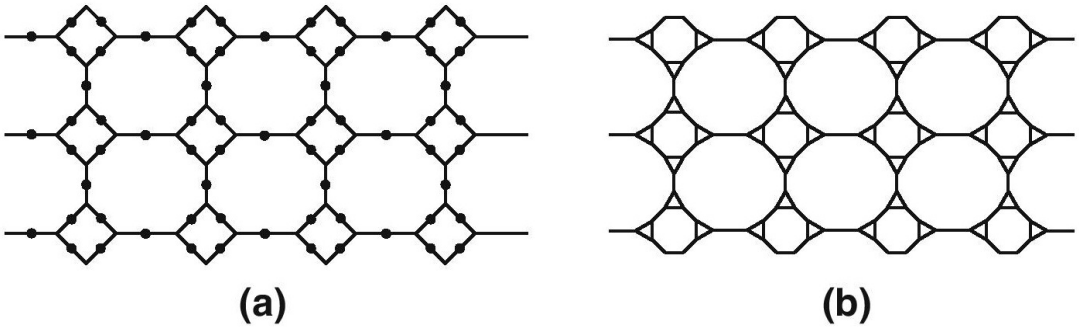


Figure 6: (a) Subdivision graph of $TUC_4C_8[4,3]$ of nanotube; (b) line graph of the subdivision graph of $TUC_4C_8[4,3]$ of nanotube.

Lemma 4.3 [21] *Let B be the line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotube. Then $M_1(B) = 108pq - 38p$, $F(B) = 324pq - 130p$ and $M_2(B) = 162pq - 67p$.*

The following result is immediate from Lemma 4.3 and Theorem 3.1.

Theorem 4.4 *Let B be the line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotube. Then $^2M_1(B) = 324pq - 142p$.*

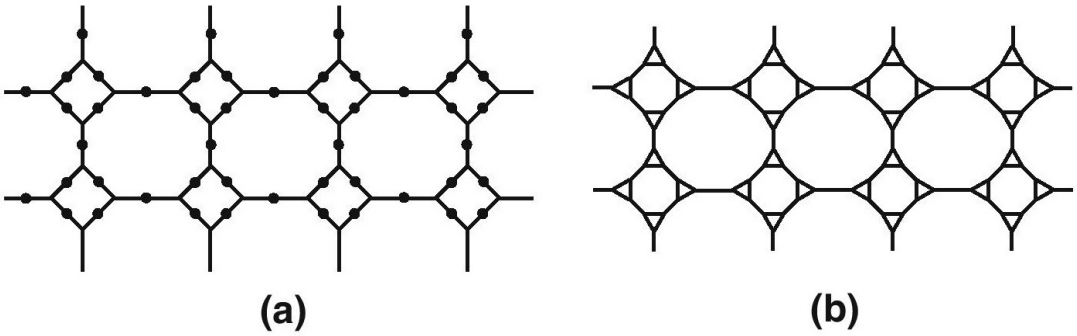


Figure 7: (a) Subdivision graph of $TUC_4C_8[4,3]$ of nanotorus; (b) line graph of the subdivision graph of $TUC_4C_8[4,3]$ of nanotorus.

Theorem 4.5 *Let C be the line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotorus. Then $^2M_1(C) = 324pq$.*

Proof. The subdivision graph of $TUC_4C_8[p,q]$ nanotorus and the graph C are shown in Figure 6 (a) and (b). The graph C is 3-regular with $12pq$ vertices. By Theorem 3.5, we get required result.

Lemma 4.6 [30, 32] (*i*) *Let X be the line graph of the subdivision graph of the tadpole graph $T_{n,k}$. Then $M_1(X) = 8n + 8k + 12$, $F(X) = 16n + 16k + 50$ and $M_2(X) = 8n + 8k + 23$.*

(*ii*) *Let Y be the line graph of the subdivision graph of the wheel graph with order $n + 1$. Then $M_1(Y) = n^3 + 27n$, $F(Y) = n^4 + 81n$ and $M_2(Y) = n(\frac{n^3-n^2+6n+72}{2})$.*

(*iii*) *Let Z be the line graph of subdivision graph of a ladder graph with order n. Then $M_1(Z) = 54n - 76$, $F(Z) = 162n - 260$ and $M_2(Z) = 81n - 132$.*

From Lemma 4.6 and Theorem 3.1, we can immediately get the following result.

Theorem 4.7 (*i*) *Let X be the line graph of the subdivision graph of the tadpole graph $T_{n,k}$. Then* $^2M_1(X) = 12n + 12k + 53$.

(*ii*) *Let Y be the line graph of the subdivision graph of the wheel graph with order $n + 1$. Then* $^2M_1(Y) = \frac{n}{2}(3n^3 - 5n^2 + 12n + 144)$.

(*iii*) *Let Z be the line graph of subdivision graph of a ladder graph with order n. Then* $^2M_1(Z) = 162n - 280$.

ACKNOWLEDGEMENT. This research was supported by UGC–SAP DRS–III, New Delhi, India for 2016–2021: F.510/3/DRS–III/2016(SAP–I) Dated: 29^{th} Feb. 2016.

REFERENCES

[1] A. R. Ashrafi, S. Yousefi, Computing Wiener index of a $TUC_4C_8(S)$ nanotorus, *MATCH Commun. Math. Comput. Chem.***57** (2007) 403–410.

[2] R Core Team, R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria. (2016) URL: https://www.R-project.org/.

[3] D. de Caen, An upper bound on the sum of squares of degrees in a graph, *Discrete Math.* **185** (1998) 245–248.

[4] K. C. Das, Sharp bounds for the sum of the squares of the degrees of a graph, *Kragujevac J. Math.* **25** (2003) 31–49.

[5] N. De, S. M. A. Nayeem, A. Pal, The F-coindex of some graph operations, *Springer Plus* (2016) 5:221, doi: 10.1186/s40064-016-1864-7.

[6] H. Deng, Catacondensed Benzenoids and Phenylenes with the extremal third–order Randić index, *MATCH Commun. Math. Comput. Chem.***64** (2010) 471– 496.

[7] M. V. Diudea, E. C. Kirby, The energetic stability of tori and single wall tubes,

Fuller. Sci. Technol. **9** (2001) 445–465.

[8] M. V. Diudea, Graphenes from 4-valent tori, *Bull. Chem. Soc. Jpn.* **75** (2002) 487–492.

[9] M. V. Diudea, Hosoya polynomial in tori, *MATCH Commun. Math. Comput. Chem.* **45** (2002) 109–122.

[10] M. V. Diudea, B. Parv, E. C. Kirby, Azulenic tori, *MATCH Commun. Math. Comput. Chem.* **47** (2003) 53–70.

[11] M. V. Diudea, M. Stefu, B. Prv, P. E. John, Wiener index of armchair polyhex nanotubes, *Croat. Chem. Acta* **77** (12) (2004) 111–115.

[12] B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190.

[13] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[14] F. Harary, *Graph Theory*, Addison-Wesley, Reading, Mass., 1969.

[15] S. M. Hosamani, Computing Sanskruti index of certain nanostructures, *J. Appl. Math. Comput.* **54** (1−2) (2017) 425–433.

[16] L. B. Kier, L. H. Hall, *Molecular Connectivity in Chemistry and Drug Research*, Academic Press, New York, 1976.

[17] L. B. Kier, L. H. Hall, W. J. Murray, M. Randić, Molecular connectivity V: connectivity series concept applied to density, *J. Pharm. Sci.* **65** (1976) 1226–1230.

[18] A. Miličević, S. Nikolić, On variable Zagreb indices, *Croat. Chem. Acta* **77** (1−2) (2004) 97–101.

[19] A. Miličević, N. Raos, Estimation of stability of coordination compounds by using topological indices, *Polyhedron* **25** (14) (2006) 2800–2808.

[20] M. F. Nadeem, S. Zafar, Z. Zahid, On certain topological indices of the line graph of subdivision graphs, *Appl. Math. Comput.* **271** (2015) 790–794.

[21] M. F. Nadeem, S. Zafar, Z. Zahid, On topological properties of the line graphs of subdivision graphs of certain nanostructures, *Appl. Math. Comput.* **273** (2016) 125–130.

[22] S. Nikolić, N. Trinajstić, S. Ivaniš, The connectivity indices of regular graphs, *Croat. Chem. Acta* **72** (4) (1999) 875–883.

[23] S. Nikolić, N. Raos, Estimation of stablity constants of mixed amino acid complexes with copper (II) from topological indices, *Croat. Chem. Acta* **74** (2001) 621–631.

[24] L. Pogliani, Molecular modeling by linear combinations of connectivity indices, *J. Phys. Chem.* **99** (3) (1995) 925–937.

[25] L. Pogliani, A strategy for molecular modeling of a physicochemical property using a linear combination of connectivity indexes, *Croat. Chem. Acta* **69** (1) (1996) 95–109.

[26] L. Pogliani, Higher-level descriptor in molecular connectivity, *Croat. Chem. Acta* **75**

(2) (2002) 409–432.

[27] J. Rada, O. Araujo, I. Gutman, Randić index of benzenoid systems and phenylenes, *Croat. Chem. Acta* **74** (2001) 225–235.

[28] J. Rada, O. Araujo, Higher order connectivity indices of starlike trees, *Discrete Appl. Math.* **119** (2002) 287–295.

[29] P. S. Ranjini, V. Lokesha, M. A. Rajan, On the Shultz index of the subdivision graphs, *Adv. Stud. Contemp. Math.* **21** (3) (2011) 279–290.

[30] P. S. Ranjini, V. Lokesha, I. N. Cangül, On the Zagreb indices of the line graphs of the subdivision graphs, *Appl. Math. Comput.* **218** (2011) 699–702.

[31] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.

[32] G. Su, L. Xu, Topological indices of the line graph of subdivision graphs and their Schur-bounds, *Appl. Math. Comput.* **253** (2015) 395–401.

[33] P. Tattar, S. Ramaiah, B. G. Manjunath, A Course in Statistics with R, John Wiley & Sons, Ltd., 2016.

[34] E. W. Weisstein, Tadpole graph, From Matheworld-A Wolfram Web Resource.

[35] J. Zhang, H. Deng, S. Chen, Second order Randic′ index of phenylenes and their corresponding hexagonal squeezes, *J. Math. Chem.* **42** (4) (2007) 941–947.

[36] J. Zhang, H. Deng, Third order Randić index of phenylenes, *J. Math. Chem.* **43** (1) (2008) 12–18.

Iranian J. Math. Chem. 8(3) September (2017) 313 – 325

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

Anti–Forcing Number of Some Specific Graphs

SAEID ALIKHANI• AND NEDA SOLTANI

Department of Mathematics, Yazd University, 89195–741, Yazd, Iran

ARTICLE INFO

Article History:

Received 9 September 2016
Accepted 14 March 2017
Published online 31 August 2017
Academic Editor: Gholam Hossein Fath–Tabar

Keywords:

Anti–forcing number
Anti–forcing set
Corona product

ABSTRACT

Let G be a simple connected graph. A perfect matching (or Kekulé structure in chemical language) of G is a set of disjoint edges which covers all vertices of G. The anti–forcing number of G is the smallest number of edges such that the remaining graph obtained by deleting these edges has a unique perfect matching and is denoted by $af(G)$. In this paper we consider some specific graphs that are of importance in chemistry and study their anti–forcing numbers.

1. INTRODUCTION

All graphs considered in this paper are undirected and simple. Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. A perfect matching or 1–factor (or Kekulé structure in chemical literature) of G is a set of disjoint edges which covers all vertices of G. Perfect matching has many practical applications, such as in dimer problem of statistical physics, Kekulé structures in organic chemistry and personnel assignment of operations research, etc. For more details on perfect matching, we refer the reader to see [8].

In 2007, Vukičević and Trinajstić [9,10] introduced the anti–forcing number of a graph G with perfect matching M. A set $S \subseteq M$ is called a forcing set of M if S cannot be contained in another perfect matching of G other than M. The forcing number (or innate degree of freedom) of M is defined as the minimum size of all forcing sets of M, denoted by $f(G,M)$ [5, 6]. The minimum forcing number of G is the minimum value of the

•Corresponding Author (Email address: alikhani@yazd.ac.ir)
DOI: 10.22052/ijmc.2017.60978.1235

forcing numbers of all perfect matchings of G, denoted by $f(G)$. Zhang et al. [11] proved that the minimum forcing number of fullerenes has a lower bound three and there are infinitely many fullerenes achieving this bound. For $S \subseteq E(G)$, let $G-S$ denote the graph obtained by removing S from G. Then S is called an anti–forcing set if $G-S$ has a unique perfect matching. The cardinality of a smallest anti–forcing set is called the anti–forcing number of G, denoted by $af(G)$. An edge e of G is called an anti–forcing edge if $G-e$ has a unique perfect matching. Note that $af(G) = |E(G)|$ if and only if G does not have any perfect matching. A graph G is called odd or even graph, if the number of vertices of G is odd or even, respectively.

Recently, Lei et al. [7] defined the anti–forcing number of a perfect matching M of a graph G as the minimal number of edges not in M whose removal to make M as a single perfect matching of the resulting graph, denoted by $af(G,M)$. By this definition, the anti–forcing number of a graph G is the smallest anti–forcing number over all perfect matchings of G.

In the next section, after computing the anti–forcing number of some specific graphs, the anti–forcing number of the link and the chain of graphs are discussed. Also we study the anti–forcing number of chain triangular cactus and chain square cactus as a special kind of the chain of graphs that are of importance in chemistry. In Section 3, we consider two graph operations, the join and the corona of two graphs and obtain some relations between the anti–forcing number of two graphs G_1 and G_2 and the anti–forcing number of the join and the corona of them under some suitable assumptions. Finally, in Section 4, we compute the anti–forcing number of some dendrimers.

2. ANTI–FORCING NUMBER OF SPECIFIC GRAPHS

In this section, we shall compute the anti–forcing number of some specific graphs. First we consider some certain graphs such as paths, cycles, wheels, friendship and Dutch–windmill graphs. The following example gives the anti–forcing number of path, cycle and wheel graphs.

Example 2.1 Let P_n, C_n and W_n be a path, cycle and wheel of order n, respectively. We have

$$af(P_n) = \begin{cases} n-1 & 2 \nmid n \\ 0 & 2 \mid n \end{cases}, af(C_n) = \begin{cases} n & 2 \nmid n \\ 1 & 2 \mid n \end{cases} \text{ and } af(W_n) = \begin{cases} 2(n-1) & 2 \nmid n \\ 2 & 2 \mid n \end{cases}.$$

As another specific graph, we consider friendship graph F_n which is a graph that can be constructed by coalescence n copies of the cycle graph C_3 with a common vertex. It is obvious that this graph does not have any perfect matching and so

$af(F_n) = |E(F_n)| = 3n$. For the stars graphs $K_{1,n}$ there is no perfect matching, thus $af(S_n) = n$, for $n \geq 2$ and $af(K_{1,1}) = 0$. Also for the n–book graph B_n which can be constructed by joining n copies of the cycle graph C_4 with a common edge $\{u,v\}$, $af(B_n) = 1$.

Let $Wd(k,n)$ be an undirected graph, constructed for $k \geq 2$ and $n \geq 2$ by joining n copies of the complete graph K_k at a shared vertex. We have $|V(G)| = (k-1)n+1$, $|E(G)| = 1/2kn(k-1)$ (see [4]). We have the following theorem for the anti–forcing number of $Wd(k,n)$.

Theorem 2.2 $af(Wd(k,n)) = \frac{1}{2}kn(k-1)$.

Proof. Suppose that n is even. Obviously, for every k, $Wd(k,n)$ is an odd graph and so the graph does not have any perfect matching. It implies that for every k, $af(Wd(k,n)) = 1/2kn(k-1)$. Now assume that n is odd, then for odd k, the order of $Wd(k,n)$ is odd too and hence the graph does not have any perfect matching. For even k, using Tutte's Theorem we have the same result. So we can conclude that $af(Wd(k,n)) = 1/2kn(k-1)$. ■

Here, we consider some graphs with specific construction that are of importance in chemistry and study their anti–forcing number. First we define the link of graphs.

Definition 2.3 [3] Let G_1, G_2, ..., G_k be a finite sequence of pairwise disjoint connected graphs and let $x_i, y_i \in V(G_i)$. The link G of the graphs $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i, y_i\}_{i=1}^k$ is obtained by joining an edge the vertex y_i of G_i with the vertex x_{i+1} of G_{i+1} for all $i = 1,2, ..., k-1$ (see Figure 1 for $k = 4$).

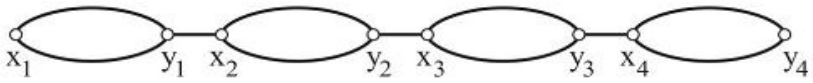


Figure 1: A link of four graphs.

Theorem 2.4 Let $L(G_1, G_2, ..., G_k)$ be the link of k graphs $G_1, G_2, ..., G_k$. If every G_i $(1 \leq i \leq k)$ has perfect matching, then

$$af(L(G_1,G_2,...,G_k)) = \sum_{i=1}^{k} af(G_i).$$

Proof. It sufficies to prove the theorem for $k = 2$. Let G_1 and G_2 be two graphs with perfect matching. Let $x_1 \in V(G_1)$, $x_2 \in V(G_2)$ and $L(G_1,G_2)$ be the link of these two graphs obtained by joining an edge the vertex x_1 with the vertex x_2. Suppose that S_1 and S_2 have the smallest cardinality over all anti–forcing sets of graphs G_1 and G_2, respectively. So $af(G_1) = |S_1|$ and $af(G_2) = |S_2|$. It is obvious that the edge x_1x_2 does not belong to any perfect matching of $L(G_1,G_2)$. So if S has the smallest cardinality over all anti–forcing sets of graph $L(G_1,G_2)$, then $S = S_1 \cup S_2$ and so,

$$af(L(G_1,G_2)) = |S| = |S_1| + |S_2| = af(G_1) + af(G_2),$$

which completes our argument. ■

Note that if there exist $1 \le i \le k$ such that G_i does not have any perfect matching, then Theorem 2.4 is not true. For example, $af(L(P_3,C_4,C_4)) = 12$, but $af(P_3) + 2af(C_4) = 4$. Now, we consider the chain of graphs and study the anti–forcing number of them for different cases.

Definition 2.5 [3] Let $G_1,G_2,...,G_k$ be a finite sequence of pairwise disjoint connected graphs and let $x_i, y_i \in V(G_i)$. The chain G of the graphs $\{G_i\}_{i=1}^{k}$ with respect to the vertices $\{x_i, y_i\}_{i=1}^{k}$ is obtained by identifying the vertex y_i with the vertex x_{i+1} for $1 \le i \le k-1$, see Figure 2 for $k = 4$.

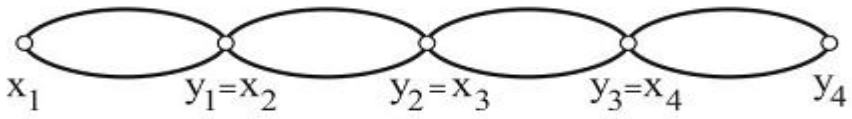


Figure 2: A chain of four graphs.

Theorem 2.6 Let $C(G_1,G_2,...,G_k)$ be the chain of k graphs $G_1,G_2,...,G_k$.

i. If $G_1,G_2,...,G_k$ are odd graphs, then $af(C(G_1,G_2,...,G_k)) = \sum_{i=1}^{k} |E(G_i)|$.

ii. If $G_1,G_2,...,G_k$ are even graphs, then for every even k we have

$$af(C(G_1,G_2,...,G_k)) = \sum_{i=1}^{k} |E(G_i)|.$$

Proof.

i. It can easily verified that $|V(C(G_1,G_2,...,G_k))| = \sum_{i=1}^{k}|V(G_i)| - (k-1)$. Thus in this case, for every k, $C(G_1,G_2,...,G_k)$ is an odd graph and so

$$af(C(G_1,G_2,...,G_k)) = |E(C(G_1,G_2,...,G_k))|.$$

Since $|E(C(G_1,G_2,...,G_k))| = \sum_{i=1}^{k}|E(G_i)|$, we have the result.

ii. It is easy to see that in this case the chain graph $C(G_1,G_2,...,G_k)$ is an odd graph and so we have the result.

Hence the result. ■

Remark 2.7 Theorem 2.6(ii), is not true for odd k. For example, $af(C(P_2,P_4,P_2)) = 0$ and $af(C(P_2,P_4,C_4)) = 1$.

As special cases of chain graphs, we can consider cactus chains. A cactus graph is a connected graph in which no edge lies in more than one cycle. Consequently, each block of a cactus graph is either an edge or a cycle. If all blocks of a cactus G are cycles of the same size k, the cactus is k–uniform. A triangular cactus is a graph whose blocks are triangles, i.e., a 3–uniform cactus. A vertex shared by two or more triangles is called a cut–vertex. If each triangle of a triangular cactus G has at most two cut–vertices, and each cut–vertex is shared by exactly two triangles, we say that G is a chain triangular cactus. The number of triangles in G is called the length of the chain. An example of a chain triangular cactus is shown in Figure 3.

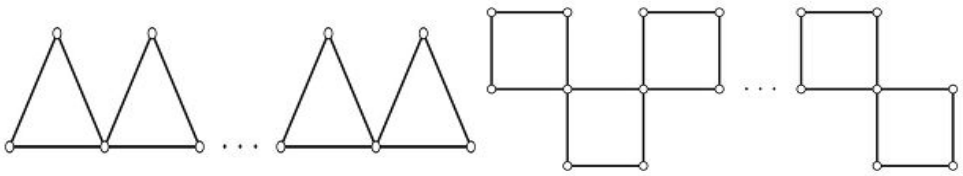


Figure 3: A chain triangular cactus T_n and square cactus O_n, respectively.

Obviously, all chain triangular cactus of the same length are isomorphic. Hence, we denote the chain triangular cactus of length n by T_n. clearly, a chain triangular cactus of length n has $2n+1$ vertices and $3n$ edges [1]. Since T_n does not have any perfect matching, we have $af(T_n) = 3n$.

By replacing triangles in chain triangular chain T_n by cycles of length 4, we obtain cactus whose every block is C_4 as shown in Figure 3. We call such cactus, square cactus and denote a chain square cactus of length n by O_n [1].

Theorem 2.8 Let O_n be a chain square cactus. We have

I. If n is even, then $af(O_n) = 4n$.

II. If n is odd, then $af(O_n) = \frac{n+1}{2}$.

Proof.

I. By Tutte's Theorem, there is no perfect matching for O_n in this case and so $af(O_n) = 4n$.

II. For this case the anti–forcing number of O_n is equal with the anti-forcing number of $L(\underbrace{C_4,...,C_4}_{(\frac{n+1}{2})-times})$. Since $af(C_4) = 1$, so we have the result by Theorem 2.4.

This proves the theorem. ■

3. ANTI–FORCING NUMBER OF SOME OPERATIONS OF GRAPHS

In this section, we shall study the anti–forcing number of some operations of two graphs. First we consider the join of two graphs. The join $G_1 + G_2$ of graphs G_1 and G_2 with disjoint point sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$ is the graph union $G_1 \cup G_2$ together with all the edges joining $V(G_1)$ and $V(G_2)$. The following theorem gives a lower bound for the anti–forcing of join of two graphs.

Theorem 3.1 Let G_1 and G_2 be two simple graphs. Then we have

$$af(G_1 + G_2) \geq af(G_1) + af(G_2).$$

Proof. Suppose that S_1, S_2 and S have the smallest cardinality over all anti–forcing sets of graphs G_1, G_2 and $G_1 + G_2$, respectively. So $af(G_1) = |S_1|$, $af(G_2) = |S_2|$ and $af(G_1 + G_2) = |S|$. By definition of $G_1 + G_2$, $|V(G_1 + G_2)| = |V(G_1)| + |V(G_2)|$ and $|E(G_1 + G_2)| > |E(G_1)| + |E(G_2)|$. Thus for the choosing the perfect matchings of $G_1 + G_2$, we have more possibilities than the number of perfect matching of G_1 plus the number of perfect matchings of G_2. It means that $|S| \geq |S_1| + |S_2|$ and so we have the result. ■

Remark 3.2 The lower bound in Theorem 3.1 is sharp. For example $af(C_3+C_3)=6=af(C_3)+af(C_3)$. Also, if G_1 is an odd graph and G_2 is an even graph, then

$$af(G_1+G_2) > af(G_1)+af(G_2).$$

Because for odd graph G_1, we have $af(G_1)=|E(G_1)|$ and for even graph G_2, $af(G_2)\le|E(G_2)|$. Also G_1+G_2 is an odd graph. So

$$af(G_1+G_2)=|E(G_1+G_2)|>|E(G_1)|+|E(G_2)|\ge af(G_1)+af(G_2).$$

Here, we consider the corona of two graphs and then we study the anti–forcing number of them. We recall that the corona of two graphs G_1 and G_2, written as $G_1\circ G_2$, is the graph obtained by taking one copy of G_1 and $|V(G_1)|$ copies of G_2, and then joining the *i*-th vertex of G_1 to every vertex in the *i*-th copy of G_2.

Theorem 3.3 Let G_1 and G_2 be two simple graphs. If both of G_1 and G_2 have perfect matching, then

$$af(G_1\circ G_2)=af(G_1)+|V(G_1)|\,af(G_2).$$

Proof. Suppose that S_1 and S_2 have the smallest cardinality over all anti–forcing sets of graphs G_1 and G_2, respectively. So $af(G_1)=|S_1|$ and $af(G_2)=|S_2|$. Let $V(G_1)=\{x_1,x_2,...,x_n\}$ and $V(G_2)=\{y_1,y_2,...,y_m\}$. For every $1\le i\le n$ and every $1\le j\le m$, the edge x_iy_j cannot be in the perfect matchings of $G_1\circ G_2$. Let S has the smallest cardinality over all anti–forcing sets of graph $G_1\circ G_2$. Then

$$S=S_1\cup\underbrace{S_2\cup...\cup S_2}_{|V(G_1)|-times}$$

and we have

$$af(G_1\circ G_2)=|S|=|S_1|+|V(G_1)||S_2|=af(G_1)+|V(G_1)|\,af(G_2).$$

This completes the proof. ■

Clearly, If G_1 has a unique perfect matching, then $af(G_1\circ G_2)=|V(G_1)|\,af(G_2)$ and if G_2 has a unique perfect matching, then $af(G_1\circ G_2)=af(G_1)$. For example $af(C_4\circ P_2)=1$ and $af(P_2\circ C_4)=2$.

Now this question comes to mind: what happens to the anti–forcing number of graph G_1oG_2, when at least one of the G_1 or G_2 does not have any perfect matching? It can easily verified that if only G_1 does not have any perfect matching, then the graph G_1oG_2 does not have any perfect matching too and so $af(G_1oG_2)=|E(G_1oG_2)|$. But if G_2 does not have perfect matching, then the anti–forcing number of G_1oG_2 just depends on G_2, because assume that $u\in V(G_1)$ and $(G_2)_u$ be a copy of G_2 such that the vertex u is adjacent to every

vertex of $(G_2)_u$. Since G_2 does not have any perfect matching, then it has at least one unsaturated vertex. Without loss of generality we can suppose that $v \in V((G_2)_u)$ is the unsaturated vertex of $(G_2)_u$. Then $uv \in M$ where M is a maximum matching of graph G_1oG_2. Thus every vertex of G_1 in M is saturated by the edges that connect G_1 with G_2. In the following propositions, we consider the anti–forcing number of G_1oG_2, when G_2 is a path, cycle or wheel of odd order n, respectively.

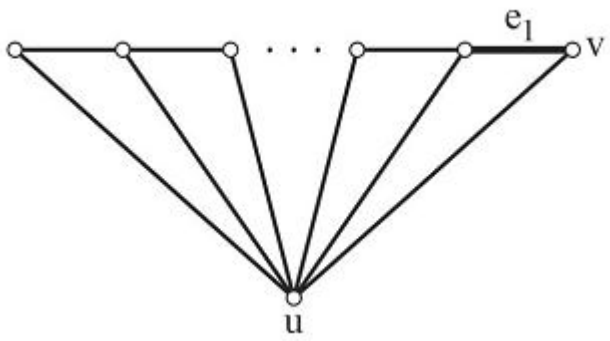


Figure 4: The $K_1 \circ P_n$ in the proof of Proposition 3.4.

Proposition 3.4 Let G be a simple graph and P_n a path of odd order n. We have

$$af(G \circ P_n) = |V(G)|.$$

Proof. Let $u \in V(G)$ and $(P_n)_u$ be a copy of P_n with the vertex set $\{v_1,...,v_n\}$ such that the vertex u is adjacent to all vertices of $(P_n)_u$. It can easily verified that if v is one of the vertices in the set $\{v_1, v_3,...,v_n\}$, then the edge uv belongs to a perfect matching of graph $G \circ P_n$. Since $P_n - v$ has unique perfect matching and there exist (n+1)/2 ways to choose vertex $v \in V(P_n)$, so we can conclude that the number of perfect matchings of $K_1 \circ P_n$ is equal to (n+1)/2. Also n is odd and so the perfect matching of $G \circ P_n$ does not related to the perfect matching of G. Thus the number of perfect matchings of $G \circ P_n$ is equal to $[(n+1)/2]^{|V(G)|}$. Let $S = \{e_1\}$ (see Figure 4). Then S has the smallest cardinality over all anti–forcing sets of graph $K_1 \circ P_n$. So for each odd n, we have $af(K_1 \circ P_n) = 1$. Obviously, the number of graphs $K_1 \circ P_n$ is equal to $|V(G)|$ and this implies the result. ■

Proposition 3.5 Let G be a simple graph and C_n be a cycle of odd order n. We have

$$af(G \circ C_n) = 2|V(G)|.$$

Proof. Let $u \in V(G)$ and $(C_n)_u$ be a copy of C_n such that the vertex u is adjacent to every vertex of $(C_n)_u$. Suppose that $v \in V((C_n)_u)$ and uv belongs to one of the perfect matchings

of graph $G \circ C_n$. Since $C_n - v = P_{n-1}$, so $C_n - v$ has an unique perfect matching. Also to choose vertex $v \in V(C_n)$ we have n possibilities. Note that since n is odd, thus the perfect matching of $G \circ C_n$ does not related to the perfect matching of G and we can conclude that the number of perfect matchings of $G \circ C_n$ is equal to $n^{|V(G)|}$. Let $S = \{e_1, e_2\}$ be as shown in Figure 5. Clearly, S has the smallest cardinality over all anti–forcing sets of graph $K_1 \circ C_n$. So for every odd n, we have $af(K_1 \circ C_n) = 2$. Also the number of graphs $K_1 \circ C_n$ is equal to $|V(G)|$. So we have the result. ■

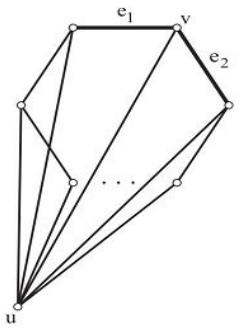


Figure 5: The graph with $S = \{e_1, e_2\}$ in the proof of Proposition 3.5.

Proposition 3.6 Let G be a simple graph and W_n a wheel of odd order n. We have

$$af(G \circ W_n) = 4|V(G)|.$$

Proof. Let $u \in V(G)$ and $(W_n)_u$ be a copy of W_n such that u is adjacent to every vertex of $(W_n)_u$. Suppose that $v \in V((W_n)_u)$ and uv belongs to one of the perfect matchings of graph $G \circ W_n$. If $v \in C_{n-1}$, then to choose other edges of perfect matching of $K_1 \circ W_n$, we have (n−1)/2 possibilities and if $v \in K_1$, then there exist two possibilities to choose other edges of perfect matching of $K_1 \circ W_n$. Since n is odd, so the perfect matching of $G \circ W_n$ does not related to the perfect matching of G. Also C_{n-1} have $n-1$ vertices. Thus to choose perfect matching of $G \circ W_n$, we have $[1/2(n-1)^2 + 2]^{|V(G)|}$ possibilities. Let $S = \{e_1, e_2, e_3, e_4\}$ as shown in Figure 6. Observe that S has the smallest cardinality over all anti–forcing sets of graph $K_1 \circ W_n$. Then for every odd n, $af(K_1 \circ W_n) = |S| = 4$ and we can conclude that $af(G \circ W_n) = 4|V(G)|$.

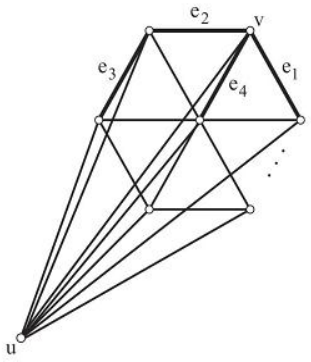


Figure 6: The graph with $S = \{e_1, e_2, e_3, e_4\}$ in the proof of Proposition 3.6.

4. ANTI–FORCING NUMBER OF SOME DENDRIMERS

Dendrimers are hyper–branched macromolecules, with a rigorously tailored architecture. They can be synthesized, in a controlled manner, either by a divergent or a convergent procedure. Dendrimers have gained a wide range of applications in supra–molecular chemistry, particularly in host guest reactions and self–assembly processes. Their applications in chemistry, biology and nano–science are unlimited [2].

In this section, we shall find the anti–forcing number of certain polyphenylene dendrimers. First we obtain the anti–forcing number of the first kind of dendrimer of generation 1–3 that has grown n stages.We denote this graph by $D_3[n]$. Figure 7 shows the first kind of dendrimer of generation 1–3 has grown 3 stages $D_3[n]$. Also we shall study the anti–forcing number of the first kind of dendrimer which has grown n steps denoted $D_1[n]$. Figure 7 shows $D_1[4]$. Note that there are three edges between each two cycle C_6 in this dendrimer.

Theorem 4.1

(i) Let $D_3[n]$ be a kind of dendrimer of generation 1–3 that has grown n stages. Then $af(D_3[n]) = 3\times 2^{n+4} - 24$.

(ii) Let $D_1[n]$ be a kind of dendrimer that has grown n stages. Then $af(D_1[n]) = 9\times 2^{n+1} - 11$.

Proof.

(i) It follows from Tutte's Theorem.

(ii) It can be observe that from Figure 7 that $D_1[n]$ is an odd graph. So $af(D_1[n]) = |E(D_1[n])| = 25 + \sum_{i=1}^{n-1}(18\times 2^i)$.

This completes our argument. ■

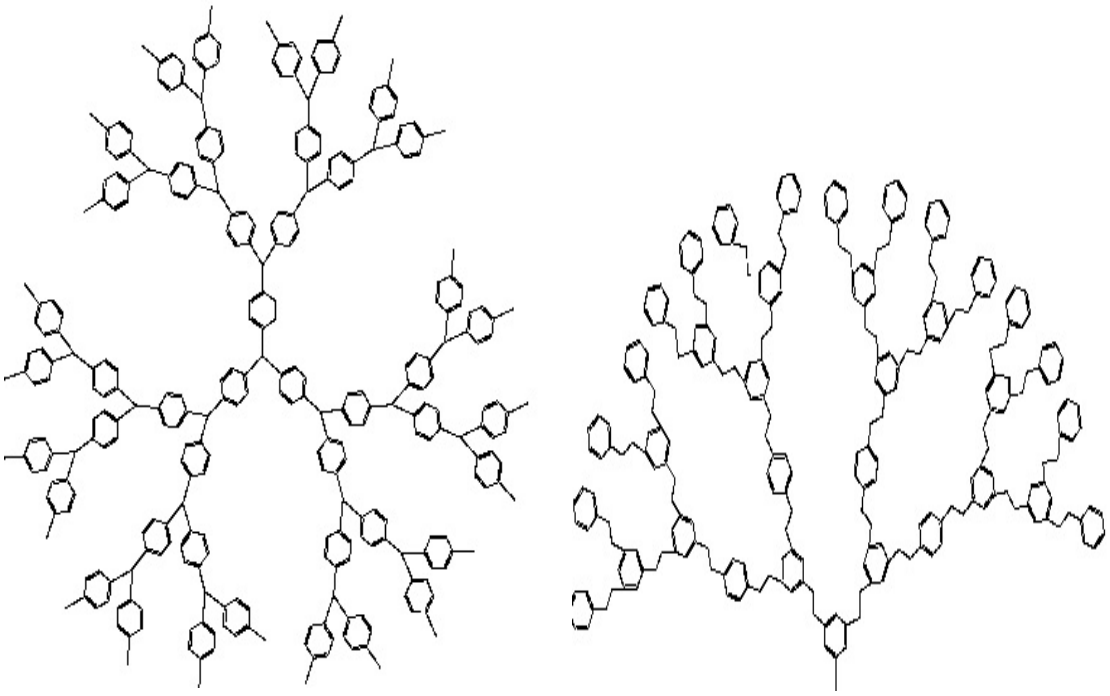


Figure 7: The dendrimers $D_3[3]$ and $D_1[4]$, respectively.

Finally we consider another type of polyphenylene dendrimer by construction of dendrimer generations G_n that has grown n stages. We simply denote this graph by $PD_2[n]$. Figure 8 shows the generations G_3 that has grown 3 stages.

Theorem 4.2 Let $PD_2[n]$ be a type of polyphenylene dendrimer by construction of dendrimer generations G_n that has grown n stages. Then we have

$$af(PD_2[n]) = 2 + \sum_{i=1}^{n}(5\times 2^{i+1}).$$

Proof. As you see in Figure 8,

$$PD_2[n] = L(\underbrace{C_6, C_6, ..., C_6}_{(2+\sum_{i=1}^{n}5\times 2^{i+1})-times}).$$

Now the result follows from Theorems 2.1 and 2.4. ■

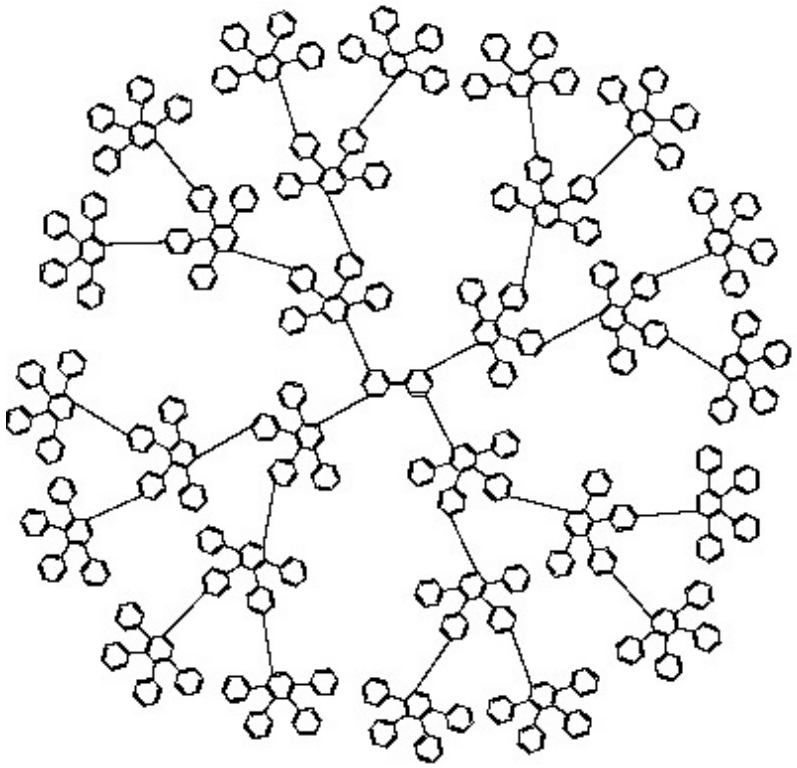


Figure 8: Polyphenylene dendrimer of generations G_3 that has grown 3 stages.

ACKNOWLEDGEMENTS. The authors would like to express their gratitude to the referees for their careful reading and helpful comments.

REFERENCES

1. S. Alikhani, S. Jahari, M. Mehryar and R. Hasni, Counting the number of dominating sets of cactus chains, *Opt. Adv. Materials–Rapid Commun*. **8** (9–10) (2014) 955–960.
2. S. Alikhani, R. Hasni, and G. C. Lau, Bounds for energy of certain polyphenylene dendrimers, *J. Comput. Theor. Nanosci*. **9** (2012) 1055–1058.
3. E. Deutsch and S. Klavžar, Computing the Hosoya polynomial of graphs from primary subgraphs, *MATCH Commun. Math. Comput. Chem*. **70** (2013) 627–644.
4. J. A. Gallian, Dynamic survey DS6: graph labeling, *Elec. J. Combin*. DS6 1–58 (2007).
5. F. Harary, D. J. Klein and T. P. Zivković, Graphical properties of polyhexes: perfect matching vector and forcing, *J. Math. Chem*. **6** (1991) 295–306.

6. D. J. Klein and M. Randić, Innate degree of freedom of a graph, *J. Comput. Chem*. **8** (1987) 516–521.
7. H. Lei, Y. N. Yeh, and H. Zhang, Anti–forcing numbers of perfect matchings of graphs, *Discrete Appl. Math.* **202** (2016) 95–105.
8. L. Lovász, M.D. Plummer, *Matching Theory*, North–Holland, Amsterdam, 1986.
9. D. Vukičević and N. Trinajstić, On the anti–forcing number of benzenoids. *J. Math. Chem*. **42** (2007) 575–583.
10. D. Vukičević and N. Trinajstić, On the anti–Kekulé number and anti–forcing number of cata–condensed benzenoids, *J. Math. Chem*. **43** (2008) 719–726.
11. H. Zhang, D. Ye and W. Shiu, Forcing matching numbers of fullerene graphs, *Discrete Appl. Math.* **158** (2010) 573–582.

Iranian J. Math. Chem. 8 (3) September (2017) 327 − 338

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

On the Forgotten Topological Index

AHMAD KHAKSARI[1] AND MODJTABA GHORBANI[•,2]

[1]Department of Mathematics, Payame Noor University, Tehran, 19395 – 3697, I. R. Iran
[2]Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785 – 136, I. R. Iran

ARTICLE INFO

Article History:

Received 13 August 2016
Accepted 15 September 2016
Published online 24 February 2017
Academic Editor: Ivan Gutman

Keywords:

Zagreb indices
Forgotten index
Graph products

ABSTRACT

The forgotten topological index of a graph G is defined as $F(G) = \Sigma_{u \in V(G)} d(u)^3$. In this paper, we compute some properties of forgotten index and then we determine it for some classes of product graphs.

1. INTRODUCTION

All graphs considered in this paper are undirected and finite without loops and multiple edges. Denoted by $V(G)$ and $E(G)$, we mean the set of vertices and the set of edges of graph G, respectively and suppose $n = |V(G)|$, $m = |E(G)|$. Two vertices are adjacent if and only if they are connected by an edge.

The ***Wiener index*** [17] is the first reported distance based topological index defined as half sum of the distances between all the pairs of vertices in a molecular graph [10,16]. ***Topological indices*** are abundantly being used in the *QSPR* and *QSAR* researches. So far, many various types of topological indices have been described.

Furtula and Gutman, in [4] introduced a new topological index namely, forgotten topological index and it is clearly stated that the forgotten index is a special case of the earlier much studied **general first Zagreb index**. They also established a few basic properties of it, see for example [1]. In 2014 unexpected chemical application of the *F*–index was discovered and it is proved that the forgotten topological index can significantly enhance the physico–chemical applicability of the first Zagreb index.

•Author to whom correspondence should be addressed (E–mail: mghorbani@srttu.edu).
DOI: 10.22052/ijmc.2017.43481

2. NOTATION AND DEFINITIONS

There are two Zagreb indices [10]: the first M_1 and the second M_2, can be defined as:

$$M_1 = M_1(G) = \sum_{u \in V(G)} d(u)^2 \tag{1}$$

and

$$M_2 = M_2(G) = \sum_{uv \in E(G)} d(u)d(v) \tag{2}$$

respectively. The first Zagreb index can be rewritten also as

$$M_1 = M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)]. \tag{3}$$

For more details on these topological indices we refer to [8,11,14,16,18]. With this notation, the *F*– index is defined as [4,5]

$$F = F(G) = \sum_{u \in V(G)} d(u)^3 = \sum_{uv \in E(G)} [d(u)^2 + d(v)^2]. \tag{4}$$

In [7] it is shown that some topological indices have one of the following three algebraic forms:

$$TI_1 = TI_1(G) = \sum_{v \in V(G)} F_1(v) \tag{5}$$

$$TI_1 = TI_1(G) = \sum_{uv \in E(G)} F_2(u,v) \tag{6}$$

$$TI_1 = TI_1(G) = \sum_{\{u,v\} \subseteq V(G), u \neq v} F_3(u,v) \tag{7}$$

where F_1, F_2 and F_3 are functions dependent of a vertex or on a pair of vertices of the molecular graph *G* and the forgotten index is of the form Eq. (5).

In 2006, bearing in mind Eqs. (1) and (2), Došlić [2] put forward the concept of the first and second Zagreb coindices, defined as

$$\overline{M}_1 = \overline{M}_1(G) = \sum_{uv \notin V(G)} [d(u) + d(v)] \tag{8}$$

and

$$\overline{M}_2 = \overline{M}_2(G) = \sum_{uv \notin E(G)} d(u)d(v) \tag{9}$$

respectively, see also [9]. In formulas (8) and (9) it is assumed that $x \neq y$. In full analogy with Eqs. (8), and (9), relying on Eq. (4), we can now define the *F*–coindex as

$$Co-F = Co-F(G) = \sum_{uv \notin E(G)} [d(u)^2 + d(v)^2]. \tag{10}$$

Let α is an arbitrary real number, the generalized version of the first Zagreb index is defined in [12,13] as follows:

$$M_\alpha = M_\alpha(G) = \sum_{u \in V(G)} d(u)^\alpha = \sum_{uv \in E(G)} [d(u)^{\alpha-1} + d(v)^{\alpha-1}]. \tag{11}$$

The generalized first Zagreb index was studied in several works such as [6,15] and the aim of this paper is to investigate the properties of $M_\alpha(G)$ where $\alpha = 3$.

The Zagreb and forgotten co–indices of a graph G and of its complement $\overline{G}$ can be represented in terms of the Zagreb indices of G and forgotten index, respectively. The respective formulas are given in [5,9].

3. RESULTS AND DISCUSSIONS

In this section, we propose several bounds for the F–index and then we compute the F–index of some composite graphs. Throughout this paper we use standard notations of graph theory. The path, star, wheel and complete graphs with n vertices are denoted by P_n, S_n, W_n and K_n, respectively.

An automorphism of the graph G is a bijection σ on which preserves the edge set E, *i.e.* if $e=uv$ is an edge of G, then $e^\sigma = u^\sigma v^\sigma$ is a member of E, where the image of vertex u is denoted by u^σ. We denote the set of all automorphisms of G by $Aut(G)$ and this set under the composition of mappings forms a group. This group acts on the set of vertices, if for any pair of vertices $u, v \in V$, there is an automorphism $\alpha \in Aut(G)$ such that $u^\sigma = v$. An isomorphism of graphs G and H is a bijection $\alpha : V(G) \to V(H)$ such that $uv \in E(G)$ if and only if $\alpha(u)\alpha(v) \in E(H)$. Two isomorphic graphs G and H are denoted by $G \cong H$.

Theorem 1. Let G be a graph with orbits $V_1, V_2, ..., V_r$ under action of Aut(G) on the set of vertices $V(G)$. Then for $u_i \in V_i$, we have

$$F(G) = \sum_{i=1}^{r} |V_i| \, \mathrm{d}(u_i)^3.$$

Proof. Let $V_1, V_2, ..., V_r$ be all orbits of Aut(G) on the set of vertices. It is a well–known fact that for two vertices $x, y \in V_i$, d(x) = d(y). Then one can verify that

$$F(G) = \sum_{i=1}^{r} \sum_{u \in V_i} \mathrm{d}(u)^3 = \sum_{i=1}^{r} |V_i| \, \mathrm{d}(u_i)^3.$$

As an application of Theorem 1, consider the dendrimer D with r layers as depicted in Figure 1. The vertex degrees of this graph are 1 and 3, thus, it is bi–regular. The vertices of every layer are in the same orbit under the action of automorphism graph on the set of vertices. Hence,

$$F(G) = \sum_{i=1}^{r} |V_i| \, \mathrm{d}(u_i)^3 = \sum_{i=1}^{r-1} |V_i| \, 3^3 + |V_r| \, .$$

This graph has $1 + 3 + 2.3 + 2^2.3 + \cdots + 2^r.3 = 1 + 3(2^{r+1} - 1)$ vertices in which the last layer has $2^r.3$ vertices. Hence,

$$F(G) = 27[1 + \sum_{i=0}^{r-1} |V_i|] + |V_r| \, .$$

This means that $F(G) = 3.2^r + 27[1 + 3(2^r - 1)] = 84.2^r - 54$.

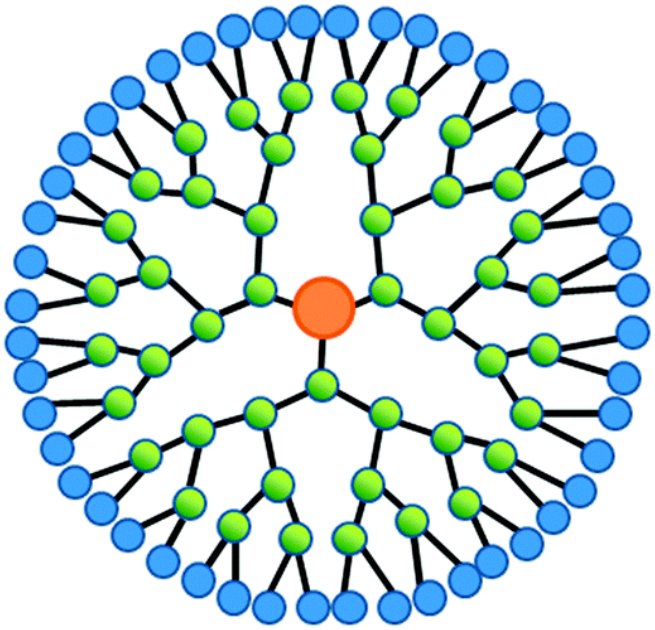


Figure 1. 2–*D* Graph of Dendrimer *D*.

Theorem 2. Let *G* be a graph on *n* vertices, then

$$F(G) \le M_1(G)^2 - 2M_2(G) \le M_1(G)^3.$$

Proof. We have

$$F(G) = \sum_{u \in V} d(u)^3 \le [\sum_{u \in V} d(u)]^3 = M_1(G)^3.$$

On the other hand,

$$\begin{aligned} F(G) &= \sum_{uv \in E(G)} [d(u)^2 + d(v)^2] \\ &= \sum_{uv \in E(G)} [(d(u) + d(v))^2 - 2d(u)d(v)] \\ &\le M_1(G)^2 - 2M_2(G). \end{aligned}$$

For two positive integers *x* and *y*, it is clear that x^3 is greater than $x^2 - 2y$ and the proof is completed.

Theorem 3. Let *G* be a graph on *n* vertices, then

$$\overline{F}(G) + F(G) \ge 2[M_2(G) + \overline{M}_2(G)].$$

Proof. For every pair of vertices $u,v \in V$, we have $(d(u)-d(v)) \geq 0$, hence $d(u)^2 + d(v)^2 \geq d(u)d(v)$ and then $F(G) \geq 2M_2(G)$. By a similar way, we can deduce that $\overline{F}(G) \geq 2\overline{M}_2(G)$. This confirms our claim.

Theorem 4. Let G be a graph on n vertices, m edges and maximum degree Δ. Then

$$\overline{F}(G) + F(G) \leq (n-1)M_1(G) + \Delta^2 m(n-3).$$

Proof. For each edge $uv \in E(G)$ and for a vertex $u \in V(G)$, the $n - 1 - d(u)$ vertices are non-adjacent with the vertex u. Let Δ be the maximum degree of G. For $uw \notin E(G)$, we have $d(u)+d(w) \leq [d(u)+\Delta][n-1-d(u)]$. So,

$$\begin{aligned}\overline{F}(G) &= \sum_{uw \notin E(G)} d(u)^2 + d(w)^2 \\ &\leq \sum_{uw \notin E(G)} [d(u)^2 + \Delta^2][n-1-d(u)] \\ &= (n-1)M_1(G) - F(G) + \Delta^2(n-1)m - \Delta^2 2m.\end{aligned}$$

Hence,

$$\overline{F}(G) \leq (n-1)M_1(G) - F(G) + \Delta^2 m(n-3).$$

Theorem 5. Let u,v be two vertices of graph G. Let $G^* = G - \{vv_1, ..., vv_s\} + \{uv_1, ..., uv_s\}$. If $d(u) + s > d(v)$ then $F(G^*) > F(G)$.

Proof. Let $d_G(u) = d(u)$, for every vertex $x \in V \setminus \{u,v\}$, we have

$$d_{G^*}(u) = d_G(u) + s, d_{G^*}(v) = d_G(v) - s, d_{G^*}(x) = d_G(x).$$

Hence, by the definition of F–index, we have

$$\begin{aligned}F(G^*) - F(G) &= d_{G^*}(u)^3 + d_{G^*}(v)^3 - d_G(u)^3 - d_G(v)^3 \\ &= (d_G(u)+s)^3 + (d_G(v)-s)^3 - d_G(u)^3 - d_G(v)^3 \\ &= 3sd_G(u)(s + d_G(u)) + 3sd_G(v)(d_G(v) - s).\end{aligned}$$

Clearly $F(G^*) - F(G) > 0$ if and only if $d_G(u)(s + d_G(u)) + d_G(v)(d_G(v) - s) > 0$. On the other hand, $\{v_1,...,v_s\} \subseteq N(v) \setminus N[u]$ implies that $d_G(v) - s > 0$ and so

$$d_G(u)(s + d_G(u)) + d_G(v)(d_G(v) - s) > 0.$$

The following bounds for the forgotten topological index were proposed in [5]:

$$F(G) \geq \frac{M_1(G)}{2m},$$

$$F(G) \geq \frac{M_1(G)^2}{m} - 2M_2(G),$$
$$F(G) \leq 2M_2(G) + m(n-1)^2.$$

Here, we establish some new bounds.

Theorem 6. Let G be a graph on n vertices and m edges. Then
$$F(G) \geq max\{6m-2n, 8m^3/n^2\}.$$

Proof. According to Bernoulli inequality, for every integer $\alpha \geq 1$, we have $(1+x)^{\alpha} \geq 1 + \alpha x$. Let $x = d(u_i) - 1$, then $d(u_i)^3 \geq 1 + 3(d(u_i) - 1) = 3d(u_i) - 2$. This means that $F(G) \geq 6m - 2n$. On the other hand, Let $x_1, ..., x_n$ be real numbers. Then, it is a well–known fact that

$$\frac{\sum_{i-1}^{n} x_i^k}{n} \geq \left(\frac{\sum_{i-1}^{n} x_i}{n} \right)^k.$$

By putting k=3 we have $F(G) \geq 8m^3/n^2$. This completes the proof.

Theorem 7. Let G be a graph on n vertices, m edges, minimum degree δ and maximum degree Δ. Then

$$F(G) \geq 6M_1(G) + 3n - 12m - \frac{2n}{\delta+1}\left(\frac{4}{(\delta+1)^2} + 3(\Delta-1)^2 + \frac{6(\Delta-1)}{\delta+1} \right).$$

Proof. For every real number a, we can prove that

$$\frac{a^2+1}{a+1} \geq \sqrt[3]{\frac{a^3+1}{2}}.$$

Thus

$$a^3 \leq 2\left(\frac{a^2+1}{a+1} \right)^3 - 1.$$

This implies that

$$F(G) = \sum_{i=1}^{n} d(u_i)^3 \leq 2\sum_{i=1}^{n}\left(\frac{d(u_i)^2+1}{d(u_i)+1} \right)^3 - n = 2\sum_{i=1}^{n}\left(\frac{d(u_i)^2-1+2}{d(u_i)+1} \right)^3 - n$$
$$= 2\left[\left(\sum_{i=1}^{n} d(u_i)^3 - 3\sum_{i=1}^{n} d(u_i)^2 + 3\sum_{i=1}^{n} d(u_i) - n \right) \right]$$
$$+ \left[8\sum_{i=1}^{n} \frac{1}{\left(1+d(u_i)\right)^3} + 6\sum_{i=1}^{n} \frac{\left(d(u_i)-1\right)^2}{\left(1+d(u_i)\right)} + 12\sum_{i=1}^{n} \frac{\left(d(u_i)-1\right)}{\left(1+d(u_i)\right)^2} \right] - n.$$

But $d(u_i) \geq 1$, and so

$$F(G) \leq 2\left[(F(G) - 3M_1(G) + 6m - n) + \frac{8n}{(\delta+1)^3} + 6\sum_{i=1}^{n}\frac{(\Delta-1)^2}{\delta+1} + 12n\frac{(\Delta-1)}{(\delta+1)^2}\right] - n.$$

Thus, the proof is completed.

Let G be a connected graph with n vertices and A be its adjacency matrix, where $\lambda_1,...,\lambda_n$ are its eigenvalues. The k–th spectral moment of G is defined as $\sum_{i-1}^{n}\lambda_i^k$ and it is equal to the number of all closed walks of length k in G. Similarly, if $\mu_1,...,\mu_n$ are Laplacian eigenvalues, than the k–th Laplacian spectral moment is as follows:

$$S_k = \sum_{i-1}^{n}\lambda_i^k.$$

Theorem 8 (**[5]**) If the graph G is triangle–free, then

$$F(G) = \sum_{xy\in E(G)}[d(x) - d(y)]^2 - 2M_1(G) + 4m + \sum_{i=1}^{n}\sum_{j=1}^{n}(A^3)_{ij}$$

where **A** is the adjacency matrix of G.

Theorem 9. Let G be a connected graph, then

$$F(G) = S_3 - 3M_1(G) + 6t.$$

Proof. Let D be a diagonal matrix whose entries are the degree of vertices in G. We have

$$\sum_{i=1}^{n}\mu_i^3 = tr(D-A)^3 = tr(D^3 - A^3 + 3A^2D)$$
$$= \sum_{i=1}^{n}d(u_i)^3 + 3\sum_{i=1}^{n}d(u_i)^2 - 6t.$$

Thus for the k–th spectral moment we have

$$F(G) = S_3 - 3\sum_{i=1}^{n}d(u_i)^2 + 6t = S_3 - 3M_1(G) + 6t.$$

Corollary 10. Let G be a triangular–free graph, then

$$F(G) = S_3 - 3M_1(G).$$

4. COMPUTING THE F–INDEX OF SOME GRAPH PRODUCTS

In this section we present explicit formulas for the F–index of several classes of graphs that arise via binary graph operations known as graph products. We start from the most common operation, the Cartesian product. The disjunction and the symmetric difference share many properties with the Cartesian product: they have the same vertex sets, they are

commutative and associative; hence they are considered next. The join of two or more graphs is also a commutative operation, but defined on the union instead on the Cartesian product of the vertex sets of the components.

4.1 CARTESIAN PRODUCT

The Cartesian product $G\times H$ of graphs G and H is a graph such that $V(G\times H)=V(G)\times V(H)$, and any two vertices (a,b) and (u,v) are adjacent in $G\times H$ if and only if either a = u and b is adjacent with v, or $b = v$ and a is adjacent with u. The degree of a vertex (u_1,u_2) of $G_1\times G_2$ is the sum of the degrees of its projections to the respective components,

$$d_{G_1\times G_2}(u_1,u_2)=d_{G_1}(u_1)+d_{G_2}(u_2).$$

Theorem 11. Let G_i (i = 1,2) be a graph on n_i vertices and m_i edges. Then

$$F(G_1\times G_2)=n_2F(G_1)+n_1F(G_2)+6m_2M_1(G_1)+6m_1M_1(G_2).$$

Proof. For $(u_1,u_2)\in G_1\times G_2$, we have $d_{G_1\times G_2}(u_1,u_2)=d_{G_1}(u_1)+d_{G_2}(u_2)$. This means that

$$\begin{aligned}F(\mathrm{G}_1\times\mathrm{G}_2)&=\sum_{(\mathrm{u}_1,\mathrm{u}_2)\in\mathrm{G}_1\times\mathrm{G}_2}d^3{}_{G_1\times G_2}(u_1,u_2)=\sum_{(\mathrm{u}_1,\mathrm{u}_2)\in\mathrm{G}_1\times\mathrm{G}_2}[d_{G_1}(u_1)+d_{G_2}(u_2)]^3\\&=\sum_{(\mathrm{u}_1,\mathrm{u}_2)\in\mathrm{G}_1\times\mathrm{G}_2}d^3{}_{G_1}(u_1)+d^3{}_{G_2}(u_2)+3d_{G_1}(u_1)d_{G_2}(u_2)[d_{G_1}(u_1)+d_{G_2}(u_2)]\\&=n_2F(\mathrm{G}_1)+n_1F(\mathrm{G}_2)+6m_2M_1(\mathrm{G}_1)+6m_1M_1(\mathrm{G}_2).\end{aligned}$$

4.2 SYMMETRIC DIFFERENCE AND DISJUNCTION

The **disjunction** $G\vee H$ of two graphs G and H is the graph with vertex set $V(G)\times V(H)$ in which (u_1,u_2) is adjacent with (v_1,v_2) whenever u_1 is adjacent with v_1 in G or u_2 is adjacent with v_2 in H. If $|V(G)| = n_1$, $|E(G)| = m_1$, $|V(H)| = n_2$, $|E(H)| = m_2$, the degree of a vertex (u_1,u_2) of $G\vee H$ is given by $\mathrm{d}_{G\vee H}((u_1,u_2)) = n_2\mathrm{d}_G(u_1) + n_1\mathrm{d}_H(u_2) - \mathrm{d}_G(u_1)\,\mathrm{d}_H(u_2)$.

Theorem 12. Let G_i (i = 1,2) be a graph on n_i vertices and m_i edges. Then

$$F(G_1\vee G_2)=n_2^2F(G_1)+n_1^2F(G_2)-4m_1m_2.$$

Proof. We have

$$\begin{aligned}F(G_1\vee G_2)&=\sum_{(u_1,u_2)\in G_1\vee G_2}d^3{}_{G_1\vee G_2}(u)=n_1\sum_{u\in G_1}d^3_{G_2}(u_2)-\sum_{u_1\in G_1}d_{G_1}(u_1)\sum_{u_2\in G_2}d_{G_2}(u_2)\\&=n_2^2F(G_1)+n_1^2F(G_2)-4m_1m_2.\end{aligned}$$

The **symmetric difference** $G\oplus H$ of two graphs G and H is the graph with vertex set $V(G)\times V(H)$ in which (u_1,u_2) is adjacent with (v_1,v_2) whenever u_1 is adjacent with v_1 in G

or u_2 is adjacent with v_2 in H, but not both. It follows from the definition that the degree of a vertex $(u_1,u_2)$of $G \oplus H$ is given by

$$d_{G\oplus H}((u_1,u_2)) = n_2 d_G(u_1) + n_1 d_H(u_2) - 2d_G(u_1)d_H(u_2).$$

Theorem 13. Let G_i (i = 1,2) be a graph on n_i vertices and m_i edges. Then

$$F(G_1 \oplus G_2) = n_1^2 F(G_2) + n_2^2 F(G_1) - 8m_1m_2.$$

Proof. The proof is similar to the proof of Theorem 12.

4.3 JOIN

The join $G = G_1 + G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph union $G_1 \cup G_2$ together with all the edges joining V_1 and V_2. Let n_1 and n_2 be number of vertices of G_1 and G_2, respectively. Then

$$d_{G_1+G_2}(u) = \begin{cases} d_{G_1}(u) + n_2 \\ d_{G_2}(u) + n_1 \end{cases}.$$

Theorem 14. Let G_i (i = 1,2) be a graph on n_i vertices and m_i edges. Then

$$F(G_1 + G_2) = F(G_1) + F(G_2) + n_1n_2^3 + n_1^3n_2 + 3n_2M_1(G_1) + 3n_1M_1(G_2) + 3n_1m_2 + 3n_2m_1.$$

Proof. We have

$$F(G_1 + G_2) = \sum_{u\in G_1+G_2} d^3{}_{G_1+G_2}(u) = \sum_{u\in G_1} (d_{G_1}(u) + n_2)^3 + \sum_{u\in G_2} (d_{G_2}(u) + n_1)^3$$
$$= F(G_1) + F(G_2) + n_1n_2^3 + n_1^3n_2 + 3n_2M_1(G_1) + 3n_1M_1(G_2) + 3n_1m_2 + 3n_2m_1.$$

4.4 COMPOSITION

The composition $G = G_1[G_2]$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 such that $|V_1| = n_1$, $|V_2| = n_2$ and edge sets E_1 and E_2 such that $|E_1| = m_1$, $|E_2| = m_2$ is the graph with vertex set $V_1 \times V_2$ and $u = (u_1,u_2)$ is adjacent with $v = (v_1,v_2)$ whenever u_1 is adjacent with v_1 or $u_1 = v_1$ and u_2 is adjacent with v_2. It follows from the definition that the degree of a vertex (u_1,u_2) of $G_1[G_2]$ is given by

$$d_{G_1[G_2]}((u_1,u_2)) = n_2 d_{G_1}(u_1) + n_1 d_{G_2}(u_2).$$

Theorem 15. Let G_i (i = 1,2) be a graph on n_i vertices and m_i edges. Then

$$F(G_1[G_2]) = n_2^3 F(G_1) + F(G_2) + 6n_2^2 m_2 M_1(G_1) + 6n_2 m_1 M_1(G_2).$$

Proof. We have

$$F(G_1[G_2]) = \sum_{(u_1,u_2)\in G_1[G_2]} d^3{}_{G_1[G_2]}(u) = \sum_{u\in G_1} [n_2 d_{G_1}(u_1) + d_{G_2}(u_2)]^3$$
$$= n_2^3 F(G_1) + F(G_2) + 6n_2^2 m_2 M_1(G_1) + 6n_2 m_1 M_1(G_2).$$

4.5 CORONA PRODUCT

The corona G_1oG_2 was defined by Frucht and Harary [3] as the graph G obtained by taking one copy of G_1 of order p_1 and p_1 copies of G_2, and then joining the i–th node of G_1 to every node in the i–th copy of G_2, see Figure 2. Suppose p_1, p_2, q_1 and q_2 are the number of vertices and the number of edges of graphs G_1 and G_2, respectively. It is easy to see that the number of vertices and the number of edges of G_1oG_2 are $p_1(1 + p_2)$ and $q_1 + p_1q_2 + p_1p_2$, respectively.

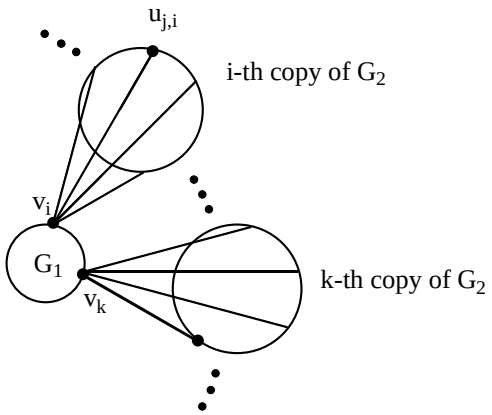


Figure 2. The Corona Product $G_1 \circ G_2$.

Example 1. For the graphs $G_1 = K_2$ and $G_2 = P_3$, the two different coronas G_1oG_2 and G_2oG_1 are shown in Figure 3.

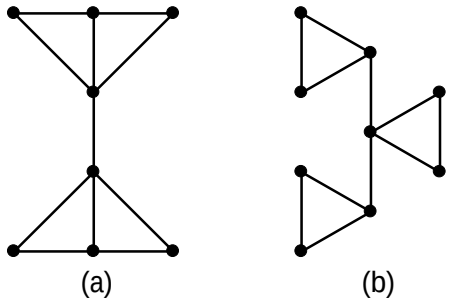


Figure 3. (*a*) The Corona Product K_2oP_3 and (*b*) P_3oK_2.

Theorem 16. Let G_i (i = 1,2) be a graph on n_i vertices and m_i edges. Then

$$F(G_1oG_2) = F(G_1) + n_1F(G_2) + n_1n_2^3 + 3n_2M_1(G_1) + 6n_2^2m_1 + n_1n_2 + 3n_1M_1(G_2) + 6n_1m_2.$$

Proof. It is not difficult to see that

$$d_{G_1oG_2}(a)=\begin{cases} d_{G_1}(a)+n_2 & a\in V(G_1) \\ d_{G_2}(u)+1 & a\in V(G_2) \end{cases}.$$

This means that

$$F(G_1oG_2)=\sum_{u\in G_1oG_2} d^3{}_{G_1oG_2}(u)=\sum_{u\in G_1} d^3_{G_1}(u)+\sum_{i=1}^{n_1}\sum_{u\in G_i} d^3_{G_i}(u)$$
$$=F(G_1)+n_1F(G_2)+n_1n_2^3+3n_2M_1(G_1)+6n_2^2m_1+n_1n_2+3n_1M_1(G_2)+6n_1m_2.$$

4.6 TENSOR PRODUCT

For given graphs G_1 and G_2 their tensor product $G_1\otimes G_2$ is defined as the graph on the vertex set $V(G_1)\times V(G_2)$ with vertices $u=(u_1, u_2)$ and $v=(v_1, v_2)$ connected by an edge if and only if either $u_1v_1\in E(G_1)$ and $u_2v_2\in E(G_2)$, see Figure 4. In other words, $G_1\otimes G_2$ has exactly n_1n_2 vertices and $2m_1+2m_2-12$ edges, where n_1, n_2 are the number of vertices and m_1, m_2 are the number of edges of G_1 and G_2, respectively.

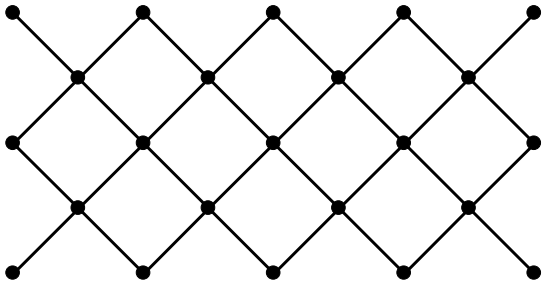


Figure 4. The Tensor Product $P_3\otimes P_5$.

Theorem 17. Let G_i (i = 1,2) be a graph on n_i vertices and m_i edges. Then

$$F(G_1\otimes G_2)=n_1F(G_2)+n_2F(G_1)+F(G_1)F(G_2)+3[2m_2(M_1(G_1)+F(G_1))+2m_1M_1(G_2)$$
$$+F(G_1)M_1(G_2)+F(G_2)M_1(G_1)]+6M_1(G_1)M_1(G_2).$$

Proof. Notice that the degree of every vertex of the tensor product can be computed as

$$\mathrm{d}_{G_1\otimes G_2}(u_1, u_2)=\mathrm{d}_{G_1}(u_1)+\mathrm{d}_{G_2}(u_2)+\mathrm{d}_{G_1}(u_1)\mathrm{d}_{G_2}(u_2).$$

Similar to the proof of Theorem 11, the proof is straightforward.

ACKNOWLEDGMENT. The authors are indebted to Professor Boris Furtula for reading the first draft of this paper and for giving us his valuable comments. This work is supported by Shahid Rajaee Teacher Training University under grant number 27774.

REFERENCES

1. K. C. Das and I. Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 103–112.
2. T. Došslić, Vertex–weighted Wiener polynomials for composite graphs, *Ars Math. Contemp.* **1** (2008) 66–80.
3. R. Frucht and F. Harary, On the corona of two graphs, *Aequationes Math.* **4** (1970) 322–324.
4. B. Furtula and I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190.
5. B. Furtula, I. Gutman, Ž. K. Vukićević ,G. Lekishvili and G. Popivoda, On an old/new degree–based topological index, *Bull. Acad. Serb. Sci. Arts* (*Cl. Sci. Math. Natur.*) **148** (2015) 19–31.
6. I. Gutman, An exceptional property of first Zagreb index, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 733–740.
7. I. Gutman, Edge decomposition of topological indices, *Iranian. J. Math. Chem.* **6** (2015) 103–108.
8. I. Gutman and K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.
9. I. Gutman, B. Furtula, Ž. Kovijanić Vukićević and G. Popivoda, On Zagreb indices and coindices, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 5–16.
10. I. Gutman, B. Ruščić, N. Trinajstić and C.F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.
11. A. Ilić and D. Stevanović, On comparing Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 681–687.
12. X. Li and H. Zhao, Trees with the first smallest and largest generalized topological indices, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 57–62.
13. X. Li and J. Zheng, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 195–208.
14. S. Nikolić, G. Kovačević, A. Miličević and N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003) 113–124.
15. G. Su, L. Xiong and L. Xu, The Nordhaus–Gaddum – type inequalities for the Zagreb index and coindex of graphs, *Appl. Math. Lett.* **25** (2012) 1701 – 1707.
16. R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.
17. H. Wiener, Structural determination of the paraffin boiling points, *J. Amer. Chem. Soc.* **69** (1947) 17–20.
18. B. Zhou and N. Trinajstić, Some properties of the reformulated Zagreb index, *J. Math. Chem.* **48** (2010) 714–719.

ABSTRACTS
IN
PERSIAN

Graphs with smallest forgotten index

I GUTMAN[1], A GHALAVAND[2], T DEHGHAN-ZADEH[2], AR ASHRAFI[2]

[1]Faculty of Science, University of Kragujevac, 34000 Kragujevac, Serbia
[2]Department of Pure Mathematics, Faculty of Mathematical Science, University of Kashan, Kashan 87317-53153, I. R. Iran

گراف ها با کمترین شاخص فراموش شده زاگرب

ادیتور رابط : حسن یوسفی آذری

چکیده

شاخص فراموش شده زاگرب گراف ملوکولی G به صورت $F(G) = \sum_{v \in V(G)} d(v)^3$ تعریف می شود که در آن d(v) درجه راس v در گراف G است. در این مقاله اولین تا ششمین درخت های با کمترین شاخص فراموش شده زاگرب، اولین تا سومین گراف های تک حلقه ای و دوحلقه ای با کمترین شاخص فراموش شده زاگرب، اولین تا چهارمین گراف سه حلقه ای با کمترین شاخص فراموش شده زاگرب و اولین و دومین گراف های چهار حلقه ای و پنج حلقه ای با کمترین شاخص فراموش شده زاگرب را بدست آمده است. این نتایج با نتایج بدست آمده برای شاخص زاگرب اول مقایسه شده اند.

لغات کلیدی:گراف تک حلقه ای، گراف دوحلقه ای، گراف سه حلقه ای، گراف جهار حلقه ای، گراف پنج حلقه ای.

On the First Variable Zagreb Index

KHOSRO MORADIAN[1], RAMIN KAZEMI[2] AND MOHAMMAD HASSAN BEHZADI[3]

[1,3]Department of Statistics, Science and Research Branch, Islamic Azad University, Tehran, Iran
[2]Department of Statistics, Faculty of Science, Imam Khomeini International University, Qazvin, Iran

شاخص زاگرب متغیر اول

ادیتور رابط : سندی کلاوزر

چکیده

شاخص زاگرب متغیر اول گراف G به‌صورت $M_1^{\lambda} = \sum_{v \in V(G)} d(v)^{2\lambda}$ تعریف می‌شود که در آن λ یک عدد حقیقی و $d(v)$ درجه راس v است. در این مقاله، چند کران پایین و بالا برای مقدار موردانتظار و تابع توزیع این متغیر در درخت‌های افزایشی تصادفی (درخت‌های بازگشتی، درخت‌های بازگشتی صفحه-جهت‌دار و درخت‌های افزایشی دودویی) ارائه می‌شود.

لغات کلیدی: شاخص زاگرب متغیر اول، درخت‌های افزایشی تصادفی، تابع توزیع، مقدار موردانتظار.

Computing the Additive Degree-Kirchhoff Index with the Laplacian Matrix

JOSE LUIS PALACIOS

Electrical and Computer Engineering Department, The University of New Mexico, Albuquerque, NM 87131, USA

محاسبهٔ شاخص کیرشهف-درجهٔ افزایشی با ماتریس لاپلاس

ادیتور رابط : علیرضا اشرفی

چکیده

معروف است که برای هرگراف همبند سادهٔ بدون جهت، می‌توان شاخص‌های کیرشهف و کیرشهف- درجه چندگانه را با استفاده از ماتریس لاپلاس محاسبه کرد. ما نشان می‌دهیم که این مسأله برای شاخص کیرشهف- درجه افزایشی نیز صادق است و یک برنامهٔ فشرده متلب ارائه می‌دهیم که هر سه شاخص کیرشهف را با استفاده از ماتریس لاپلاس به عنوان تنها ورودی محاسبه می‌کند.

لغات کلیدی: شاخص کیرشهف- درجه، ماتریس لاپلاس

On the Spectra of Reduced Distance Matrix of the Generalized Bethe Trees

ABBAS HEYDARI

Department of Science, Arak University of Technology, Arak, Iran

طیف ماتریس کاهش‌فاصله درخت‌های بت تعمیم‌یافته

ادیتور رابط : بیژن طائری

چکیده

فرض کنید G یک گراف سادهٔ همبند با مجموعهٔ رئوس آویختهٔ (رئوس با درجهٔ یک) $\{v_1, v_2, v_3, \dots, v_k\}$ باشد. ماتریس کاهش‌فاصله گراف G، ماتریسی مربعی از مرتبهٔ k است که درایهٔ (i,j)-ام آن برابر فاصلهٔ توپولوژیکی بین رئوس آویختهٔ v_i و v_j است. یک درخت ریشه‌دار، درخت بت تعمیم‌یافته نامیده می‌شود هرگاه درجات رئوس واقع بر یک سطح آن برابر باشند. در این مقاله، ما مجموعه طیف‌های ماتریس کاهش‌فاصله درخت‌های بت تعمیم‌یافته را محاسبه می‌کنیم..

لغات کلیدی: ماتریس کاهش‌فاصله، درخت بت تعمیم‌یافته، طیف‌ها.

On the Second Order First Zagreb Index

B. BASAVANAGOUD[1], S. PATIL[1] AND H. DENG[2]

[1]Department of Mathematics, Karnatak University, Dharwad − 580 003, Karnataka, India [2]Key Laboratory of High Performance Computing and Stochastic Information Processing, College of Mathematics and Computer Science, Hunan Normal University, Changsha, Hunan, 410081, P. R. China

اولین شاخص زاگرب مرتبهٔ دوم

ادیتور رابط : علیرضا اشرفی

چکیده

دراینجا با الهام از کاربردهای شیمیایی شاخص اتصال درجهٔ بالاتر (یا شاخص راندیک)، اولین شاخص زاگرب مرتبهٔ بالاتر از یک گراف مولکولی را در نظر می‌گیریم. در این مقاله، آنالیز رگرسیون خطی اولین شاخص زاگرب مرتبهٔ دوم را با آنتروپی و عامل خارج از مرکز ایزومرهای اکتان، مطالعه می‌کنیم. مدل خطی که بر پایهٔ اولین شاخص زاگرب مرتبهٔ دوم است، از مدلهای مرتبط با شاخص اول زاگرب و شاخص-F بهتر است. بعلاوه، اولین شاخص زاگرب نوع دوم گرافهای یالی از گرافهای زیربخش شبکهٔ 2D-، نانو تیوب و نانو لوله از $TUC_4C_8[p,q]$، گرافهای بچه قورباغه، گرافهای چرخ و گرافهای نردبانی را محاسبه میکنیم.

لغات کلیدی: شاخص توپولوژیکی، گراف یالی، گراف زیربخش، نانوسازه، گراف بچه قورباغه.

Anti-Forcing Number of Some Specific Graphs

SAEID ALIKHANI AND NEDA SOLTANI

Department of Mathematics, Yazd University, 89195-741, Yazd, Iran

عدد آنتی‌فورسینگ برخی از گرافهای خاص

ادیتور رابط : غلامحسین فتح‌تبار

چکیده

فرض کنید $G = (V, E)$ گرافی ساده و همبند است. منظور از یک جورسازی کامل گراف G، مجموعه‌ای از یالهای مجزای G است که همهٔ رئوس گراف را پوشش می‌دهند. آنتی فورسینگ گراف G که با نماد $af(G)$ نشان داده می‌شود، برابر با کمترین تعداد یالهایی از گراف است که باید از گراف برداشته شوند تا گراف حاصل دارای یک جورسازی کامل منحصربفرد باشد. در این مقاله گرافهای خاصی که در شیمی اهمیت دارند را درنظر گرفته و اعداد آنتی‌فورسینگ آنها را مطالعه می‌کنیم.

لغات کلیدی: عدد آنتی‌فورسینگ، مجموعهٔ آنتی‌فورسینگ، ضرب کرونا.

On the Forgotten Topological Index

AHMAD KHAKSARI[1] AND MODJTABA GHORBAN[2]

[1]Department of Mathematics, Payame Noor University, Tehran, 19395-3697, I. R. Iran
[2]Department of mathematics, Shahid Rajaee Teacher Training University, Tehran, 16785 – 136, I. R. Iran

شاخص توپولوژیکی فراموش‌شده

ادیتور رابط : ایوان گوتمن

چکیده

شاخص توپولوژیکی فراموش‌شده به صورت مجموع توان سوم درجات تعریف می شود. در این مقاله ما بعضی ویژگی‌های شاخص فراموش شده را محاسبه کرده و سپس این شاخص را برای برخی کلاسهای گراف حاصلضربی مشخص می‌کنیم.

لغات کلیدی: شاخص‌های زاگرب، شاخص فراموش‌شده، گراف حاصلضربی.

این نشریه طبق مجوز شماره 89/3/11/104372 مورخه 89/11/27 دارای اعتبار **علمی -پژوهشی** از وزارت علوم ، تحقیقات و فناوری می باشد. همچنین این مجله در پایگاه اطلاعاتی ISC (Islamic World Science Citation Center) وابسته به وزارت علوم ، تحقیقات و فناوری نمایه می شود.

IRANIAN JOURNAL OF MATHEMATICAL CHEMISTRY

CONTENTS

ISSN

2228-6489 (Print Version)

2008-9015 (Online Version)