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)

Iranian Journal of Mathematical Chemistry

Vol. 9, No. 4 December 2018

CONTENTS **pages**

Iranian J. Math. Chem. 9 (4) December (2018) 241 − 254

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

The Extremal Graphs for (Sum-) Balaban Index of Spiro and Polyphenyl Hexagonal Chains

YANG ZUO, YAQIAN TANG AND HANYUAN DENG•

College of Mathematics and Statistics, Hunan Normal University, Changsha, Hunan 410081, P. R. China

ARTICLE INFO

Article History:

Received 9 August 2018
Accepted 1 October 2018
Published online 15 December 2018
Academic Editor: Sandi Klavžar

Keywords:

Balaban index
Sum-Balaban index
Spiro hexagonal chain
Polyphenyl hexagonal chain

ABSTRACT

As highly discriminant distance-based topological indices, the Balaban index and the sum-Balaban index of a graph G are defined as $J(G) = \frac{m}{\mu+1}\sum_{uv\in E}\frac{1}{\sqrt{D_G(u)D_G(v)}}$ and $SJ(G) = \frac{m}{\mu+1}\sum_{uv\in E}\frac{1}{\sqrt{D_G(u)+D_G(v)}}$, respectively, where $D_G(u) = \sum_{v\in V} d(u,v)$ is the distance sum of a vertex u in G, m is the number of edges and μ is the cyclomatic number of G. They are useful distance-based descriptor in chemometrics. In this paper, we focus on the extremal graphs of spiro and polyphenyl hexagonal chains with respect to the Balaban index and the sum-Balaban index.

1 INTRODUCTION

Polyphenyl and spiro hexagonal chains have been widely investigated, and they represent a relevant area of interest in mathematical chemistry because they have been used to study intrinsic properties of molecular graphs. Polyphenyls and their derivatives, which can be used in organic synthesis, drug synthesis, heat exchangers, etc., attracted the attention of chemists for many years [7, 8, 20, 21, 26, 28, 30]. Spiro compounds are an important class of cycloalkanes in organic chemistry. A spiro union in spiro compounds is a linkage between two rings that consists of a single atom common to both rings and a free spiro union is a linkage that consists of the only direct union between the rings. Several works have been developed to analyze extremal values and extremal graphs for many topological indices on the spiro and polyphenyl hexagonal chains. Some results on energy, Merrifield-Simmons index, Hosoya index, Wiener index and Kirchhoff index of the spiro and

•Corresponding Author (Email address: hydeng@hunnu.edu.cn)
DOI: 10.22052/ijmc.2018.143823.1381

polyphenyl chains were reported in [2, 9, 12, 13, 16, 17, 35, 32]. In this paper, we will consider the extremal values and the extremal graphs for the Balaban index and the sum-Balaban index on polyphenyl and spiro chains.

As a highly discriminant distance-based topological index, the Balaban index [3] was defined on the basis of the Randić formula but using distance sums for vertices instead of vertex degrees. The Balaban index is a variant of connectivity index, represents extended connectivity and is a good descriptor for the shape of the molecules. It shows a good isomer discrimination ability and produces good correlations with some physical properties, such as the motor octane number [6], and it appears in theoretical models for predicting and screening drug candidates in rational drug design strategies [22]. It is of interest in combinatorial chemistry. It turned out to be applicable to several questions of molecular chemistry.

Throughout this paper we consider only simple and connected graphs. For a graph G with vertex set $V(G)$ and edge set $E(G)$. The distance between vertices u and v in G, denoted by $d_G(u,v)$, is the length of a shortest path connecting u and v. Let $D_G(u) = \sum_{v\in V(G)} d(u,v)$, which is the distance sum of vertex u in G.

The cyclomatic number μ of G is the minimum number of edges that must be removed from G in order to transform it to an acyclic graph. Let $|V(G)| = n$, $|E(G)| = m$, it is known that $\mu = m - n + 1$.

The Balaban index of a connected graph G is defined as

$$J(G) = \frac{m}{\mu+1}\sum_{uv\in E(G)} \frac{1}{\sqrt{D_G(u)\cdot D_G(v)}}.$$

It was introduced by A. T. Balaban in [3, 4], which is also called the average distance-sum connectivity or J index. It appears to be a very useful molecular descriptor with attractive properties. In 2010, Balaban et al. [5] also proposed the sum-Balaban index $SJ(G)$ of a connected graph G, which is defined as

$$SJ(G) = \frac{m}{\mu+1}\sum_{uv\in E(G)} \frac{1}{\sqrt{D_G(u)+D_G(v)}}.$$

The Balaban index and the sum-Balaban index were used in various quantitative structure-property relationship and quantitative structure activity relationship studies. Until now, the Balaban index and the sum-Balaban index have gained much popularity and new results related to them are constantly being reported, see [1, 10, 11, 14, 15, 18, 19, 25, 27, 29, 31, 33, 34].

Let G be a cactus graph in which each block is either an edge or a hexagon. G is called a polyphenyl hexagonal chain if each hexagon of G has at most two cut-vertices, and each cut-vertex is shared by exactly one hexagon and one cut-edge. The number of hexagons in G is called the length of G. An example of a polyphenyl hexagonal chain is shown in Figure 1.

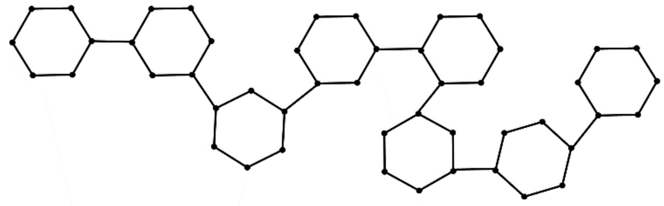

Figure 1: A polyphenyl hexagonal chain of length 8.

Let $PPC_n = H_1H_2 \cdots H_n (n \geq 3)$ be a polyphenyl hexagonal chain of length n. There is a cut-edge $v_{n-1}u_n$ between PPC_{n-1} and H_n, see Figure 2.

Note that any polyphenyl hexagonal chain of length n has $6n$ vertices and $7n-1$ edges. A vertex v of H_k is said to be ortho-, meta-, and para-vertex if the distance between v and u_k is 1, 2 and 3, denoted by o_k, m_k and p_k, respectively. Example of Figure 2, $o_n = x_2, x_6$, $m_n = x_3, x_5$, $p_n = x_4$. Obviously, every hexagon has two ortho-vertices, two meta-vertices and one para-vertex except the first hexagon H_1.

A polyphenyl hexagonal chain PPC_n is a polyphenyl ortho-chain if $v_k = o_k$ for $2 \leq k \leq n-1$. The polyphenyl meta-chain and polyphenyl para-chain are defined in a completely analogous manner.

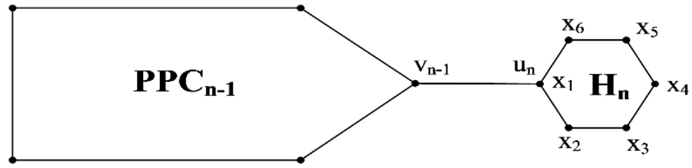

Figure 2: A polyphenyl hexagonal chain of length n.

The polyphenyl ortho-, meta-, and para-chains of length n are denoted by O_n, M_n and P_n, respectively. Examples of polyphenyl ortho-, meta-, and para-chains are shown in Figure 3.

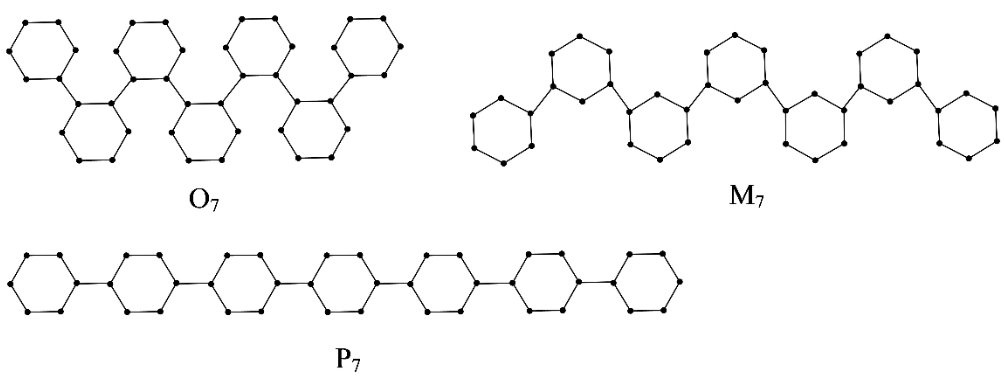

Figure 3: Polyphenyl hexagonal ortho-, meta-, and para-chains of length 7.

The definition of spiro hexagonal chain is same as definition of polyphenyl hexagonal chain. A hexagonal cactus is a connected graph in which every block is a hexagon. A vertex shared by two or more hexagon is called a cut-vertex. If each hexagon of a hexagonal cactus G has at most two cut-vertices, and each cut-vertex is shared by exactly two hexagons, then G is called a spiro hexagonal chain. The number of hexagon in G is called the length of G. An example of a spiro hexagonal chain is shown in Figure 4.

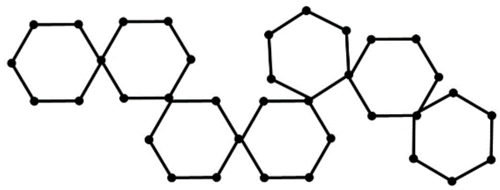

Figure 4: A spiro hexagonal chain of length 7.

Obviously, a spiro hexagonal chain of length n has $5n + 1$ vertices and $6n$ edges. Let $SPC_n = \overline{H}_1\overline{H}_2 \cdots \overline{H}_n (n \geq 3)$ be a spiro hexagonal chain of length n. There is a cut-vertex u_n between SPC_{n-1} and H_n, see Figure 5.

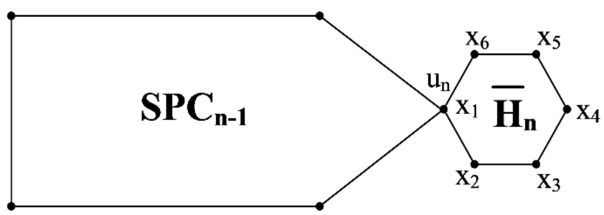

Figure 5: A spiro hexagonal chain of length n.

A vertex v of $\overline{H}_k$ is said to be ortho-, meta-, and para- vertex if the distance between v and u_k is 1, 2 and 3, denoted by $\overline{o}_k$, $\overline{m}_k$ and $\overline{p}_k$, respectively. A spiro hexagonal chain is a spiro ortho-chain if $u_k = \overline{o}_k$ for $2 \leq k \leq n$. The spiro meta-chain and para-chains are defined in a completely analogous manner. The spiro ortho-, meta-, and para-chains of length n are denoted by SO_n, SM_n and SP_n, respectively.

The following lemmas will be used in the next section.

Lemma 1 ([14]) *Let $x, y, a \in R^+$ such that $x \geq y + a$. Then $\frac{1}{\sqrt{xy}} \geq \frac{1}{\sqrt{(x-a)(y+a)}}$ with equality if and only if $x = y + a$.*

Lemma 2 ([15]) *Let $r_1, t_1, r_2, t_2 \in R^+$ such that $r_1 > t_1$ and $r_2 - r_1 = t_2 - t_1 > 0$. Then $\frac{1}{\sqrt{r_1}} + \frac{1}{\sqrt{t_2}} < \frac{1}{\sqrt{r_2}} + \frac{1}{\sqrt{t_1}}$.*

Lemma 3 ([14]) *Let $a, w, x, y, z \in R^+$ such that $\frac{a}{x} \geq \frac{a}{w}, \frac{a}{y} \geq \frac{a}{z}$. Then*

$$\frac{1}{\sqrt{(w+a)(z+a)}} + \frac{1}{\sqrt{xy}} \geq \frac{1}{\sqrt{wz}} + \frac{1}{\sqrt{(x+a)(y+a)}}.$$

2. (SUM-) BALABAN INDEX OF POLYPHENYL HEXAGONAL CHAINS

In this section, we first give two cut-edge transformations on PPC_n, and then determine the extremal graphs by using the transformations.

The first cut-edge transformation on $\boldsymbol{PPC_n}$: Let $G_n = H_1H_2 \cdots H_n (n \geq 3)$ be a polyphenyl hexagonal chain of length n. x_1 and x_4 are two cut-vertices in the $k-th$ hexagon H_k, and the distance between x_1 and x_4 is 3. If G' is the graph obtained from G by deleting the cut edge x_4u_{k+1} between H_k and H_{k+1}, and adding a new cut-edge x_3u_{k+1} between H_k and H_{k+1} (see Figure 6), then we say that G' is obtained from G by the first cut-edge transformation.

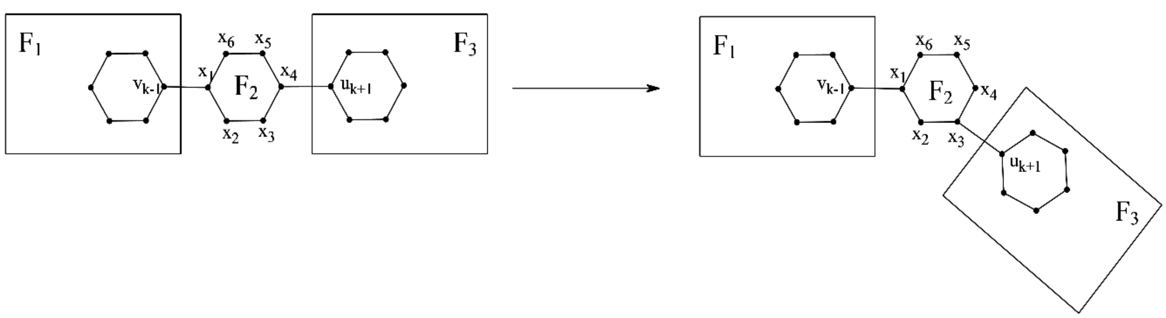

Figure 6: The first cut-edge transformation.

Lemma 4 *Let $G_n = H_1H_2 \cdots H_n (n \geq 3)$ be a polyphenyl hexagonal chain of length n. G' is obtained from G by the first cut-edge transformation. Then $J(G) < J(G')$ and $SJ(G) < SJ(G')$.*

Proof. Let $F_1 = H_1H_2 \cdots H_{k-1}$, $F_2 = H_k$, $F_3 = H_{k+1}H_{k+2} \cdots H_n$. The length of F_1 is $a = k-1$ and the length of F_3 is $b = n-k$. Obviously, $a + b = n-1$. Without loss of generality, let $a \geq b$. For a vertex $v_x \in F_1$, we have

$$D_G(v_x) = \textstyle\sum_{u \in F_1} d_G(v_x, u) + \sum_{u \in F_2} d_G(v_x, u) + \sum_{u \in F_3} d_G(v_x, u),$$

$$D_{G'}(v_x) = \textstyle\sum_{u \in F_1} d_{G'}(v_x, u) + \sum_{u \in F_2} d_{G'}(v_x, u) + \sum_{u \in F_3} d_{G'}(v_x, u)$$

$$\textstyle\sum_{u \in F_1} d_G(v_x, u) = \sum_{u \in F_1} d_{G'}(v_x, u),$$

$$\textstyle\sum_{u \in F_2} d_G(v_x, u) = \sum_{u \in F_2} d_{G'}(v_x, u),$$

$$\textstyle\sum_{u \in F_3} d_G(v_x, u) = \sum_{u \in F_3} d_{G'}(v_x, u) + 6b.$$

So, $D_G(v_x) - D_{G'}(v_x) = 6b$ and $D_G(v_x) > D_{G'}(v_x)$. For a vertex $v_y \in F_3$, we have

$$D_G(v_y) = \textstyle\sum_{u \in F_1} d_G(v_y, u) + \sum_{u \in F_2} d_G(v_y, u) + \sum_{u \in F_3} d_G(v_y, u),$$

$$D_{G'}(v_y) = \textstyle\sum_{u \in F_1} d_{G'}(v_y, u) + \sum_{u \in F_2} d_{G'}(v_y, u) + \sum_{u \in F_3} d_{G'}(v_y, u).$$

Furthermore,

$\sum_{u\in F_1} d_G(v_y,u) = \sum_{u\in F_1} d_{G'}(v_y,u)$,
$\sum_{u\in F_2} d_G(v_y,u) = \sum_{u\in F_2} d_{G'}(v_y,u)$,
$\sum_{u\in F_3} d_G(v_y,u) = \sum_{u\in F_3} d_{G'}(v_y,u) + 6a$. So, $D_G(v_y) - D_{G'}(v_y) = 6a$
$D_G(v_y) > D_{G'}(v_y)$.

For a vertex in $V(F_2) = \{x_1,x_2,x_3,x_4,x_5,x_6\}$, it is easy to see that
$D_G(x_1) - D_{G'}(x_1) = D_G(x_2) - D_{G'}(x_2) = D_G(x_3) - D_{G'}(x_3) = 6b$,
$D_{G'}(x_4) - D_G(x_4) = D_{G'}(x_5) - D_G(x_5) = D_{G'}(x_6) - D_G(x_6) = 6b$.

(I) For an edge $v_xv_y \in E(F_1)\cup E(F_3)$, we have

$$\frac{1}{\sqrt{D_{G'}(v_x)D_{G'}(v_y)}} > \frac{1}{\sqrt{D_G(v_x)D_G(v_y)}} \tag{1}$$

and

$$\frac{1}{\sqrt{D_{G'}(v_x)+D_{G'}(v_y)}} > \frac{1}{\sqrt{D_G(v_x)+D_G(v_y)}} \tag{2}$$

since $D_G(v_x) > D_{G'}(v_x)$ and $D_G(v_y) > D_{G'}(v_y)$.

(II) In what follows, we consider an edge in $\{x_1x_2,x_2x_3,x_3x_4,x_4x_5,x_5x_6,x_6x_1,x_1v_{k-1},x_4u_{k+1}\}$. Let $M = \sum_{u\in F_1} d_G(x_1,u) + \sum_{u\in F_3} d_G(x_4,u) + \sum_{u\in F_2} d_G(x,u)$, where $x\in\{x_1,x_2,x_3,x_4,x_5,x_6\}$. Then $M = \sum_{u\in F_1} d_{G'}(x_1,u) + \sum_{u\in F_3} d_{G'}(x_3,u) + \sum_{u\in F_2} d_{G'}(x,u)$. It can be checked directly that

$D_G(x_1) = M + 18bD_{G'}(x_1) = M + 12b$
$D_G(x_2) = M + 6a + 12bD_{G'}(x_2) = M + 6a + 6b$
$D_G(x_3) = M + 12a + 6bD_{G'}(x_3) = M + 12a$
$D_G(x_4) = M + 18aD_{G'}(x_4) = M + 18a + 6b$
$D_G(x_5) = M + 12a + 6bD_{G'}(x_5) = M + 12a + 12b$
$D_G(x_6) = M + 6a + 12bD_{G'}(x_6) = M + 6a + 18b$.

(i) For the edges $x_1v_{k-1}, x_4u_{k+1} \in E(G)$ and $x_1v_{k-1}, x_3u_{k+1} \in E(G')$, we have

$$\frac{1}{\sqrt{D_{G'}(x_1)D_{G'}(v_{k-1})}} + \frac{1}{\sqrt{D_{G'}(x_3)D_{G'}(u_{k+1})}} > \frac{1}{\sqrt{D_G(x_1)D_G(v_{k-1})}} + \frac{1}{\sqrt{D_G(x_4)D_G(u_{k+1})}} \tag{3}$$

and

$$\frac{1}{\sqrt{D_{G'}(x_1)+D_{G'}(v_{k-1})}} + \frac{1}{\sqrt{D_{G'}(x_3)+D_{G'}(u_{k+1})}} > \frac{1}{\sqrt{D_G(x_1)+D_G(v_{k-1})}} + \frac{1}{\sqrt{D_G(x_4)+D_G(u_{k+1})}}. \tag{4}$$

since $D_G(x_1) > D_{G'}(x_1)$, $D_G(v_{k-1}) > D_{G'}(v_{k-1})$, $D_G(x_4) > D_{G'}(x_3)$, $D_G(u_{k+1}) > D_{G'}(u_{k+1})$.

(ii) For the edges $x_1x_6, x_3x_4 \in E(G)$, we have $D_{G'}(x_6) \geq D_{G'}(x_1) + 6b$, $D_G(x_1) = D_{G'}(x_1) + 6b$ and $D_G(x_6) = D_{G'}(x_6) - 6b$. By Lemma 1, we can get

$$\frac{1}{\sqrt{D_{G'}(x_1)D_{G'}(x_6)}} \geq \frac{1}{\sqrt{D_G(x_1)D_G(x_6)}} \tag{5}$$

and

$$\frac{1}{\sqrt{D_{G'}(x_1)+D_{G'}(x_6)}} \geq \frac{1}{\sqrt{D_G(x_1)+D_G(x_6)}} \tag{6}$$

Also, $D_{G'}(x_4) \geq D_{G'}(x_3) + 6b$, $D_G(x_3) = D_{G'}(x_3) + 6b$ and $D_G(x_4) = D_{G'}(x_4) - 6b$, by Lemma 1, we have

$$\frac{1}{\sqrt{D_{G'}(x_3)D_{G'}(x_4)}} \geq \frac{1}{\sqrt{D_G(x_3)D_G(x_4)}} \tag{7}$$

and

$$\frac{1}{\sqrt{D_{G'}(x_3)+D_{G'}(x_4)}} \geq \frac{1}{\sqrt{D_G(x_3)+D_G(x_4)}} \tag{8}$$

(iii) For the edges $x_1x_2, x_4x_5 \in E(G)$, let $x = D_{G'}(x_1)$, $y = D_{G'}(x_2)$, $w = D_G(x_4)$, $z = D_G(x_5)$. Then $D_G(x_1) = x + 6b$, $D_G(x_2) = y + 6b$, $D_{G'}(x_4) = w + 6b$, $D_{G'}(x_5) = z + 6b$. Note that $w > x$, $z > y$ and $\frac{6b}{x} > \frac{6b}{w}, \frac{6b}{y} > \frac{6b}{z}$, by Lemma 3, we have

$$\frac{1}{\sqrt{D_{G'}(x_1)D_{G'}(x_2)}} + \frac{1}{\sqrt{D_{G'}(x_4)D_{G'}(x_5)}} \geq \frac{1}{\sqrt{D_G(x_1)D_G(x_2)}} + \frac{1}{\sqrt{D_G(x_4)D_G(x_5)}} \tag{9}$$

Now, let $r_1 = D_G(x_4) + D_G(x_5) = 2M + 30a + 6b$, $r_2 = D_{G'}(x_4) + D_{G'}(x_5) = 2M + 30a + 18b$, $t_1 = D_{G'}(x_1) + D_{G'}(x_2) = 2M + 6a + 18b$, $t_2 = D_G(x_1) + D_G(x_2) = 2M + 6a + 30b$. Then $r_2 - r_1 = t_2 - t_1 = 12b > 0$, $r_1 - t_1 = 24a - 12b > 0$ (since $a \geq b > 0$). By Lemma 2, we have

$$\frac{1}{\sqrt{D_{G'}(x_1)+D_{G'}(x_2)}} + \frac{1}{\sqrt{D_{G'}(x_4)+D_{G'}(x_5)}} > \frac{1}{\sqrt{D_G(x_1)+D_G(x_2)}} + \frac{1}{\sqrt{D_G(x_4)+D_G(x_5)}} \tag{10}$$

(iv) For the edges $x_2x_3, x_5x_6 \in E(G)$, by the same ways as in (iii), we can get

$$\frac{1}{\sqrt{D_{G'}(x_2)D_{G'}(x_3)}} + \frac{1}{\sqrt{D_{G'}(x_5)D_{G'}(x_6)}} \geq \frac{1}{\sqrt{D_G(x_2)D_G(x_3)}} + \frac{1}{\sqrt{D_G(x_5)D_G(x_6)}} \tag{11}$$

$$\frac{1}{\sqrt{D_{G'}(x_2)+D_{G'}(x_3)}} + \frac{1}{\sqrt{D_{G'}(x_5)+D_{G'}(x_6)}} > \frac{1}{\sqrt{D_G(x_2)+D_G(x_3)}} + \frac{1}{\sqrt{D_G(x_5)+D_G(x_6)}} \tag{12}$$

From Equations (1–12) and the definition of the Balaban index and the sum-Balaban index, we have $J(G) < J(G')$ and $SJ(G) < SJ(G')$. ■

The second cut-edge transformation on PPC_n: Let $G_n = H_1H_2 \cdots H_n (n \geq 3)$ be a polyphenyl hexagonal chain of length n. x_1 and x_3 are two cut-vertices in the $k-th$ hexagon H_k, and the distance between x_1 and x_4 is 2. If G' is the graph obtained from G by deleting the cut edge x_3u_{k+1} between H_k and H_{k+1}, and adding a new cut-edge x_2u_{k+1} between H_k and H_{k+1} (see Figure 7), then we say that G' is obtained from G by the second cut-edge transformation.

Lemma 5 *Let $G_n = H_1H_2 \cdots H_n (n \geq 3)$ be a polyphenyl hexagonal chain of length n. G' is obtained from G by the second cut-edge transformation. Then $J(G) < J(G')$ and $SJ(G) < SJ(G')$.*

Proof. Let $F_1 = H_1 H_2 \cdots H_{k-1}$, $F_2 = H_k$, $F_3 = H_{k+1} H_{k+2} \cdots H_n$. The length of F_1 is $a = k - 1$ and the length of F_3 is $b = n - k$. Obviously, $a + b = n - 1$. Without loss of generality, let $a \geq b$.

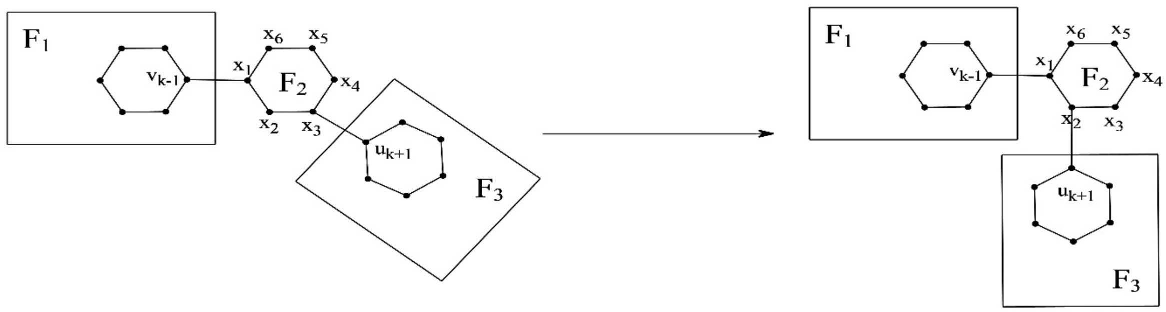

Figure 7: The second cut-edge transformation.

For a vertex $v_x \in F_1$, we have

$$D_G(v_x) = \sum_{u \in F_1} d_G(v_x, u) + \sum_{u \in F_2} d_G(v_x, u) + \sum_{u \in F_3} d_G(v_x, u),$$

$$D_{G'}(v_x) = \sum_{u \in F_1} d_{G'}(v_x, u) + \sum_{u \in F_2} d_{G'}(v_x, u) + \sum_{u \in F_3} d_{G'}(v_x, u)$$

and $\sum_{u \in F_1} d_G(v_x, u) = \sum_{u \in F_1} d_{G'}(v_x, u)$, $\sum_{u \in F_2} d_G(v_x, u) = \sum_{u \in F_2} d_{G'}(v_x, u)$, $\sum_{u \in F_3} d_G(v_x, u) = \sum_{u \in F_3} d_{G'}(v_x, u) + 6b$. So, $D_G(v_x) - D_{G'}(v_x) = 6b$ and $D_G(v_x) > D_{G'}(v_x)$. For a vertex $v_y \in F_3$, we have

$$D_G(v_y) = \sum_{u \in F_1} d_G(v_y, u) + \sum_{u \in F_2} d_G(v_y, u) + \sum_{u \in F_3} d_G(v_y, u),$$

$$D_{G'}(v_y) = \sum_{u \in F_1} d_{G'}(v_y, u) + \sum_{u \in F_2} d_{G'}(v_y, u) + \sum_{u \in F_3} d_{G'}(v_y, u)$$

and $\sum_{u \in F_3} d_G(v_y, u) = \sum_{u \in F_3} d_{G'}(v_y, u)$, $\sum_{u \in F_2} d_G(v_y, u) = \sum_{u \in F_2} d_{G'}(v_y, u)$, $\sum_{u \in F_1} d_G(v_y, u) = \sum_{u \in F_1} d_{G'}(v_y, u) + 6a$. So, $D_G(v_y) - D_{G'}(v_y) = 6a$ and $D_G(v_y) > D_{G'}(v_y)$. For a vertex in $F_2 = \{x_1, x_2, x_3, x_4, x_5, x_6\}$, let

$M = \sum_{u \in F_1} d_G(x_1, u) + \sum_{u \in F_3} d_G(x_2, u) + \sum_{u \in F_2} d_G(x, u) = \sum_{u \in F_1} d_{G'}(x_1, u) + \sum_{u \in F_3} d_{G'}(x_2, u) + \sum_{u \in F_2} d_{G'}(x, u)$, where $x \in \{x_1, x_2, x_3, x_4, x_5, x_6\}$. It can be checked directly that

$$D_G(x_1) = M + 12bD_{G'}(x_1) = M + 6b$$

$$D_G(x_2) = M + 6a + 6bD_{G'}(x_2) = M + 6a$$

$$D_G(x_3) = M + 12aD_{G'}(x_3) = M + 12a + 6b$$

$$D_G(x_4) = M + 18a + 6bD_{G'}(x_4) = M + 18a + 12b$$

$$D_G(x_5) = M + 12a + 12bD_{G'}(x_5) = M + 12a + 18b$$

$$D_G(x_6) = M + 6a + 18bD_{G'}(x_6) = M + 6a + 12b.$$

(I) For an edge $v_x v_y \in E(F_1) \cup E(F_3)$, we have $D_G(v_x) > D_{G'}(v_x)$, $D_G(v_y) > D_{G'}(v_y)$. So,

$$\frac{1}{\sqrt{D_{G'}(v_x)D_{G'}(v_y)}} > \frac{1}{\sqrt{D_G(v_x)D_G(v_y)}} \tag{13}$$

and

$$\frac{1}{\sqrt{D_{G'}(v_x)+D_{G'}(v_y)}} > \frac{1}{\sqrt{D_G(v_x)+D_G(v_y)}} \tag{14}$$

(II) In what follows, we consider an edge in $\{x_1x_2, x_2x_3, x_3x_4, x_4x_5, x_5x_6, x_6x_1, x_1v_{k-1}, x_3u_{k+1}\}$.

(i) For the edges $x_1v_{k-1}, x_3u_{k+1} \in E(G)$ and $x_1v_{k-1}, x_2u_{k+1} \in E(G')$, it is easy to know that $D_G(x_1) > D_{G'}(x_1)$, $D_G(v_{k-1}) > D_{G'}(v_{k-1})$, $D_G(x_3) > D_{G'}(x_2)$, $D_G(u_{k+1}) > D_{G'}(u_{k+1})$. And

$$\frac{1}{\sqrt{D_{G'}(x_1)D_{G'}(v_{k-1})}} + \frac{1}{\sqrt{D_{G'}(x_2)D_{G'}(u_{k+1})}} > \frac{1}{\sqrt{D_G(x_1)D_G(v_{k-1})}} + \frac{1}{\sqrt{D_G(x_3)D_G(u_{k+1})}}, \tag{15}$$

$$\frac{1}{\sqrt{D_{G'}(x_1)+D_{G'}(v_{k-1})}} + \frac{1}{\sqrt{D_{G'}(x_2)+D_{G'}(u_{k+1})}} > \frac{1}{\sqrt{D_G(x_1)+D_G(v_{k-1})}} + \frac{1}{\sqrt{D_G(x_3)+D_G(u_{k+1})}}. \tag{16}$$

(ii) For the edges $x_2x_3, x_5x_6 \in E(G)$, because $D_{G'}(x_3) > D_{G'}(x_2) + 6b$, by Lemma 1, we have

$$\frac{1}{\sqrt{D_{G'}(x_2)D_{G'}(x_3)}} \geq \frac{1}{\sqrt{D_G(x_2)D_G(x_3)}} \tag{17}$$

and

$$\frac{1}{\sqrt{D_{G'}(x_2)+D_{G'}(x_3)}} = \frac{1}{\sqrt{D_G(x_2)+D_G(x_3)}}. \tag{18}$$

Also, because $D_{G'}(x_5) = D_{G'}(x_6) + 6b$, by Lemma 1, we have

$$\frac{1}{\sqrt{D_{G'}(x_5)D_{G'}(x_6)}} \geq \frac{1}{\sqrt{D_G(x_5)D_G(x_6)}} \tag{19}$$

and

$$\frac{1}{\sqrt{D_{G'}(x_5)+D_{G'}(x_6)}} = \frac{1}{\sqrt{D_G(x_5)+D_G(x_6)}}. \tag{20}$$

(iii) For the edges $x_1x_2, x_3x_4 \in E(G)$, let $x = D_{G'}(x_2)$, $y = D_{G'}(x_1)$, $w = D_G(x_3)$, $z = D_G(x_4)$, then $x + 6b = D_G(x_2)$, $y + 6b = D_G(x_1)$, $w + 6b = D_{G'}(x_3)$, $z + 6b = D_{G'}(x_4)$. Note that $w > x, z > y, \frac{6b}{x} > \frac{6b}{w}, \frac{6b}{y} > \frac{6b}{z}$, by Lemma 3, we have

$$\frac{1}{\sqrt{D_{G'}(x_1)D_{G'}(x_2)}} + \frac{1}{\sqrt{D_{G'}(x_3)D_{G'}(x_4)}} > \frac{1}{\sqrt{D_G(x_1)D_G(x_2)}} + \frac{1}{\sqrt{D_G(x_3)D_G(x_4)}}. \tag{21}$$

Let $r_1 = D_G(x_3) + D_G(x_4) = 2M + 30a + 6b$, $r_2 = D_{G'}(x_3) + D_{G'}(x_4) = 2M + 30a + 18b$, $t_1 = D_{G'}(x_1) + D_{G'}(x_2) = 2M + 6a + 6b$, $t_2 = D_G(x_1) + D_G(x_2) = 2M + 6a + 18b$. Then $r_2 - r_1 = t_2 - t_1 = 12b > 0, r_1 - t_1 = 24a > 0$. By Lemma 2, we have

$$\frac{1}{\sqrt{D_{G'}(x_1)+D_{G'}(x_2)}} + \frac{1}{\sqrt{D_{G'}(x_3)+D_{G'}(x_4)}} \geq \frac{1}{\sqrt{D_G(x_1)+D_G(x_2)}} + \frac{1}{\sqrt{D_G(x_3)+D_G(x_4)}} \tag{22}$$

(iv) For the edges $x_1x_6, x_4x_5 \in E(G)$, by the same way as in (iii), we have

$$\frac{1}{\sqrt{D_{G'}(x_1)D_{G'}(x_6)}} + \frac{1}{\sqrt{D_{G'}(x_4)D_{G'}(x_5)}} \geq \frac{1}{\sqrt{D_G(x_1)D_G(x_6)}} + \frac{1}{\sqrt{D_G(x_4)D_G(x_5)}}, \tag{23}$$

$$\frac{1}{\sqrt{D_{G'}(x_1)+D_{G'}(x_6)}} + \frac{1}{\sqrt{D_{G'}(x_4)+D_{G'}(x_5)}} > \frac{1}{\sqrt{D_G(x_1)+D_G(x_6)}} + \frac{1}{\sqrt{D_G(x_4)+D_G(x_5)}}. \tag{24}$$

From Equations (13−24) and the definitions of the Balaban index and the sum-Balaban index, we have $J(G) < J(G')$ and $SJ(G) < SJ(G')$. ■

Using the transformations above, we can get the extremal graphs for the (sum-) Balaban index on polyphenyl hexagonal chains.

Theorem 6 *Let PPC_n be a polyphenyl hexagonal chain of length n. Then*

$$J(P_n) \leq J(PPC_n) \leq J(O_n), \qquad SJ(P_n) \leq SJ(PPC_n) \leq SJ(O_n),$$

with equalities if and only if $PPC_n = O_n$, $PPC_n = P_n$, respectively.

Proof. Suppose on the contrary that $G = H_1H_2 \cdots H_n (n \geq 3)$, a polyphenyl hexagonal chain of length n, has the maximum (sum-) Balaban index, and $G \ncong O_n$. Then there is $1 < k < n$ such that the distance between two cut-vertices u_k and v_k, which belongs to the k-th hexagon H_k, is 2 or 3. Let G' be the graph obtained from G by using the first or the second cut-edge transformation. By Lemmas 4 and 5, we have $J(G) < J(G')$ and $SJ(G) < SJ(G')$, a contradiction. So, O_n is the unique graph with the maximum (sum-) Balaban index. Similarly, we can show that P_n is the unique graph with the minimum (sum-) Balaban index. ■

3. (SUM-) BALABAN INDEX OF SPIRO HEXAGONAL CHAINS

As in the last section, we first give two transformations on SPC_n.

The first cut-vertex transformation on SPC_n: Let $G = \overline{H}_1\overline{H}_2 \cdots \overline{H}_n (n \geq 3)$ be a spiro hexagonal chain of length n, $v_k = x_1$ and $v_{k+1} = x_4$ are two cut-vertices in k-th hexagon $\overline{H_k}$. If G' is the graph obtained from G by taking two cut-vertices $v_k = x_1$ and $v_{k+1} = x_3$ in k-th hexagon $\overline{H_k}$, then we say that G' is obtained from G by the first cut-vertex transformation, see Figure 8.

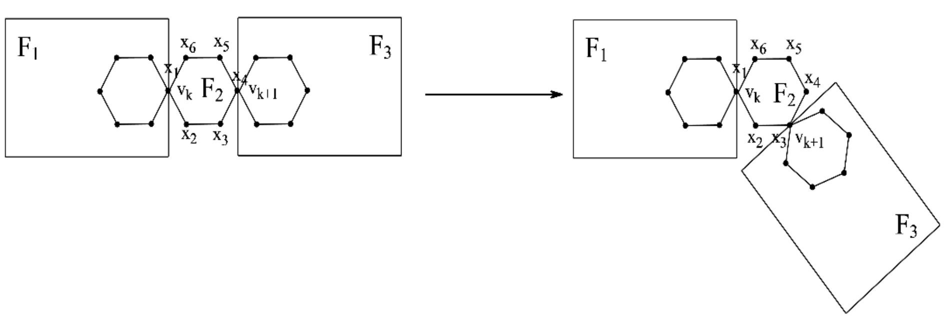

Figure 8: The first cut-vertex transformation.

Lemma 7 *Let $G = \overline{H}_1\overline{H}_2\cdots\overline{H}_n(n \geq 3)$ be a spiro hexagonal chain of length n. G' is obtained from G by the first cut-vertex transformation. Then $J(G) < J(G')$ and $SJ(G) < SJ(G')$.*

Proof. Let $F_1 = \overline{H}_1\overline{H}_2\cdots\overline{H}_{k-1}$, $F_2 = \overline{H_k}$, $F_3 = \overline{H}_{k+1}\overline{H}_{k+2}\cdots\overline{H}_n$ in Figure 8. $V(F_2) = \{x_1, x_2, x_3, x_4, x_5, x_6\}$ and the length of F_1 and F_3 is a and b, respectively, $a + b = n - 1$. Let $M = \sum_{u\in F_1} d_G(x_1, u) + \sum_{u\in F_3} d_G(x_4, u) + \sum_{u\in F_2} d_G(x, u)$, where $x \in V(F_2)$. Then $M = \sum_{u\in F_1} d_{G'}(x_1, u) + \sum_{u\in F_3} d_{G'}(x_3, u) + \sum_{u\in F_2} d_{G'}(x, u)$.
For a vertex $v_x \in F_1$, we have

$$D_G(v_x) = \sum_{u\in F_1} d_G(v_x, u) + \sum_{u\in F_2} d_G(v_x, u) + \sum_{u\in F_3} d_G(v_x, u),$$
$$D_{G'}(v_x) = \sum_{u\in F_1} d_{G'}(v_x, u) + \sum_{u\in F_2} d_{G'}(v_x, u) + \sum_{u\in F_3} d_{G'}(v_x, u),$$

and $\sum_{u\in F_1} d_G(v_x, u) = \sum_{u\in F_1} d_{G'}(v_x, u)$, $\sum_{u\in F_2} d_G(v_x, u) = \sum_{u\in F_2} d_{G'}(v_x, u)$, $\sum_{u\in F_3} d_G(v_x, u) = \sum_{u\in F_3} d_{G'}(v_x, u) + 6b$. So, $D_G(v_x) - D_{G'}(v_x) = 6b$ and $D_G(v_x) > D_{G'}(v_x)$. Similarly, we have $D_G(v_y) - D_{G'}(v_y) = 6a$ for a vertex $v_y \in F_3$. For a vertex in $V(F_2) = \{x_1, x_2, x_3, x_4, x_5, x_6\}$, it can be check directly that

$$D_G(x_1) = M + 18b, D_{G'}(x_1) = M + 12b$$
$$D_G(x_2) = M + 6a + 12b, D_{G'}(x_2) = M + 6a + 6b$$
$$D_G(x_3) = M + 12a + 6b, D_{G'}(x_3) = M + 12a$$
$$D_G(x_4) = M + 18a, D_{G'}(x_4) = M + 18a + 6b$$
$$D_G(x_5) = M + 12a + 6b, D_{G'}(x_5) = M + 12a + 12b$$
$$D_G(x_6) = M + 6a + 12b, D_{G'}(x_6) = M + 6a + 18b.$$

Using the method as in Lemma 4, we can get Lemma 7. ■

The second cut-vertex transformation on SPC_n: Let $G = \overline{H}_1\overline{H}_2\cdots\overline{H}_n(n \geq 3)$ be a spiro hexagonal chain of length n, $v_k = x_1$ and $v_{k+1} = x_3$ are two cut-vertices in k-th hexagon $\overline{H_k}$. If G' is the graph obtained from G by taking two cut-vertices $v_k = x_1$ and $v_{k+1} = x_2$ in k-th hexagon $\overline{H_k}$, then we say that G' is obtained from G by the second cut-vertex transformation (see Figure 9).

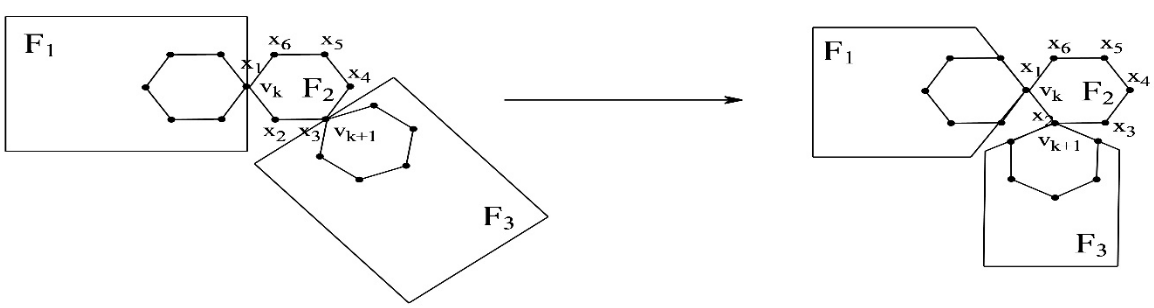

Figure 9: The second cut-vertex transformation.

Lemma 8 *Let* $G = \overline{H}_1\overline{H}_2 \cdots \overline{H}_n (n \geq 3)$ *be a spiro hexagonal chain of length* n. G' *is obtained from* G *by the second cut-vertex transformation. Then* $J(G) < J(G')$ *and* $SJ(G) < SJ(G')$.

Proof. The proof is similar to Lemma 5, we omit it here.

Using the first and the second cut-vertex transformations and Lemmas 7-8, we can directly obtain the following result, which determines the extremal graphs for the (sum-) Balaban index on spiro hexagonal chains.

Theorem 9 *Let* SPC_n *be a spiro hexagonal chain of length* n. *Then*

$$J(SP_n) \leq J(SPC_n) \leq J(SO_n) \text{and} SJ(SP_n) \leq SJ(SPC_n) \leq SJ(SO_n),$$

with equalities if and only if $SPC_n = SO_n$ and $SPC_n = SP_n$, respectively.

Theorem 9 also shows that SO_n and SP_n are the unique graph with the maximum and the minimum (sum-) Balaban index among all spiro hexagonal chains of length n.

ACKNOWLEDGEMENT. Project supported by Hunan Provincial Natural Science Foundation of China (2018JJ2249).

REFERENCES

1. V. Andová, M. Knor, R. Škrekovski, Distance based indices in nanotubical graphs: part 2, *J. Math. Chem.* DOI: 10.1007/s10910-018-0933-2.
2. Y. Bai, B. Zhao, P. Zhao, Extremal Merrifild-Simmons index and Hosoya index of polyphenyl chains, *MATCH Commun. Math. Comput. Chem*. **62** (2009) 649–656.
3. A. T. Balaban, Highly discriminating distance-based topological index, *Chem. Phys. Lett.* 89 (1982) 399–404.
4. A. T. Balaban, Topological index based on topological distance in molecular graphs, *Pure Appl. Chem.* **55** (1983) 199–206.
5. A. T. Balaban, P. V. Khadikar, S. Aziz, Comparison of topological index based on iterated 'sum' versus 'product' operations, *Iranian J. Math. Chem*. **1** (2010) 43–67.
6. A. T. Balaban, L. B. Kier, N. Joshi, Structure-property analysis of octane numbers for hydrocarbons (alkanes, cycloalkanes, alkenes), *MATCH Commun. Math. Comput. Chem.* **28** (1992) 13–27.
7. D. Bonchev, E. J. Markel, A. H. Dekmezian, Long chain branch polymer chain dimensions: application of topology to the Zimm-Stockmayer model, *Polymer* **43** (2002) 203–222.

8. M. Bureš, V. Pekárek, T. Ocelka, Thermochemical properties and relative stability of polychlorinated biphenyls, *Environ. Tox. Pharm.* **25** (2008) 2610–2617.
9. X. Chen, B. Zhao, P. Zhao, Six-membered ring spiro chains with extremal Merrifild-Simmons index and Hosoya index, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 657–665.
10. H. Deng, On the Balaban index of trees, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 253–260.
11. H. Deng, On the Sum-Balaban index, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 273–284.
12. H. Deng, Wiener indices of spiro and polyphenyl hexagonal chains, *Math. Comput. Modelling* **55** (2012) 634–644.
13. H. Deng, Z. Tang, Kirchhoff indices of spiro and polyphenyl hexagonal chains, *Util. Math.* **95** (2014) 113–128.
14. H. Dong, X. Guo, Character of graphs with extremal Balaban index, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 799–812.
15. H. Dong, X. Guo, Character of trees with extremal Balaban index, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 261–272.
16. T. Došlić, M. Litz, Matchings and independent sets in polyphenylene chains, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 313–330.
17. T. Došlić, F. Måløy, Chain hexagonal cacti: Matchings and independent sets, *Discrete Math.* **310** (2010) 1676–1690.
18. W. Fang, Y. Gao, Y. Shao, W. Gao, G. Jing, Z. Li, Maximum Balaban index and Sum-Balaban index of bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **75** (2016) 129–156.
19. W. Fang, H. Yu, Y. Gao, X. Li, G. Jing, Z. Li, Maximum Balaban index and Sum-Balaban index of tricyclic graphs, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 717–742.
20. D. R. Flower, On the properties of bit string-based measures of chemical similarity, *J. Chem. Inf. Comput. Sci.* **38** (1998) 379–386.
21. A. Graja, *Low-Dimensional Organic Conductors*, World Scientific, Singapore, 1992.
22. G. Grassy, B. Calas, A. Yasri, R. Lahana, J. Woo, S. Iyer, M. Kaczorek, F. Floch, R. Buelow, Computer-assisted rational design of immunosuppressive compounds, *Nat. Biotechnol.* **16** (1998) 748–752.
23. G. Huang, M. Kuang, H. Deng, The extremal graph with respect to the matching energy for a random polyphenyl chain, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 121–131.

24. G. Huang, M. Kuang, H. Deng, The expected values of Hosoya index and Merrifield-Simmons index in a random polyphenylence chain, *J. Combin. Opt.* **32** (2) (2016) 550–562.
25. M. Knor, R. Škrekovski, A. Tepeh, Balaban index of cubic graphs, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 519–528.
26. Q. R. Li, Q. Yang, H. Yin, S. Yang, Analysis of by-products from improved Ullmann reaction using TOFMS and GCTOFMS, *J. Univ. Sci. Technol. China* **34** (2004) 335–341.
27. S. Li, B. Zhou, On the Balaban index of trees, *Ars Combin.* **101** (2011) 503–512.
28. G. Luthe, J. A. Jacobus, L. W. Robertson, Receptor interactions by polybrominated diphenyl ethers versus polychlorinated biphenyls: A theoretical structure-activity assessment, *Environ. Tox. Pharm.* **25** (2008) 202–210.
29. L. Sun, Bounds on the Balaban index of trees, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 813–818.
30. S. Tepavčević, A. T. Wroble, M. Bissen, D. J. Wallace, Y. Choi, L. Hanley, Photoemission studies of polythiophene and polyphenyl films produced via surface polymerization by ion-assisted deposition, *J. Phys. Chem. B* **109** (2005) 7134–7140.
31. R. Xing, B. Zhou, A. Graovac, On Sum-Balaban index, *Ars Combin.* **104** (2012) 211–223.
32. W. Yang, F. Zhang, Wiener index in random polyphenyl chains, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 371–376.
33. L. You, X. Dong, The maximum Balaban index (Sum-Balaban index) of unicyclic graphs, *J. Math. Res. Appl.* **34** (2014) 292–402.
34. L. You, H. Han, The maximum Balaban index (Sum-Balaban index) of trees with given diameter, *Ars Combin.* **112** (2013) 115–128.
35. P. Zhao, B. Zhao, X. Chen, Y. Bai, Two classes of chains with maximal and minmal total π-electron energy, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 525–536.

Iranian J. Math. Chem. 8(4) December (2017) 255 – 261

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

An Application of Geometrical Isometries in Non–Planar Molecules

A. A. REZAEI[a,•], A. REISI–VANANI[b] AND S. MASOUM[c]

[a]Department of Pure Mathematics, Faculty of Mathematical Sciences, University of Kashan, Kashan, I. R. Iran
[b]Department of Physical Chemistry, Faculty of Chemistry, University of Kashan, Kashan, I. R. Iran
[c]Department of Analytical Chemistry, Faculty of Chemistry, University of Kashan, Kashan, I. R. Iran

ARTICLE INFO

Article History:

Received 6 April 2016
Accepted 24 April 2016
Published online 14 October 2018
Academic Editor: Ivan Gutman

Keywords:

Frame
Isometry
Orthogonal transformation
Polygon
Non-planar polycyclic molecule

ABSTRACT

In this paper we introduce a novel methodology to transmit the origin to the center of a polygon in a molecule structure such that the special axis be perpendicular to the plane containing the polygon. The mathematical calculations are described completely and the algorithm will be showed as a computer program.

1. INTRODUCTION

An isometry is a distance-preserving injective map between metric spaces. The isometries associated with the Euclidean metric, are called Euclidean motions or rigid motions, which forms a Lie group under composition. This *ancient* group is among the oldest and most studied implicitly, long before the concept of group was invented.

One of the applications of isometries is to transfer or rotate the coordinate system in order to simplify the computations or visions. This usually happens in all branches of sciences which apply the analytic geometry.

•Corresponding Author (Email: a_rezaei@kashanu.ac.ir)
DOI: 10.22052/ijmc.2017.51462.1186

In computational chemistry, sometimes, one needs to calculate some properties in each point on the area of molecule or above and below it, so one must put ghost (Bq) atom in an arbitrary point, exactly. Evaluation of the aromaticity, antiaromaticity and nonaromaticity of compounds by nucleus independent chemical shift criterion (NICS), is an example for it. To NICS calculation at each point above and below of the all polygons, one must put some Bq atoms in various distances on the z axis, straightforwardly. In non-planar molecule, vertically putting Bq atoms in various distances of the rings in different sheets is not very hard, but estimation of components of the nuclear magnetic shielding tensors $\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \ldots$ is very hard and for more complex molecules is impossible. But, using our proposed method and doing calculation separately for each polygon facilitate estimation of nuclear magnetic shielding tensors components. We refer to [3] as a good review published which has collected a large number of works related to NICS criterion.

By mathematical language, in this paper we transfer the origin to the center of a pentagon (or hexagon) in the space, such that the z-axes is perpendicular to the plane containing the polygon (or hexagon). Our motivation is the study of the geometric structure of some molecules such as *Corannulene* and *Sumanene* which are polycyclic aromatic hydrocarbons. This method can be used for other molecules which have polygons in their structure (*Fullerenes*, for example). Thanks to this technique the authors investigated the evaluation of aromaticity of some non-planar molecules in [7]. The content of this article is the mathematical description of the mentioned process. To see the related chemical issues, we refer the reader to [1] and [10].

We begin with a quick review on isometries and frames, and then obtain the desire isometry for our purpose. Finally, as an example we will apply the program for some molecules.

2. ISOMETRIES AND FRAMES

In this section, we shall investigate the isometries of Euclidean space, and see how two frames uniquely determine an isometry.

Definition 2. 1. An isometry, or rigid motion, of Euclidean space is a mapping that preserves the Euclidean distance d between points. More precisely, an isometry is a mapping $F: \mathbb{R}^3 \to \mathbb{R}^3$ for which $d(F(p), F(q)) = d(p, q)$, for all $p, q \in \mathbb{R}^3$.

The most important examples of isometries are translations and orthogonal transformations.

Definition 2. 2. Translation by a point $a \in \mathbb{R}^3$ is a map $T: \mathbb{R}^3 \to \mathbb{R}^3$, for which $T(u) = u + a$. An orthogonal transformation of $\mathbb{R}^3$ is a linear transformation $C: \mathbb{R}^3 \to \mathbb{R}^3$ which preserves inner product, namely $C(p).C(q) = p.q$.

For instance, rotations around a coordinate axis are orthogonal transformations. By simple computations, one can show that If F and G are isometries of $\mathbb{R}^3$, then the composite mapping $G \circ F$ is also an isometry of $\mathbb{R}^3$. A vital theorem in differential geometry asserts that If F is an isometry of $\mathbb{R}^3$, then there exists a unique translation T and a unique orthogonal transformation C such that $F = T \circ C$ [6].

Definition 2. 3. A set $\{e_1, e_2, e_3\}$ of pair-wise orthogonal unit vectors tangent to $p \in \mathbb{R}^3$ is called a frame at p.

For example, $\{i = (1,0,0), j = (0,1,0), k = (0,0,1)\}$ is a frame at each point of $\mathbb{R}^3$, which is called the standard frame. It is clear that at each point of the Euclidean space, there exist uncountable frames. Depending on the application, certain frames are used. For example in local curve theory, the Frenet frame [5], determines the geometric properties of the curve. Here we use the frames to obtain an important isometry. First we state a vital theorem in differential geometry, see [6] for example.

Theorem 2. 4. For any two frames $\{e_1, e_2, e_3\}$ and $\{f_1, f_2, f_3\}$ at the points $p, q \in \mathbb{R}^3$ respectively, there exists a unique isometry F of $\mathbb{R}^3$ such that F maps the tangent vector e_i to tangent vector f_i, for $i = 1, 2, 3$.

To compute the isometry F in the above theorem, let $e_i = (a_{i1}, a_{i2}, a_{i3})$, $f_i = (b_{i1}, b_{i2}, b_{i3})$, $A = (a_{ij})$, $B = (b_{ij})$, and $C = B^t A$. A and B are the attitude matrices of the $\{e_i\}$ and $\{f_i\}$ frames, respectively. Now C is an orthogonal transformation and $C(e_i) = f_i$. If T be the translation by the point $q - C(p)$, then $F = T \circ C$ is the desired isometry.

3. APPLICATION AND ILLUSTRATION

Here we apply the last theorem in previous section to transfer the origin and the standard frame to the center of an arbitrary pentagon or hexagon in a polycyclic molecule (corannulene, sumanene, or fullerene), such that the z-axis will be perpendicular on this polygon. To do so, we need a frame on the center point of polygon.

Although we don't investigate the chemical aspects of these compounds, a brief introduction may be interesting (for some mathematical facets of Fullerenes, see [2], [8], and [9]).

Corannulene is a polycyclic aromatic hydrocarbon with one central pentagonal ring and five peripheral hexagonal rings, Figure 1(a). Sumanene is a polycyclic aromatic hydrocarbon with one central hexagonal ring and three peripheral hexagonal and three peripheral pentagonal rings, alternately, Figure 1(b). Fullerenes are a family of carbon allotropes which composed entirely of carbon, in the form of a sphere, ellipsoid, cylinder, or tube. The structure of fullerenes is composed of hexagonal, pentagonal or sometimes heptagonal and octagonal rings, Figure 1(c).

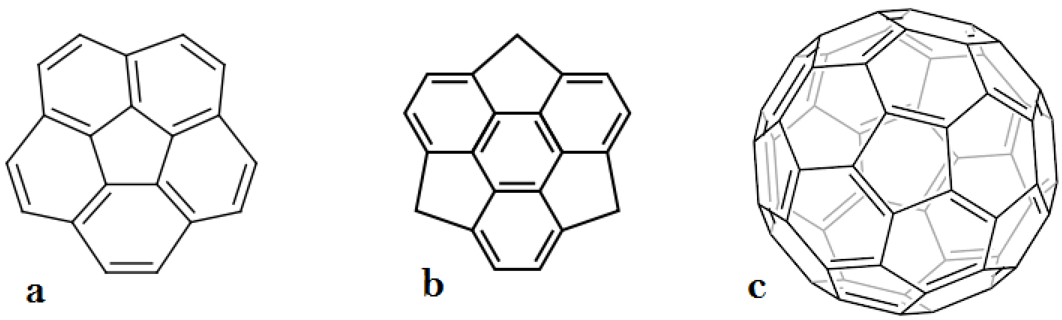

Figure 1. Structure of: (a) corannulene, (b) sumanene, and (c) a fullerene molecules.

We describe the method for a hexagon, the case pentagon is similar. Let p_1, p_2 and p_3 are three consecutive vertices of the hexagon. Then the vector $\overrightarrow{p_1p_2} \times \overrightarrow{p_1p_3}$ is perpendicular to the plane containing the hexagon. Dividing this vector by its own length, we have the unit vector

$$u_3 = \frac{\overrightarrow{p_1p_2} \times \overrightarrow{p_1p_3}}{|\overrightarrow{p_1p_2} \times \overrightarrow{p_1p_3}|}.$$

Multiply u_3 by the unit vector $u_1 = \frac{\overrightarrow{p_1p_2}}{|\overrightarrow{p_1p_2}|}$ to get the unit vector $u_2 = u_3 \times u_1$. Now the set $\{u_1, u_2, u_3\}$ is a frame. To obtain an isometry F which maps the frame $\{u_1, u_2, u_3\}$ to the standard frame $\{i, j, k\}$, let $u_1 = (a_{11}, a_{12}, a_{13})$, $u_2 = (a_{21}, a_{22}, a_{23})$, $u_3 = (a_{31}, a_{32}, a_{33})$, then $A = (a_{ij})$ and B is the identity matrix, so $C = B^t A = A$, namely:

$$C = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix},$$

i.e. if $q = (x, y, z)^t$ be the primary coordinate of the point q, then its new coordinate is given by:

$$F(q) = \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

We did all calculations of coordinate transformation in MATLAB environment. This program has been shown in the following lines.

```
function [B,Fx]=Transfer(A);

%      A: First coordination of the molecule
%      B: New coordination after origin transfer
%      Fx: Final coordination
clc
n1=input('n1=');n2=input('n2=');n3=input('n3=');
n4=input('n4=');n5=input('n5=');n6=input('n6=');
c=mean([A(n1,:);A(n2,:);A(n3,:);A(n4,:);A(n5,:);A(n6,:)])*(-1);
B=[(A(:,1)+c(1,1)),(A(:,2)+c(1,2)),(A(:,3)+c(1,3))];
p1=B(n1,:);p2=B(n2,:);p3=B(n3,:);
p1p2=[p2(1,1)-p1(1,1),p2(1,2)-p1(1,2),p2(1,3)-p1(1,3)];
p1p3=[p3(1,1)-p1(1,1),p3(1,2)-p1(1,2),p3(1,3)-p1(1,3)];
u4=[(p2(1,2)-p1(1,2))*(p3(1,3)-p1(1,3))-(p2(1,3)-p1(1,3))*
(p3(1,2)-p1(1,2)),(p2(1,3)-p1(1,3))*(p3(1,1)-p1(1,1))-(p2(1,1)-p1(1,1))*
(p3(1,3)-p1(1,3)),(p2(1,1)-p1(1,1))*(p3(1,2)-p1(1,2))-(p2(1,2)-p1(1,2))*
(p3(1,1)-p1(1,1))];
Q=norm(p1p2);T=norm(u4);
a11=(p2(1,1)-p1(1,1))/Q;
a12=(p2(1,2)-p1(1,2))/Q;
a13=(p2(1,3)-p1(1,3))/Q;
a31=((p2(1,2)-p1(1,2))*(p3(1,3)-p1(1,3))-(p2(1,3)-p1(1,3))*(p3(1,2)-p1(1,2)))/T;
a32=((p2(1,3)-p1(1,3))*(p3(1,1)-p1(1,1))-(p2(1,1)-p1(1,1))*(p3(1,3)-p1(1,3)))/T;
a33=((p2(1,1)-p1(1,1))*(p3(1,2)-p1(1,2))-(p2(1,2)-p1(1,2))*(p3(1,1)-p1(1,1)))/T;
a21=(a13*a32)-(a12*a33);
a22=(a11*a33)-(a13*a31);
a23=(a12*a31)-(a11*a32);
u1=[a11 a12 a13];
u2=[a21 a22 a23];
u3=[a31 a32 a33];
w=u1*u2';z=u2*u3';v=u3*u2';
H=[a11 a21 a31;a12 a22 a32;a13 a23 a33];
F=B';G=[F(1,:);F(2,:);F(3,:)];
Fx=(H'*G)';
```

As an example we apply the program for corannulene molecule. Figure 2 shows the structure of molecule before and after translating and rotating the coordinate system.

4. CONCLUSION AND REMARK

Proposed methodology in this work helps ones to transmit origin of coordinate to an arbitrary point and changes the axes coordinate direction perpendicular to an arbitrary polygon. It facilitates estimation of components of the nuclear magnetic shielding tensors in non-planar molecules and can be used for any calculation that needs to such coordinate change. Although our discussion was based on z-axis, but it can be used for other axes by a simple rotation.

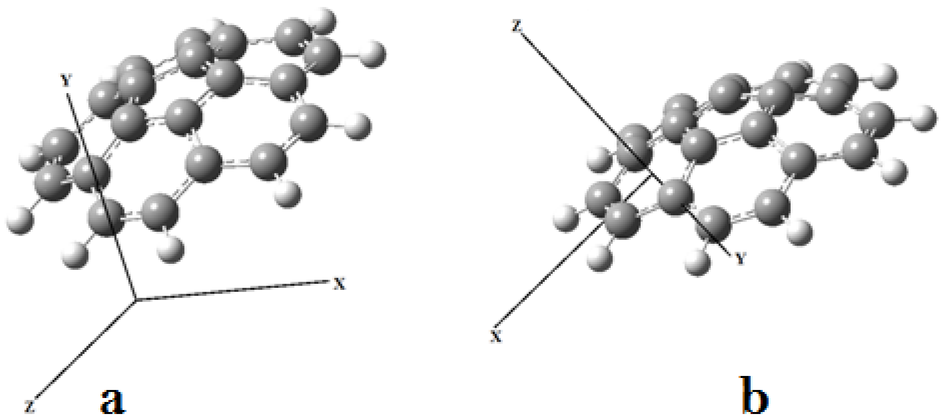

Figure 2. Corannulene molecule: (a) origin coordinate in in arbitrary point, (b) molecule was rotated with uncertain angle such that z-axis is perpendicular to hexagon.

ACKNOWLEDGEMENT. The authors are grateful to the University of Kashan for supporting this work by Grant No. 572767.

REFERENCES

1. W. E. Barth, R. G. Lawton, Dibenzo[ghi,mno]fluoranthene, *J. Am. Chem. Soc.* **88** (1966) 380–381.
2. F. Cataldo, A. Graovac, O. Ori, *The Mathematics and Topology of Fullerenes*, Springer, Verlag, Berlin, 2011.
3. Z. Chen, C. S. Wannere, C. Corminboeuf, R. Puchta, P. V. R. Schleyer, Nucleus-independent chemical shifts (NICS) as an aromaticity criterion, *Chemical Reviews-Columbus* **105** (2005) 3842–3888.
4. H. Fallah Bagher Shaidaei, C. S. Wannere, C. Corminboeuf, R. Puchta, P. V. R. Schleyer, Which NICS aromaticity index for planar rings is best?, *Organic Letters* **8** (2006) 863–866.
5. R. Millman and G. Parker, *Elements of Differential Geometry*, Prentice-Hall, 1977.
6. B. O'Neill, *Elementary Differential Geometry*, 2nd ed. Academic Press, 1997.
7. A. Reisi−Vanani, A. A. Rezaei, Evaluation of the aromaticity of non-planar and bowl-shaped molecules by NICS criterion, *J. Mol. Graph. Model.* **61** (2015) 85–88.

8. A. A. Rezaei, Polygonal tiling of some surfaces containing fullerene molecules, *Iranian J. Math. Chem.* **5** (2) (2014) 2 99–105.
9. A. A. Rezaei, Tiling fullerene surface with heptagon and octagon, *Fullerenes, Nanotubes, Carbon Nanostructures* **23** (12) (2015) 1033–1036.
10. H. Sakurai, T. Daiko, T. Hirao, A synthesis of sumanene, a fullerene fragment, *Science* **301** (2003) 1878–1878.

Iranian J. Math. Chem. 9 (4) December (2018) 263 − 277

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

On ev−Degree and ve−Degree Topological Indices

B. ŞAHIN[1,•] AND S. EDIZ[2]

[1]Faculty of Science, Selçuk University, Konya, Turkey
[2]Faculty of Education, Yuzuncu Yil University, Van, Turkey

ARTICLE INFO

Article History:

Received 10 January 2017
Accepted 25 March 2017
Published online 31 December 2018
Academic Editor: Tomislav Došlić

Keywords:

ev−Degree
ve−Degree
ev−Degree topological index
ve−Degree topological index

ABSTRACT

Recently two new degree concepts have been defined in graph theory: *ev*-degree and *ve*-degree. Also the *ev*-degree and *ve*-degree Zagreb and Randić indices have been defined very recently as parallel of the classical definitions of Zagreb and Randić indices. It was shown that *ev*-degree and *ve*-degree topological indices can be used as possible tools in QSPR researches [2]. In this paper, we define the *ve*-degree and *ev*-degree Narumi–Katayama indices, investigate the predicting power of these novel indices and extremal graphs with respect to these novel topological indices. Also we give some basic mathematical properties of *ev*-degree and *ve*-degree Narumi-Katayama and Zagreb indices.

1. INTRODUCTION

Topological indices have important place in theoretical chemistry. Many topological indices were defined by using vertex degree concept. The Zagreb and Randić indices are the most used degree based topological indices so far in mathematical and chemical literature among the all topological indices. Very recently, Chellali, Haynes, Hedetniemi and Lewishave published a seminal study: On *ve*-degrees and *ev*-degrees in graphs [1]. The authors defined two novel degree concepts in graph theory; *ev*-degrees and *ve*-degrees and investigate some basic mathematical properties of both novel graph invariants with regard to graph regularity and irregularity [1]. After given the equality of the total *ev*-degree and total *ve*-degree for any graph, also the total *ev*-degree and the total *ve*-degree were stated as in relation to the first Zagreb index. It was proposed in the article that the chemical applicability of the total *ev*-degree (and the total *ve*-degree) could be an interesting problem in view of chemistry and chemical graph theory. In the light of this suggestion, one of the

•Corresponding author (Email: shnbnymn25@gmail.com)
DOI: 10.22052/ijmc.2017.72666.1265

present author has carried these novel degree concepts to chemical graph theory by defining the *ev*-degree and *ve*-degree Zagreb and Randić indices [2]. It was compared these new group *ev*-degree and *ve*-degree indices with the other well-known and most used topological indices in literature such as; Wiener, Zagreb and Randić indices by modeling some physicochemical properties of octane isomers [2]. It was shown that the *ev*-degree Zagreb index, the *ve*-degree Zagreb and the *ve*-degree Randić indices give better correlation than Wiener, Zagreb and Randić indices to predict the some specific physicochemical properties of octanes [2]. Also it was given the relations between the second Zagreb index and *ev*-degree and *ve*-degree Zagreb indices and some mathematical properties of *ev*-degree and *ve*-degree Zagreb indices [2]. In this paper we define the *ve*-degree and *ev*-degree Narumi–Katayama indices, investigate the predicting power of these novel indices and extremal graphs with respect to these topological indices. Also we give some basic mathematical properties of *ev*-degree and *ve*-degree Zagreb indices.

A graph $G = (V,E)$ consists of two nonempty sets V and 2-element subsets of V namely E. The elements of V are called vertices and the elements of E are called edges. For a vertex v, $\deg(v)$ show the number of edges that incident to v. The set of all vertices which adjacent to v is called the open neighborhood of v and denoted by $N(v)$. If we add the vertex v to $N(v)$, then we get the closed neighborhood of v, $N[v]$.

The first and second Zagreb indices [3] defined as follows: The first Zagreb index of a connected graph G, defined as,

$$M_1 = M_1(G) = \sum_{u\in V(G)} \deg(u)^2 = \sum_{uv\in E(G)}(\deg(u) + \deg(v)).$$

and the second Zagreb index of a connected graph G, defined as

$$M_2 = M_2(G) = \sum_{uv\in E(G)} \deg(u) . \deg(v).$$

The authors investigated the relationship between the total π-electron energy on molecules and Zagreb indices [3]. For the details see the references [4−6]. Randić investigated the measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons via Randić index [7]. The Randić index of a connected graph G defined as;

$$R = R(G) = \sum_{uv\in E(G)}(\deg(u) . \deg(v))^{-1/2} .$$

We refer the interested reader to [8−10] and the references therein for the up to date arguments about the Randić index.

The forgotten topological index for a connected graph G is defined as,

$$F = F(G) = \sum_{u\in V(G)} \deg(u)^3 = \sum_{uv\in E(G)}(\deg(u)^2 + \deg(v)^2) .$$

It was showed in [11] that the predictive power of the forgotten topological index is very close to the first Zagreb index for the entropy and eccentric factor. For further studies about the forgotten topological index we refer to the interested reader [11−13] and references therein.

In the 1980s, Narumi and Katayama considered the production of the degrees of vertices

$$NK = NK(G) = \prod_{v\in V(G)} \deg(v)$$

and named it the "simple topological index'' [14]. Later for this graph invariant, the name ''Narumi-Katayama index'' was used in [15–17]. The extremal graphs with respect to NK index was studied by Gutman and Ghorbani [15], Zolfi and Ashrafi [20]. Some relations between the Narumi-Katayama index and the first Zagreb index were introduced in the more recent paper [21].

Multiplicative version of the first Zagreb index of a connected graph was defined by Eliasi et. al. in [22] as:

$$\Pi_1^* = \Pi_1^*(G) = \prod_{uv\in E(G)} (\deg(u) + \deg(v)).$$

For detailed discussions of the multiplicative version of Zagreb indices, we refer the interested reader to [23] and the references cited therein.

In the following section, we will give basic definitions of *ev*-degree and *ve*-degree concepts, *ve*-degree and *ev*-degree Zagreb indices and as well as the basic mathematical properties of these novel topological indices. And also we give the definitions of *ev*-degree and *ve*-degree Narumi-Katayama indices.

2. ve-Degree and ev-Degree Concepts and Corresponding Topological Indices

In this section we give the definitions of *ev*-degree and *ve*-degree concepts which were given by Chellali et al. in [1] and the definitions and properties of *ev*-degree and *ve*-degree topological indices.

Definition 2.1 [1] *Let G be a connected graph and $v \in V(G)$. The ve-degree of the vertex v, $deg_{ve}(v)$, equals the number of different edges that incident to any vertex from the closed neighborhood of v. For convenience we prefer to show the ve-degree of the vertex v, by c_v.*

Definition 2.2 [1] *Let G be a connected graph and $e = uv \in E(G)$. The ev-degree of the edge e, $deg_{ev}(e)$, equals the number of vertices of the union of the closed neighborhoods of u and v. For convenience we prefer to show the ev-degree of the edge $e = uv$, by c_e or c_{uv}.*

Definition 2.3 [1] *Let G be a connected graph and $v \in V(G)$. The total ev-degree of the graph G is defined as $T_e = T_e(G) = \sum_{e\in E(G)} c_e$ and the total ve-degree of the graph G is defined as $T_v = T_v(G) = \sum_{v\in V(G)} c_v$.*

Observation 2.4 [1] *For any connected graph G, $T_e(G) = T_v(G)$.*

Observation 2.5 [1] *For any triangle free connected graph* G, $c_e = c_{uv} = \deg(u) + \deg(v)$.

The following theorem states the relationship between the first Zagreb index and the total *ve*-degree of a connected graph G.

Theorem 2.6 [1] *For any connected graph* G, $T_e(G) = T_v(G) = M_1(G) - 3n(G)$, *where* $n(G)$ *denotes the total number of triangles in* G.

In [1], the authors suggested the idea that to carry these novel degree concepts to mathematical chemistry. One of the present author following this suggestion defined *ev*-degree and *ve*-degree Zagreb indices and showed that these novel group Zagreb and Randić indices give better correlation than well-known topological indices such as; Wiener, Zagreb and Randić indices to modeling some physicochemical properties of octane isomers [2]. And now, we give the definitions and some basic mathematical properties of ev-degree and ve-degree Zagreb indices which were given in [2].

Definition 2.7 [2] *Let* G *be a connected graph and* $e \in E(G)$. *The ev-degree Zagreb index of the graph* G *is defined as* $S = S(G) = \sum_{e \in E(G)} c_e^{\,2}$.

Definition 2.8 [2] *Let* G *be a connected graph and* $v \in V(G)$. *The first ve-degree Zagreb alpha index of the graph* G *is defined as* $S^{\alpha} = S^{\alpha}(G) = \sum_{v \in V(G)} c_v^{\,2}$.

Definition 2.9 [2] *Let* G *be a connected graph and* $uv \in E(G)$. *The first ve-degree Zagreb beta index of the graph* G *is defined as* $S^{\beta} = S^{\beta}(G) = \sum_{uv \in E(G)} (c_u + c_v)$.

Definition 2.10 [2] *Let* G *be a connected graph and* $uv \in E(G)$. *The second ve-degree Zagreb index of the graph* G *is defined as* $S^{\mu} = S^{\mu}(G) = \sum_{uv \in E(G)} c_u c_v$.

Definition 2.11 [2] *Let* G *be a connected graph and* $uv \in E(G)$. *The ve-degree Randić index of the graph* G *is defined as* $R^{\alpha} = R^{\alpha}(G) = \sum_{uv \in E(G)} (c_u c_v)^{-1/2}$.

And now we restate the some basic properties of ev-degree and ve-degree Zagreb indices which were given in [2].

Lemma 2.12 [2] *Let* T *be a tree and* $v \in V(T)$ *then,* $c_v = \sum_{u \in N(v)} \deg(u)$.

Theorem 2.13 [2] *Let T be a tree with the vertex set* $V(T) = \{v_1, v_2, \ldots, v_n\}$ *then,* $S^{\beta}(T) = 2M_2(T)$.

Theorem 2.14 [2] *Let G be a triangle free connected graph, then;* $S(G) = F(G) + 2M_2(G)$.

Corollary 2.15 *Let T be a tree then,* $S(T) = F(T) + S^{\beta}(T)$.

And now we give the definitions of *ev*-degree and *ve*-degree Narumi-Katayama indices for a graph *G*.

Definition 2.16 *The ve-Narumi-Katayama index of a graph G is defined with the following equation* $NK_{ve} = NK_{ve}(G) = \prod_{v \in V(G)} c_v$.

If a graph has an isolated vertex, its $NK_{ve} = 0$ which is the minimal value of NK_{ve}. We take the graphs without isolated vertices in the following results which will be introduced in the section four.

Definition 2.17 *The ev-Narumi-Katayama index of a graph G is defined with the following equation* $NK_{ev} = NK_{ev}(G) = \prod_{e \in E(G)} c_e$.

In the next section we investigate the predicting power of these novel topological indices and after that we investigate some mathematical properties of these novel indices.

3. New Tools for QSPR Researches: The ev−Narumi−Katayama Index and the ve−Narumi−Katayama Index

In this section we compare the Narumi-Katayama index and its corresponding versions ofthe *ev*-Narumi-Katayama and *ve*-Narumi-Katayama indices with each other by using strong correlation coefficients acquired from the chemical graphs of octane isomers. We get the experimental results at the www.moleculardescriptors.eu (see Table 1). The following physicochemical features have been modeled:

- Entropy,
- Acentric factor (AcenFac),
- Enthalpy of vaporization (HVAP),
- Standard enthalpy of vaporization (DHVAP).

We select those physicochemical properties of octane isomers for which give reasonably good correlations, i.e. the absolute value of correlation coefficients are larger than 0.8959 (see Table 2). Also we find the Narumi-Katayama index of octane isomers values at thewww.moleculardescriptors.eu (see Table 3). We also calculate and show the *ev*-Narumi-Katayama and the *ve*-Narumi-Katayama indices of octane isomers values in Table 3.

Table 1. Some physicochemical properties of octane isomers.

Molecule	Entropy	AcenFac	HVAP	DHVAP
n-octane	111.70	0.39790	73.19	9.915
2-methyl-heptane	109.80	0.37792	70.30	9.484
3-methyl-heptane	111.30	0.37100	71.30	9.521
4-methyl-heptane	109.30	0.37150	70.91	9.483
3-ethyl-hexane	109.40	0.36247	71.70	9.476
2,2-dimethyl-hexane	103.40	0.33943	67.70	8.915
2,3-dimethyl-hexane	108.00	0.34825	70.20	9.272
2,4-dimethyl-hexane	107.00	0.34422	68.50	9.029
2,5-dimethyl-hexane	105.70	0.35683	68.60	9.051
3,3-dimethyl-hexane	104.70	0.32260	68.50	8.973
3,4-dimethyl-hexane	106.60	0.34035	70.20	9.316
2-methyl-3-ethyl-pentane	106.10	0.33243	69.70	9.209
3-methyl-3-ethyl-pentane	101.50	0.30690	69.30	9.081
2,2,3-trimethyl-pentane	101.30	0.30082	67.30	8.826
2,2,4-trimethyl-pentane	104.10	0.30537	64.87	8.402
2,3,3-trimethyl-pentane	102.10	0.29318	68.10	8.897
2,3,4-trimethyl-pentane	102.40	0.31742	68.37	9.014
2,2,3,3-tetramethylbutane	93.06	0.25529	66.20	8.410

Table 2. Topological indices of octane isomers.

Molecule	Nar	*ev*Nar	*ve*Nar
n-octane	4.159	9.129	9.129
2-methyl-heptane	3.871	9.640	9.757
3-methyl-heptane	3.871	9.575	9.575
4-methyl-heptane	3.871	9.575	9.510
3-ethyl-hexane	3.871	9.510	9.352
2,2-dimethyl-hexane	3.466	10.491	10.738
2,3-dimethyl-hexane	3.584	10.045	10.098
2,4-dimethyl-hexane	3.584	10.085	10.163
2,5-dimethyl-hexane	3.584	10.150	10.386
3,3-dimethyl-hexane	3.466	10.386	10.450
3,4-dimethyl-hexane	3.584	9.980	9.940
2-methyl-3-ethyl-pentane	3.584	9.980	9.911
3-methyl-3-ethyl-pentane	3.466	10.281	10.240
2,2,3-trimethyl-pentane	3.178	10.869	11.075
2,2,4-trimethyl-pentane	3.178	11.002	11.298
2,3,3-trimethyl-pentane	3.178	10.828	11.010
2,3,4-trimethyl-pentane	3.296	10.515	10.658
2,2,3,3-tetramethylbutane	2.773	11.736	12.210

Table 3. The correlation coefficients between new and old topological indices and some physicochemical properties of octane isomers.

Index	Entropy	AcenFac	HVAP	DHVAP
Nar	0.9398	0.9700	0.8959	0.9410
ve-Nar	-0.9192	-0.9092	-0.9236	-0.9490
ev-Nar	-0.9369	-0.9486	-0.9202	-0.9568

Table 4. The squares of correlation coefficients between topological indices and some physicochemical properties of octane isomers.

Index	Entropy	AcenFac	HVAP	DHVAP
Nar	0.8832	0.9409	0.8026	0.8854
ve-Nar	0.8449	0.8266	0.8530	0.9006
ev-Nar	0.8778	0.8998	0.8468	0.9154

Note that the all values in Table 2 are given by using natural logarithm. It can be seen from the Table 2 that the most convenient indices which are modeling the Entropy, Enthalpy of vaporization (HVAP), Standard enthalpy of vaporization (DHVAP) and Acentric factor (AcenFac) are Narumi-Katayama index (S) for entropy and Acentric Factor, *ve*-Narumi-Katayama index for the Enthalpy of vaporization (HVAP) and *ev*-Narumi-Katayama index for the Standard enthalpy of vaporization (DHVAP), respectively. But notice that the Narumi-Katayama index show the positive strong correlation and the *ve*-Narumi-Katayama and the*ev*-Narumi-Katayama indices show the negative strong correlation. Because of this fact we can compare these graph invariants with each other by using the squares of correlation coefficients for ensure the compliance between the positive and negative correlation coefficients (see Table 4).

The cross-correlation matrix of the indices are given in Table 5.

Table 5. The cross-correlation matrix of the topological indices.

Index	Nar	*ve*-Nar	*ev*-Nar
Nar	1.0000		
ve-Nar	-0.9901	1.0000	
ev-Nar	-0.9715	0.9931	1.0000

It can be shown from the Table 5 that the absolute value of the minimum correlation efficient among the indices is 0.9715 which is indicate strong correlation among all these indices. From the above arguments, we can say that the *ve*-Narumi-Katayama index and *ev*-Narumi-Katayama index are possible tools for QSPR researches.

4. MAIN RESULTS

In this section, we firstly give some basic mathematical properties of *ve*-degree, *ev*-Narumi-Katayama and *ve*-Narumi-Katayama indices. Secondly, we investigate certain mathematical properties of *ev*-degree and *ve*-degree Zagreb indices.

Lemma 4.1. *Let G be a connected graph, then* $\sum_{v\in V(G)} n_v = \sum_{e\in E(G)} n_e = 3n(G)$, *where* n_v, n_e , $n(G)$ *denote the number of triangles in G containing the vertex v, the number of triangles in G containing the edge e and the total number of triangles in G, respectively.*

Proof. The second part of this equality were given in [1]. The first part comes from that since every triangle consists of three vertices and edges, we count every triangle exactly three times for each vertex. Since the total number of triangles in the graph *G* will not be changed, the desired result acquired easily. □

Lemma 4.2. *Let G be a connected graph and* $v \in V(G)$, *then* $c_v = \sum_{u\in N(v)} \deg(u) - n_v$.

Proof. From the Definition 2.1, we know that c_v equals the number of different edges incident to any vertex of $N(v)$. Therefore $c_v = \sum_{u\in N(v)} \deg(u)$ if v does not lie in a triangle. But if v belongs a triangle then the edge that does not incident to v of this triangle must be counted twice in the sum $\sum_{u\in N(v)} \deg(u)$. Therefore we must minus one from the sum $\sum_{u\in N(v)} \deg(u)$ for we find the exact number of different edges incident to $N(v)$. Thus if v lies in more than one triangle then we must minus n_v from the the sum $\sum_{u\in N(v)} \deg(u)$ for we find the exact number of different edges incident to $N(v)$. □

Corollary 4.3. *For the n-vertex triangle graph G, the ve-degree Narumi-Katayama index* $NK_{ve}(G)$ *is calculated by the following equation:*

$$NK_{ve}(G) = \prod_{v\in V}\left(\sum_{u\in N(v)} \deg(u)\right).$$

Example 4.4. *Consider the* P_2 *path graph* $c_{v_1} = c_{v_2} = 1$ *and* $NK_{ve}(P_2) = 1$. *For* P_3 *path graph* $c_{v_1} = c_{v_2} = c_{v_3} = 2$ *and* $NK_{ve}(P_3) = 8$. *For* P_4, $c_{v_1} = c_{v_4} = 2$ *and* $c_{v_2} = c_{v_3} = 3$ *so that* $NK_{ve}(P_4) = 36$. *We take the* P_n *such that* $n \geq 5$. $c_{v_1} = c_{v_n} = 2$ *and* $c_{v_2} = c_{v_{n-1}} = 3$ *and the* ve*-degree of the other vertices are 4. Therefore* $NK_{ve}(P_n) = 9.4^{n-3}$.

Example 4.5. *Consider the C_3 cycle $c_{v_1} = c_{v_2} = c_{v_3} = 3$ and $NK_{ve}(C_3) = 27$. For $n \geq 4$ every cycle 4_{ve}-regular and $NK_{ve}(C_n) = 4^n$.*

Example 4.6. *Consider the S_n-star graph on n vertices. Every vertices have the same ve-degree such that $(n-1)$. This means $NK_{ve}(S_n) = (n-1)^n$.*

Example 4.7. *Consider the K_n-complete graph with n vertices. K_n is a m_{ve}-regular graph with the size $m = n(n-1)/2$. Therefore, $NK_{ve}(K_n) = m^n$.*

Proposition 4.8. *Let G be a graph with n vertices, then $NK_{ve}(G) \leq NK_{ve}(K_n)$.*

Proof. Note that contribution each edge is positive. Hence, $NK_{ve}(G)$ reaches its maximum value for the complete graphs. □

Proposition 4.9. *For the P_n-path graph with n vertices such that $n \geq 4$, $NK_{ve}(P_n) = NK_{ev}(P_n) = 9.4^{n-3}$.*

Proof. We have already known that $NK_{ve}(P_n) = 9.4^{n-3}$ from the Example 4.4. There are $n-3$ edges with their *ev*-degrees equal 4 and 2 edges with their *ev*-degrees equal 3 for the *n*-vertex path. Therefore, the proof is complete. □

Proposition 4.10. *For the cycle C_n on n vertices such that $n \geq 4$,$NK_{ve}(C_n) = NK_{ev}(C_n) = 4^n$.*

Proof. From the Example 4.5 we can directly write that $NK_{ve}(C_n) = 4^n$. Clearly, from the definition of *ev*-degree, every edge of C_n is 4_{ev}-regular. The proof comes from this fact. □

Proposition 4.11. *For the S_n-star graph with n vertices such that $n \geq 4$, $NK_{ev}(S_n) = n^{n-1} < NK_{ve}(S_n) = (n-1)^n$.*

Proof. We make the proof by induction on n. For $n = 4$, $NK_{ev}(S_4) = 4^3 = 64 < NK_{ve}(S_4) = 3^4 = 81$, as desired. We assume that the claim is true for $n = k$ and we will show that it is true $n = k+1$. For $n = k$, $k^{k-1} < (k-1)^k$ is equivalent to

$$\left(1 + \frac{1}{k-1}\right)^{k-1} < k-1$$

and for $n = k+1$, $(k+1)^k < k^{k+1}$. Thus we want to show that

$$\left(1 + \frac{1}{k}\right)^k < k. \ \left(1 + \frac{1}{k}\right)^k < \left(1 + \frac{1}{k-1}\right)^k = \left(1 + \frac{1}{k-1}\right)^{k-1}\left(1 + \frac{1}{k-1}\right) < (k-1)\frac{k}{k-1} = k.$$

So, the proof is complete. □

Theorem 4.12. (*a*) *The n-vertex tree with maximal* NK_{ve} *is* S_n *such that* $NK_{ve}(S_n) = (n-1)^n$.
(*b*) *The* n*-vertex unicyclic graph with the maximal* NK_{ve} *is* $S_n + e$ (*depicted in Figure 1*) *such that* $NK_{ve}(S_n + e) = n^3(n-1)^{n-3}$.
(*c*) *The* n*-vertex bicyclic graph with the maximal* NK_{ve} *is* Z_n (*depicted in Figure 1*) *such that* $NK_{ve}(Z_n) = (n+1)^4(n-1)^{n-4}$.

Figure 1. The graphs $S_n + e$ and Z_n.

Theorem 4.13. (a) *The* n*-vertex tree with minimal* NK_{ve} *is* $P_n (n \geq 4)$ *such that* $NK_{ve}(P_n) = 9.4^{n-3}$.
(b) *The* n*-vertex unicyclic graph with the minimal* NK_{ve} *is* R_n (*depicted in Figure 2*) *such that* $NK_{ve}(R_n) = 2.3.5^2.4^{n-4}$.
(*c*) *The* n*-vertex bicyclic graph with the minimal* NK_{ve} *is* T_n (*depicted in Figure 2*) *such that* $NK_{ve}(T_n) = 5^4.4^{n-4}$.

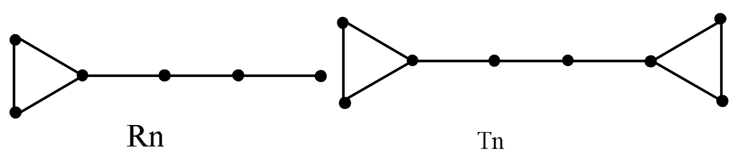

Figure 2. Graphs which are used for Theorem 2.

Theorem 4. 14. (*a*) *The* n*-vertex tree with second maximal* NK_{ve} *is* X_n (*depicted in Figure 3*) *such that* $NK_{ve}(X_n) = 2(n-1)^2(n-2)^{n-3}$.
(*b*) *The* n*-vertex unicyclic graph with second maximal* NK_{ve} *is* $S_n + e + e'$ (*depicted in Figure 4*) *such that* $NK_{ve}(S_n + e + e') = 4.n^3(n-2)^{n-4}$.
(*c*) *The* n*-vertex bicyclic graph with second maximal* NK_{ve} *is* L_n (*depicted in Figure 3*) *such that* $NK_{ve}(L_n) = 5.(n+1)^2 n^2 (n-2)^{n-5}$.

Theorem 4.15. (*a*) *The* n*-vertex tree with second minimal* NK_{ve} *is the* Q*-graph* (*depicted in Figure 5*) *such that* $NK_{ve}(Q) = 2^2.3^3.5^3.4^{n-8}$.
(*b*) *The* n*-vertex unicyclic graph with second minimal* NK_{ve} *is the* R*-graph* (*depicted in Figure 6*) *such that* $NK_{ve}(R) = 2.3^2.5^5.4^{n-8}$.

(*c*) *The n-vertex bicyclic graph with second minimal NK_{ve} is the S-graph* (*depicted in Figure 7*) *such that* $NK_{ve}(S) = 3.5^7.4^{n\text{-}8}$.

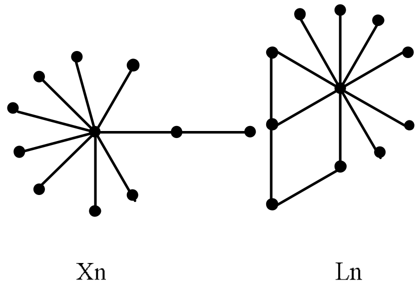

Figure 3. The graph X_n and L_n.

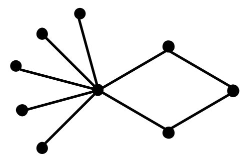

Figure 4. The graph $S_n + e + e'$.

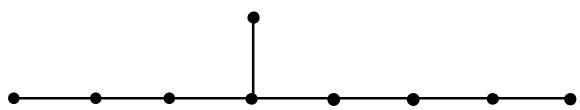

Figure 5. The graph Q.

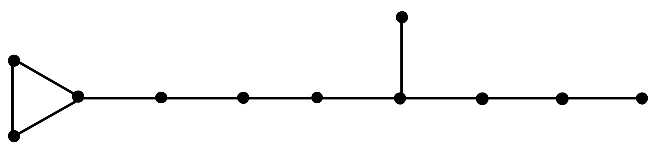

Figure 6. The graph R.

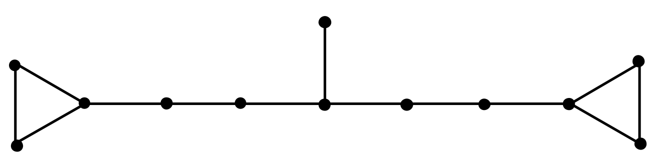

Figure 7. The graph S.

Corollary 4.16. *For any triangle-free graph G,* $NK_{ev}(G) = \prod_1^*(G)$.

Proof. The proof directly comes from the Observation 2.5, the Definition 2.17 and the definition of multiplicative version of the first Zagreb index. □

Now, we give some mathematical properties of *ev*-degree and *ve*-degree Zagreb indices in terms of the forgotten topological index and the total number of the triangles *n(G)* of a connected graph *G*. Before giving propositions, we give following terminologies which be used.

Theorem 4.17. *Let G be a connected graph, then*

$$S(G) = F(G) + 2M_2(G) - 2\sum_{uv\in E(G)}(\deg(u) + \deg(v))\, n_e + \sum_{e=uv\in E(G)} {n_e}^2 .$$

Proof. We know that $c_{e=uv} = \deg(u) + \deg(v) - n_e$ and $S = S(G) = \sum_{e\in E(G)} {c_e}^2$. Therefore,

$$\begin{aligned} S = S(G) &= \sum_{e=uv\in E(G)} {c_e}^2 = (\deg(u) + \deg(v) - n_e)^2 \\ &= \sum_{e=uv\in E(G)} (\deg(u) + \deg(v))^2 - 2\sum_{e=uv\in E(G)}(\deg(u) + \deg(v))\, n_e \\ &+ \sum_{e=uv\in E(G)} {n_e}^2 \\ &= \sum_{e=uv\in E(G)}(\deg(u)^2 + \deg(v)^2) + 2\sum_{e=uv\in E(G)} \deg(u)\deg(v) \\ &-2\sum_{e=uv\in E(G)}(\deg(u) + \deg(v))\, n_e + \sum_{e=uv\in E(G)} {n_e}^2 \\ &= F(G) + 2M_2(G) - 2\sum_{uv\in E(G)}(\deg(u) + \deg(v))\, n_e + \sum_{e=uv\in E(G)} {n_e}^2 . \end{aligned}$$

□

Theorem 4.18. *Let G be a connected graph, then* $S^\beta(G) = 2M_2(G) - 6n(G)$, *where* $n(G)$ *denotes the total number of triangles in G.*

Proof. From the definition of the first *ve*-degree Zagreb beta index and Lemma 4.2 we get

$$\begin{aligned} S^\beta(G) &= \sum_{uv\in E(G)}(c_u + c_v) \\ &= \sum_{uv\in E(G)}\left[\left(\sum_{w\in N(u)} \deg(w) - n_u\right) + \left(\sum_{w\in N(v)} \deg(w) - n_v\right)\right] \\ &= \sum_{uv\in E(G)}\left(\sum_{w\in N(u)} deg(w) + \sum_{w\in N(v)} deg(w)\right) - \sum_{uv\in E(G)}(n_u + n_v) \\ &= S^\beta(G) = 2M_2(G) - 6n(G). \end{aligned}$$

□

Theorem 4.19. *Let G be a connected graph, then*

$$S^\alpha(G) = F(G) - 2\sum_{v\in V(G)}\left(\sum_{u\in N(v)} \deg(u) n_v\right) + \sum_{v\in V(G)} {n_v}^2$$

where n_v *denotes the number of triangles in G containing the vertex v.*

Proof. From the definition of the first *ve*-degree Zagreb alpha index and Lemma 4.2 we get

$$
\begin{aligned}
S^{\alpha}(G) &= \sum_{v\in V(G)} c_v^{\,2} = \sum_{v\in V(G)} \sum_{u\in N(v)} (\deg(u) - n_v)^2 \\
&= \sum_{v\in V(G)} \left[\left(\sum_{u\in N(v)} \deg(u) \right)^2 - 2\sum_{u\in N(v)} \deg(u) n_v + n_v^{\,2} \right] \\
&= \sum_{v\in V(G)} \left(\sum_{u\in N(v)} \deg(u) \right)^2 - 2\sum_{v\in V(G)} \left(\sum_{u\in N(v)} \deg(u) n_v \right) + \sum_{v\in V(G)} n_v^{\,2} \\
&= \sum_{v\in V(G)} \deg(v)^3 - 2\sum_{v\in V(G)} \left(\sum_{u\in N(v)} \deg(u) n_v \right) + \sum_{v\in V(G)} n_v^{\,2} \\
&= F(G) - 2\sum_{v\in V(G)} \left(\sum_{u\in N(v)} \deg(u) n_v \right) + \sum_{v\in V(G)} n_v^{\,2}.
\end{aligned}
$$

□

It is very surprisingly to see that for any triangle free graph the forgotten topological index and the first *ve*-degree Zagreb alpha index equal each other. The following corollary states this fact.

Corollary 4.20. *Let G be a triangle-free connected graph, then* $S^{\alpha}(G) = F(G)$.

5. Conclusion

In this study we defined *ev*-degree and *ve*-degree Narumi-Katayama indices and showed that these novel degree based topological indices can be used possible tools for QSPR researches. Also we investigated some basic mathematical properties of *ev*-degree and *ve*-degree Narumi-Katayama and Zagreb indices. It can be interesting to compute the exact value of *ev*-degree and *ve*-degree topological indices for some graph operations. It can also be interesting to investigate the *ev*-degree and *ve*-degree concepts for the other topological indices for further studies.

References

1. M. Chellali, T.W. Haynes, S.T. Hedetniemi, T.M. Lewis, On ve-degrees and *ev*-degrees in graphs, *Discrete Math.* **340** (2017) 31−38.
2. S. Ediz, Predicting some physicochemical properties of octane isomers: A topological approach using *ev*-degree and *ve*-degree Zagreb indices, *Int. J. Syst. Sci. Appl. Math.* **2** (2017), 87−92.
3. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535−538.
4. B. Horoldagva, K. Das, T. Selenge, Complete characterization of graphs for direct comparing Zagreb indices, *Discrete Appl. Math.* **215** (2016) 146−154.
5. A. Ali, Z. Raza, A. Bhatti, A note on the augmented Zagreb index of cacti with fixed number of vertices and cycles, *Kuwait J. Sci.* **43** (2016) 11−17.

6. S. Ediz, Reduced second Zagreb index of bicyclic graphs with pendent vertices, *Le Mathematiche* **71** (2016) 135−147.
7. M. Randić, Characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609−6615.
8. R. K. Kincaid, S. J. Kunkler, M. D. Lamar, D. J. Phillips, Algorithms and complexity results for findings graphs with extremal Randić index, *Networks* **67** (2016) 338−347.
9. A. Banerjee, R. Mehatari, An eigenvalue localization theorem for stochastic matrices and its application to Randić matrices, *Linear Algebra Appl.* **505** (2016) 85−96.
10. R. Gu, F. Huang, X. Li, Skew Randić matrix and skew Randić energy, *Trans. Comb.* **5** (2016) 1−14.
11. B. Furtula, I. Gutman, A forgotten topological index, *J Math. Chem.* **53** (2015) 1184−1190.
12. N. De, S. M. Abu Nayeem, Computing the F-index of nanostar dendrimers, *Pacific Sci. Rev. A: Nat. Sci. Eng.* **18** (2016) 14−21.
13. W. Gao, M. K. Siddiqui, M. Imran, M. K. Jamil, M. R. Farahani, Forgotten topological index of chemical structure in drugs, *Saudi Pharm. J.* **24** (2016) 258−264.
14. H. Narumi, M. Katayama, Simple topological index. a newly devised index characterizing the topological nature of structural isomers of saturated hydrocarbons, *Mem. Fac. Engin. Hokkaido Univ.* **16** (1984) 209−214.
15. I. Gutman, M. Ghorbani, Some properties of the Narumi-Katayama index, *Appl. Math. Lett.* **25** (2012) 1435−1438.
16. D. J. Klein, V. R. Rosenfeld, The degree–product index of Narumi and Katayama, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 607−618.
17. D. J. Klein, V. R. Rosenfeld, The Narumi–Katayama degree–product index and the degree–product polynomial, in: I. Gutman, B. Furtula (Eds.), Novel Molecular Structure Descriptors—Theory and Applications II, Univ. Kragujevac, Kragujevac, 2010, pp. 79−90.
18. R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley–VCH, Weinheim, 2009, p. 868.
19. A. Zolfi, A. R. Ashrafi, Extremal properties of Narumi-Katayama index of chemical trees, *Kragujevac J. Sci.* **35** (2013), 71−76.
20. K. C. Das, N. Akgüneş, M. Togan, A. Yurttaş, İ. N. Cangül, A. S. Çevik, On the first Zagreb index and multiplicative Zagreb coindices of graphs, *An. St. Univ. Ovidius Constanta-Seria Matematica* **24** (2016), 153−176.

21. M. Eliasi, I. Gutman, A. Iranmanesh, Multiplicative versions of first Zagreb index, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 217−230.
22. B. Basavanagoud, S. Patil, Multiplicative Zagreb indices and co-indices of some derived graphs, *Opuscula Math.* **36** (2016), 287−299.

Iranian J. Math. Chem. 9 (4) December (2018) 279 − 287

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

The Second Geometric–Arithmetic Index for Trees and Unicyclic Graphs

NASRIN DEHGARDI[a], **HAMIDEH ARAM**[b] **AND ABDOLLAH KHODKAR**[•]

[a]Department of Mathematics and Computer Science, Sirjan University of Technology, Sirjan, Iran
[b]Department of Mathematics, Gareziaeddin Center, Khoy Branch, Islamic Azad University, Khoy, Iran
[•]Department of Mathematics, University of West Georgia, Carrollton, GA 30118, USA

ARTICLE INFO

Article History:

Received 1 April 2017
Accepted 29 August 2017
Published online 31 December 2018
Academic Editor: Hamid Reza Maimani

Keywords:

Second geometric-arithmetic index
Tree
Unicyclic graph

ABSTRACT

Let G be a finite and simple graph with edge set $E(G)$. The second geometric-arithmetic Index is defined as

$$GA_2(G) = \sum_{uv\in E(G)} \frac{2\sqrt{n_u n_v}}{n_u+n_v},$$

where n_u denotes the number of vertices in G lying closer to u than to v. In this paper we find a sharp upper bound for $GA_2(T)$, where T is tree, in terms of the order and maximum degree of the tree. We also find a sharp upper bound for $GA_2(G)$, where G is a unicyclic graph, in terms of the order, maximum degree and girth of G. In addition, we characterize the trees and unicyclic graphs which achieve the upper bounds.

1 INTRODUCTION

Let G be a simple connected graph with vertex set $V = V(G)$ and edge set $E = E(G)$. The integers $n = n(G) = |V(G)|$ and $m = m(G) = |E(G)|$ are the order and the size of the graph G, respectively. We write $deg_G(v) = deg(v)$ for the degree of a vertex v and $\Delta = \Delta(G)$ for the maximum degree of G. Let $u, v \in V(G)$, then the distance $d_G(u,v)$ between u and v is defined as the length of a shortest path in G connecting u and v.

[•] Corresponding Author (Email address:akhodkar@westga.edu)
DOI: 10.22052/ijmc.2017.81079.1277

In [5], a new class of topological descriptors, based on some properties of the vertices of a graph is presented. These descriptors are named as geometric-arithmetic indices, GA_{general}, and defined as:

$$GA_{\text{general}}(G) = \sum_{uv\in E(G)} \frac{2\sqrt{Q_u Q_v}}{Q_u+Q_v},$$

where Q_u is some quantity that in a unique manner can be associated with the vertex u of the graph G. The geometric-arithmetic index GA is defined in [6] as:

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{deg(u)deg(v)}}{deg(u)+deg(v)}.$$

The geometric-arithmetic index is well studied in the literature, see for example [2, 4, 7]. Let uv be an edge of G. Define $N(u,G) = \{x \in V(G) \mid d_G(u,x) < d_G(u,x)\}$. In other words, $N(u,G)$ consists of vertices of G which are closer to u than to v. Note that the vertices equidistant to u and v are not included into either $N(u,G)$ or $N(v,G)$. Such vertices exist only if the edge uv belongs to an odd cycle. Hence, in trees, $n_u + n_v = n$ for all edges of the tree. It is also worth noting that $u \in N(u,G)$ and $v \in N(v,G)$, which implies that $n_u \geq 1$ and $n_v \geq 1$. The second geometric-arithmetic index GA_2 is defined in [5] as:

$$GA_2(G) = \sum_{uv\in E(G)} \frac{2\sqrt{n_u n_v}}{n_u+n_v},$$

where $n_u = n_u(G) = |N(u,G)|$. See [1, 3, 8] for more information on this index.

The following statements can be found in [5].

Theorem A. The path P_n is the n-vertex tree with maximum second geometric-arithmetic index.

Theorem B. Let S_n be a star of order n, then $GA_2(G) = \frac{2(n-1)\sqrt{n-1}}{n}$.

In this paper we first present some examples. Then we prove that for any tree T of order $n \geq 2$ with maximum degree Δ,

$$GA_2(T) \leq \frac{2}{n}\left((\Delta-1)\sqrt{n-1} + \sum_{i=1}^{n-\Delta}\sqrt{i(n-i)}\right).$$

Finally, we prove that for any unicyclic graph G of order $n \geq 3$ with maximum degree $\Delta \geq 3$ and girth k, if k is odd, then

$$GA_2(G) \leq \frac{2}{n}\left((\Delta-2)\sqrt{n-1} + \sum_{i=1}^{n-k-\Delta+2}\sqrt{i(n-i)}\right) + \frac{2(k-1)}{n-1}\sqrt{\left(\frac{k-1}{2}+\Delta-2\right)\left(n-\frac{k-1}{2}-\Delta+1\right)} + \frac{2}{\Delta+k-3}\sqrt{\frac{k-1}{2}\left(\frac{k-1}{2}+\Delta-2\right)} + \frac{2}{n-\Delta+1}\sqrt{\frac{k-1}{2}\left(n-\frac{k-1}{2}-\Delta+1\right)},$$

and if k is even, then

$$GA_2(G) \le \frac{2}{n}\left((\Delta-2)\sqrt{n-1} + \sum_{i=1}^{n-k-\Delta+2}\sqrt{i(n-i)} + k\sqrt{\left(\frac{k}{2}+\Delta-2\right)\left(n-\frac{k}{2}-\Delta+2\right)}\right).$$

We also characterize the trees and unicyclic graphs which achieve the upper bounds.

2 EXAMPLES

Dendrimers are nanostructures that can be precisely designed and manufactured for a wide variety of applications, such as drug delivery, gene delivery and diagnostic tests. In this section we calculate the second geometric-arithmetic index for Dendrimers of types A and B and for Tecto Dendrimers. See Figure 1.

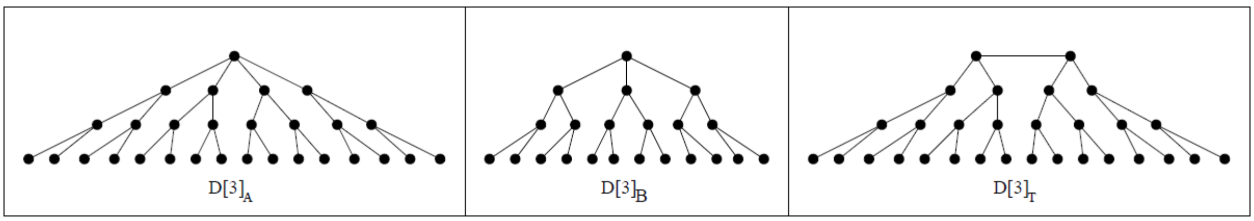

Figure 1: Dendrimers of types A and B and Tecto Dendrimers.

Example 1. In Dendrimers $D[n]$ type A, denoted $D[n]_A$, there are $4(2^n-1)+1$ vertices and $4(2^n-1)$ edges. Let e be an edge between the ith and the $(i+1)$th layers. Then

$$f_i(e) = \sqrt{(2^{n-i}-1)(2^{n+2}-2^{n-i}-2)} \text{ for } i = 1,2,\ldots,n-1.$$

In addition, there are 2^{i+2} edges between the ith and the $(i+1)$th layers. Therefore, for $n \ge 2$,

$$GA_2(D[n]_A) = \frac{2}{4(2^n-1)+1}\left(4\sqrt{(2^n-1)(3(2^n-1)+1)} + \sum_{i=1}^{n-1} 2^{i+2} f_i(e)\right)$$

$$= \frac{8}{4(2^n-1)+1}\left(\sqrt{(2^n-1)(3(2^n-1)+1)} + \sum_{i=1}^{n-1} 2^{i} f_i(e)\right).$$

For examples,

$GA_2(D[2]_A) = \frac{8}{13}\left(\sqrt{30}+2\sqrt{12}\right) = 7.63$ *and*

$GA_2(D[3]_A) = \frac{8}{29}\left(\sqrt{154}+2\sqrt{78}+4\sqrt{28}\right) = 14.13.$

Example 2. In Dendrimers $D[n]$ type B, denoted $D[n]_B$, there are $3(2^n-1)+1$ vertices and $3(2^n-1)$ edges. Let e be an edge between the ith and the $(i+1)$th layers. Then

$$f_i(e) = \sqrt{(2^{n-i}-1)(3(2^n)-2^{n-i}-1)} \text{ for } i = 1,2,\ldots,n-1.$$

In addition, there are $3(2^i)$ edges between the ith and the $(i + 1)$th layers. Therefore, for $n \geq 2$,

$$GA_2(D[n]_B) = \frac{8}{3(2^n-1)+1}\left(\sqrt{3(2^n-1)(2(2^n-1)+1)} + \sum_{i=1}^{n-1} 3(2^i)\, f_i(e)\right).$$

For example,

$GA_2(D[2]_B) = \frac{2}{10}\left(3\sqrt{21} + 18\right) = 6.35$ and

$GA_2(D[3]_B) = \frac{2}{22}\left(3\sqrt{105} + 6\sqrt{57} + 12\sqrt{21}\right) = 11.91.$

Example 3. In Tecto Dendrimers $D[n]_T$, there are $2^{n+2} - 2$ vertices and $2^{n+2} - 3$ edges. Let e be an edge between the ith and the $(i + 1)$th layers. Then

$$f_i(e) = \sqrt{(2^{n-i}-1)(2^{n+2}-2^{n-i}-1)} \text{ for } i = 1,2,\ldots,n-1.$$

In addition, there are 2^{i+2} edges between the ith and the $(i + 1)$th layers. Therefore, for $n \geq 2$,

$$GA_2(D[n]_T) = \frac{8}{2^{n+2}-2}\left(4\sqrt{(2^n-1)(3(2^n)-1)} + \sum_{i=1}^{n-1} 2^{i+2} f_i(e) + 2^{n+1} - 1\right).$$

For example,

$GA_2(D[2]_T) = \frac{2}{14}\left(4\sqrt{33} + 8\sqrt{13} + 7\right) = 8.40$ and

$GA_2(D[3]_T) = \frac{2}{30}\left(4\sqrt{161} + 8\sqrt{81} + 16\sqrt{29} + 15\right) = 14.93.$

2 AN UPPER BOUND ON THE SECOND GEOMETRIC–ARITHMETIC OF TREES

In this section we present a sharp upper bound for the second geometric-arithmetic index of trees in terms of their order and maximum degree. We also characterize all trees whose the second geometric-arithmetic index achieves the upper bound. A *leaf* of a tree T is a vertex of degree 1, a *support vertex* is a vertex adjacent to a leaf and a *strong support vertex* is a support vertex adjacent to at least two leaves. An end-support vertex is a support vertex whose all neighbors with exception at most one are leaves. A *rooted tree* is a tree having a distinguished vertex v, called the *root*. Let $T_{n,\Delta}$ be the set of trees of order n and maximum degree Δ. Let T be a tree of order n and let $f : E(T) \to Z^+$ is a function defined by $f(xy) = \sqrt{n_x n_y}$. Hence $GA_2(T) = \frac{2}{n}\sum_{uv\in E(G)} f(uv)$. We start with an easy but useful observation.

Observation 4. Let $x \geq y \geq 1$ and $n \geq x + y + 2$ be positive integers. Then for every $1 \leq k \leq y$, $(x + k)(n - x - k) > (y - k + 1)(n - y + k - 1)$.

Proof. First note that $(x+k)(n-x-k)-(y-k+1)(n-y+k-1) = n(2k+x)-(x+k)^2$. Since $n \geq x+y+2$, it follows that $n(2k+x)-(x+k)^2 > 0$. So the result follows.

Lemma 5. Let T be a tree of order n with maximum degree Δ and v be a vertex of maximum degree. If T has a vertex of degree at least three different from v, then there is a tree $T' \in T_{n,\Delta}$ such that $GA_2(T) < GA_2(T')$.

Proof. Let T be the rooted tree at v. Let $u \neq v$ be a vertex of degree $deg(u) = k \geq 3$ such that $d(u,v)$ is as large as possible and let $N(u) = \{u_1, u_2, \dots, u_{k-2}, u_{k-1}, u_k\}$. Now we distinguish three cases.

Case 1. u is an end-support vertex.

We may assume that u_k is the parent of u. Let $S = \{uu_1, uu_2, \dots, uu_{k-2}, uu_{k-1}\}$ and let T' be the tree obtained by attaching the path $uu_1u_2 \dots u_{k-2}u_{k-1}$ to $T - \{u_1, u_2, \dots, u_{k-1}\}$. Suppose that $S' = \{uu_1, u_1u_2, \dots, u_{k-2}u_{k-1}\}$. Clearly, $T' \in T_{n,\Delta}$ and

$$\sum_{uv\in E(T)-S} f(uv) = \sum_{uv\in E(T')-S'} f(uv).$$

By definition

$$\frac{n}{2}GA_2(T) = \sum_{uv\notin S} f(uv) + \sum_{uv\in S} f(uv) = \sum_{uv\in E(T)-S} f(uv) + (k-1)\sqrt{n-1}, \qquad (1)$$

and

$$\frac{n}{2}GA_2(T') = \sum_{uv\notin S'} f(uv) + \sum_{uv\in S'} f(uv) = \sum_{uv\in E(T')-S'} f(uv) + \sum_{i=1}^{k-1}\sqrt{i(n-i)}. \qquad (2)$$

Combining (1), (2) and the fact that $k \geq 3$, we obtain $GA_2(T) < GA_2(T')$, as desired.

Case 2. u is a support vertex.

By Case 1, we may assume that u is not an end-support vertex and $deg(u_1) = 1$. Suppose $deg(u_2) = 2$ and T_{u_2} is the component of $T - uu_2$ containing u_2. Since, by the choice of vertex u, $d(u,v)$ is as large as possible, we may assume that T_{u_2} is the path $u_2x_1x_2 \dots x_t, t \geq 1$. Let T' be the tree obtained from $T - uu_1$ by adding the pendant edge x_tu_1 to this graph. Let $S = \{uu_1, uu_2, u_2x_1, x_1x_2, \dots, x_{t-1}x_t\}$ and $S' = \{uu_2, u_2x_1, x_1x_2, \dots, x_{t-1}x_t, u_1x_t\}$. Clearly, $T' \in T_{n,\Delta}$ and

$$\sum_{uv\in E(T)-S} f(uv) = \sum_{uv\in E(T')-S'} f(uv).$$

By definition

$$\frac{n}{2}GA_2(T) = \sum_{uv\in E(T)-S} f(uv) + \sum_{i=1}^{t+1}\sqrt{i(n-i)} + \sqrt{n-1}, \qquad (3)$$

and

$$\frac{n}{2}GA_2(T') = \sum_{uv\in E(T')-S'} f(uv) + \sum_{i=1}^{t+2}\sqrt{i(n-i)}. \qquad (4)$$

By (3), (4) and the fact that $n \geq t+4$, we obtain $GA_2(T) < GA_2(T')$.

Case 3. u is not a support vertex.

Suppose T_{u_1} and T_{u_2} are the components of $T-\{uu_1,uu_2\}$ containing u_1 and u_2, respectively. By the choice of vertex u, we may assume that $T_{u_1}=u_1x_1x_2\ldots x_s$, $s\geq 1$ and $T_{u_2}=u_2y_1y_2\ldots y_t$, $t\geq 1$. Then $deg(x_i)=deg(y_j)=2$, $1\leq i\leq s-1$, $1\leq j\leq t-1$, and $deg(x_s)=deg(y_t)=1$. Let T' be the tree obtained from $T-T_{u_2}$ by adding the path $x_sy_ty_{t-1}\ldots y_1u_2$ to this graph. Let

$$S=\{uu_1,u_1x_1,x_1x_2,\ldots,x_{s-1}x_s\}\cup\{uu_2,u_2y_1,y_1y_2,\ldots,y_{t-1}y_t\},$$

and

$$S'=\{uu_1,u_1x_1,x_1x_2,\ldots,x_{s-1}x_s\}\cup\{x_sy_t,u_2y_1,y_1y_2,\ldots,y_{t-1}y_t\}.$$

Clearly, $T'\in T_{n,\Delta}$ and

$$\sum_{uv\in E(T)-S}f(uv)=\sum_{uv\in E(T')-S'}f(uv).$$

By definition we have

$$\frac{n}{2}GA_2(T)=\sum_{uv\in E(T)-S}f(uv)+\sum_{i=1}^{s+1}\sqrt{i(n-i)}+\sum_{i=1}^{t+1}\sqrt{i(n-i)}, \tag{5}$$

and

$$\frac{n}{2}GA_2(T')=\sum_{uv\in E(T')-S'}f(uv)+\sum_{i=1}^{s+t+2}\sqrt{i(n-i)}. \tag{6}$$

Applying Observation 4 and inequalities (5) and (6), we conclude that $GA_2(T)<GA_2(T')$. This complete the proof.

A spider is a tree with at most one vertex of degree more than 2, called the center of the spider (if no vertex is of degree more than two, then any vertex can be the center). A leg of a spider is a path from the center to a vertex of degree 1. Thus, a star with *k* edges is a spider of *k* legs, each of length 1, and a path is a spider of 1 or 2 legs.

Lemma 6. Let *T* be a spider of order *n* with $k\geq 3$ legs. If *T* has two legs of length at least 2, then there is a spider T' of order *n* with *k* legs such that $GA_2(T)<GA_2(T')$.

Proof. Let *v* be the center of *T* and $N(v)=\{v_1,v_2,\ldots,v_k\}$. Root *T* at *v*. Assume, without loss of generality, that $deg(v_1)=deg(v_2)=2$ and let $v_1x_1x_2\ldots x_s$ and $v_2y_1y_2\ldots y_t$ be two legs of *T*. Let T' be the tree obtained from *T* be deleting the edges $x_1x_2,\ldots,x_{s-1}x_s$ and adding the edges $x_1y_t,x_1x_2,\ldots,x_{s-1}x_s$. Suppose

$$S=\{vv_1,v_1x_1,x_1x_2,\ldots,x_{s-1}x_s\}\cup\{vv_2,v_2y_1,y_1y_2,\ldots,y_{t-1}y_t\},$$

and

$$S'=\{vv_1,y_tx_1,x_1x_2,\ldots,x_{s-1}x_s\}\cup\{vv_2,v_2y_1,y_1y_2,\ldots,y_{t-1}y_t\}.$$

Clearly

$$\sum_{uv\in E(T)-S}f(uv)=\sum_{uv\in E(T')-S'}f(uv).$$

By definition we have

$$\frac{n}{2}GA_2(T)=\sum_{uv\in E(T)-S}f(uv)+\sum_{i=1}^{s+1}\sqrt{i(n-i)}+\sum_{i=1}^{t+1}\sqrt{i(n-i)}, \tag{7}$$

and

$$\frac{n}{2}GA_2(T')=\sum_{uv\in E(T')-S'}f(uv)+\sum_{i=1}^{s+t+1}\sqrt{i(n-i)}+\sqrt{n-1}. \tag{8}$$

By Observation 4, equalities (7) and (8) and the fact that $n \geq s + t + 4$ we obtain $GA_2(T) < GA_2(T')$.

We are now ready to prove the main theorem of this section.

Theorem 7. For any tree $T \in T_{n,\Delta}$ of order $n \geq 2$,

$$GA_2(T) \leq \frac{2}{n}\left((\Delta - 1)\sqrt{n-1} + \sum_{i=1}^{n-\Delta}\sqrt{i(n-i)}\right).$$

The equality holds if and only if T is a spider with at most one leg of length at least two.

Proof. Let T_1 be a tree of order $n \geq 2$ with maximum degree Δ such that

$$GA_2(T_1) = \max\{GA_2(T) \mid T \text{ is a tree of order } n \text{ with maximum degree } \Delta\}.$$

Let v be a vertex with maximum degree Δ. Root T_1 at v. If $\Delta = 2$, then T_1 is a path of order n and the result follows by Theorem A. Let $\Delta \geq 3$. By the choice of T_1, we deduce from Lemma 5 that T_1 is a spider with center v. It follows from Lemma 6 and the choice of T_1 that T_1 has at most one leg of length at least two. First let all legs of T_1 have length one. Then T_1 is a star of order n and the result follows by Theorem B. Now let T_1 have only one leg of length at least two. Then

$$GA_2(T) = \frac{2}{n}\left((\Delta - 1)\sqrt{n-1} + \sum_{i=1}^{n-\Delta}\sqrt{i(n-i)}\right).$$

This completes the proof.

3 UNICYCLIC GRAPHS

A connected graph with precisely one cycle is called a unicyclic graph. Let the set $\varphi_{n,\Delta,k}$consist of all unicycle graphs of order n, maximum degree $\Delta \geq 3$ and grith k, where $3 \leq k \leq n$. Note that if G is a cycle of order n, then $GA_2(G) = n$. Let $G \in \varphi_{n,\Delta,k}$. In this section we assume that the k-cycle of G is $C_k = (w_1, w_2, \ldots, w_k)$. In addition for a vertex $u \in V(C_k)$ we let T_u be the connected component of $G \setminus E(C_k)$ containing u. Note that T_u is a tree and we assume u is the root of this tree. Without loss of generality, we also assume one of the vertices of T_{w_1}, say v, is of degree Δ.

Lemma 8. *Let $G \in \varphi_{n,\Delta,k}$ and v be a vertex of maximum degree Δ. Let C be the only cycle of G, $u \in V(C)$ and $u \neq v$. If T_u is a spider with at least two legs, then there is a graph $G' \in \varphi_{n,\Delta,k}$such that $GA_2(G) < GA_2(G')$.*

Proof. Assume T_u has ℓ legs with lengths $t_1, t_2, \ldots, t_\ell$ and $\sum_{i=1}^{\ell} t_i = s$. Let the graph G' be obtained from $G \setminus E(T_u)$ by attaching a path P_s to vertex u. Obviously, $G' \in \varphi_{n,\Delta,k}$. A simple calculation shows that

$$GA_2(G') - GA_2(G) = \frac{2}{n}\left[\sum_{i=1}^{s}\sqrt{i(n-i)} - \sum_{j=1}^{\ell}\sum_{i=1}^{t_j}\sqrt{i(n-i)}\right].$$

Apply Observation 4 to obtain $GA_2(G') - GA_2(G) > 0$.

Lemma 9. *Let* $G \in \varphi_{n,\Delta,k}$ *and* $deg(u) \geq 3$*, where* $u \in T_{w_i}$, $u \neq w_i$*, for some* $2 \leq i \leq k$*. Then there is a graph* $G' \in \varphi_{n,\Delta,k}$ *such that* $GA_2(G) < GA_2(G')$.

Proof. Without loss of generality, we may assume u has the largest distance from w_i among all the vertices of T_{w_i} whose degree is at least 3. This implies that T_u is a spider with at least two legs. Let G' be the graph obtained from G by replacing T_u with a path with the same order as T_u. A calculation similar to that presented in Lemma 8 shows that $GA_2(G') - GA_2(G) > 0$.

Lemma 10. *Let* $G \in \varphi_{n,\Delta,k}$ *and* T_{w_i} *and* T_{w_j} *be paths of length at least 1 for some* $2 \leq i, j \leq k, i \neq j$*. Then there is a graph* $G' \in \varphi_{n,\Delta,k}$ *such that* $GA_2(G) < GA_2(G')$.

Proof. Let ℓ_1 and ℓ_2 be the length of the paths T_{w_i} and T_{w_j}, respectively. Let G' be the graph obtained from G by removing T_{w_i} and T_{w_j} and attaching a path of length $\ell_1 + \ell_2$ to the vertex u. Then as before one can see that $GA_2(G) < GA_2(G')$.

Lemma 11. *Let* $G \in \varphi_{n,\Delta,k}$ *and assume the vertices of the cycle* C_k *are all of degree two except* w_1 *and* w_i*,* $i \neq 1$*. If the distance of* w_i *from* w_1 *is not* $\lceil (k-1)/2 \rceil$*, then there is a graph* $G' \in \varphi_{n,\Delta,k}$ *such that* $GA_2(G) < GA_2(G')$.

Proof. Let G' be the graph obtained from G by removing T_{w_i} and attaching it to vertex w_j, where $j = \lceil (k-1)/2 \rceil$. Then one can see that $GA_2(G) < GA_2(G')$.

Now we consider the graph $G \in \varphi_{n,\Delta,k}$ with $deg(w_i) = 2$ for all $2 \leq i \leq k, i \neq \lceil (k-1)/2 \rceil$ and $deg(w_j) \geq 2$, where $j = \lceil (k-1)/2 \rceil$. By Lemma 9, in order to maximize $GA_2(G)$, T_v must be a spider and $deg_G(w_1) = 3$ if $w_1 \neq v$.

Lemma 12. Let $G \in \varphi_{n,\Delta,k}$ and $w_1 \neq v$. Then there is a graph $G' \in \varphi_{n,\Delta,k}$ *such that* $GA_2(G) < GA_2(G')$.

Proof. Let G' be the graph obtained from $G \backslash T_{w_1}$ by attaching a path of order $|V(T_{w_1})| - \Delta + 2$ to the end vertex of the path T_{w_j} which is different from w_j, $j = \lceil (k-1)/2 \rceil$ and adding $\Delta - 2$ pendant edges at vertex w_1. Obviously, $G' \in \varphi_{n,\Delta,k}$ and it is straightforward to verify that $GA_2(G) < GA_2(G')$.

By Lammas 8–12 we obtain the following result.

Corollary 13. *Let $H \in \varphi_{n,\Delta,k}$ be the graph which consists of a cycle $C_k = (w_1, w_2, \dots, w_k)$ with $\Delta - 2$ pendant edges at vertex w_1 and a path of order $n - k - \Delta + 2$ at vertex w_j, where $j = \lceil (k-1)/2 \rceil$. Then for every $G \in \varphi_{n,\Delta,k}$, $GA_2(G) \le GA_2(H)$.*

We are now ready to state the main theorem of this section.

Theorem 14. For any unicycle graph G of order *n*, girth *k* and maximum degree $\Delta \ge 3$, if *k* is odd, then

$$GA_2(G) \le \frac{2}{n}\left((\Delta-2)\sqrt{n-1} + \sum_{i=1}^{n-k-\Delta+2} \sqrt{i(n-i)}\right) + \frac{2(k-1)}{n-1}\sqrt{\left(\frac{k-1}{2}+\Delta-2\right)\left(n-\frac{k-1}{2}-\Delta+1\right)} + \frac{2}{\Delta+k-3}\sqrt{\frac{k-1}{2}\left(\frac{k-1}{2}+\Delta-2\right)} + \frac{2}{n-\Delta+1}\sqrt{\frac{k-1}{2}\left(n-\frac{k-1}{2}-\Delta+1\right)},$$

and if *k* is even, then

$$GA_2(G) \le \frac{2}{n}\left((\Delta-2)\sqrt{n-1} + \sum_{i=1}^{n-k-\Delta+2} \sqrt{i(n-i)} + k\sqrt{\left(\frac{k}{2}+\Delta-2\right)\left(n-\frac{k}{2}-\Delta+2\right)}\right).$$

The equality holds if and only if G is the graph H given in Corollary 13.

REFERENCES

1 K. Ch. Das, I. Gutman and B. Furtula, *On second geometric-arithmetic index of graphs*, Iranian J. Math. Chem. **1** (2010), 17–28.

2 K. Ch. Das, I. Gutman and B. Furtula, *On the first geometric-arithmetic index of graphs*, Discrete Appl. Math. **159** (2011), 2030–2037.

3 H. Hua, *Trees with given diameter and minimum second geometric-arithmetic index*, J. Math. Chem. **64** (2010), 631–638.

4 A. Madanshekaf and M. Moradi, *The first geometric-arithmetic index of some nanostar dendrimers*, Iranian J. Math. Chem. **5** (2014), 1–6.

5 G. H. Fath-Tabar, B. Furtula and I. Gutman, *A new geometric-arithmetic index*, J. Math. Chem. **47** (2010), 477–486.

6 D. Vukicevic and B. Furtula, *Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges*, J. Math. Chem. **4** (2009), 1369–1376.

7 Y. Yuan, B. Zhou and N. Trinajstic, *On geometric-arithmetic index*, J. Math. Chem. **47** (2010), 833–841.

ABSTRACTS
IN
PERSIAN

The Extremal Graphs for (Sum-) Balaban Index of Spiro and Polyphenyl Hexagonal Chains

YANG ZUO, YAQIAN TANG AND HANYUAN DENG

College of Mathematics and Statistics, Hunan Normal University, Changsha, Hunan 410081, P. R. China

گراف‌های اکسترمال برای شاخص (مجموع-) بالابان زنجیرهای شش‌ضلعی پلی‌فنیل و اسپیرو

ادیتور رابط : سندی کلاوزر

چکیده

به عنوان شاخص‌های توپولوژیکی مبتنی بر فاصلهٔ بسیار متمایزکننده، شاخص بالابان و شاخص مجموع- بالان یک گراف G، به ترتیب به صورت $J(G)=\frac{m}{\mu+1}\sum_{u,v\in E}\frac{1}{\sqrt{DG(u)DG(v)}}$ و $SJ(G)=\frac{m}{\mu+1}\sum_{u,v\in E}^{\infty}\frac{1}{\sqrt{DG(u)+DG(v)}}$ تعریف می‌شوند که $D_G(u)=\sum_{v\in V} d(u,v)$ مجموع فاصلهٔ یک رأس u در G، m تعداد یال‌ها و μ عدد سیکلوماتیک G است. آنها توصیف‌گرهای مفید مبتنی بر فاصله در شیمی‌درمانی‌ها هستند. دراین مقاله، ما روی گراف‌های اکسترمال زنجیرهای شش‌ضلعی پلی‌فنیل و اسپیرو، با توجه به شاخص بالابان و شاخص مجموع- بالابان تمرکز می‌کنیم.

لغات کلیدی: شاخص بالابان، شاخص مجموع- بالابان، زنجیر شش‌ضلعی اسپیرو، زنجیر شش‌ضلعی پلی‌فنیل

An Application of Geometrical Isometries in Non-planar Molecules

A. A. REZAEI[a], A. REISI-VANANI[b] AND S. MASOUM[c]

[a]Department of Pure Mathematics, Faculty of Mathematical Sciences, University of Kashan,Kashan, I. R. Iran
[b]Department of Physical Chemistry, Faculty of Chemistry, University of Kashan, Kashan, I. R. Iran
[c]Department of Analytical Chemistry, Faculty of Chemistry, University of Kashan, Kashan, I. R. Iran

کاربردی از ایزومتری‌های هندسی در مولکول‌های غیرمسطح

ادیتور رابط : ایوان گوتمن

چکیده

در این مقاله، روشی جدید برای انتقال مبدأ به مرکز یک چندضلعی در یک ساختار مولکولی معرفی می کنیم، به طوری که یک محور بخصوص، بر صفحهٔ حاوی چند ضلعی مورد نظر عمود باشد .محاسبات ریاضی را به طور کامل تشرح می‌کنیم و الگوریتم آن را به عنوان یک برنامهٔ کامپیوتری ارائه می‌دهیم.

لغات کلیدی: قاب، ایزومتری، تبدیل متعامد، چندضلعی، مولکول چندحلقه‌ای غیرمسطح.

On ev–Degree and ve–Degree Topological Indices

B. SAHIN[1] AND S. EDIZ[2]

[1]Faculty of Science, Selçuk University, Konya, Turkey
[2]Faculty of Education, YuzuncuYil University, Van, Turkey

شاخص‌های توپولوژیکی ev-درجه و ve-درجه

ادیتور رابط : تومیسلاو داسلیک

چکیده

اخیرا دو مفهوم جدید از درجه در نظریۀ گراف تعریف شده است: ev- درجه و ve- درجه. همچنین شاخص‌های زاگرب و راندیک ev- درجه و ve- درجه نیز به موازات تعاریف کلاسیک شاخص‌های زاگرب و راندیک، تعریف شده‌اند. نشان داده شده است که شاخص‌های توپولوژیکی ev- درجه و ve- درجه می‌توانند به عنوان ابزارهای ممکن در تحقیقات QSPR استفاده شوند. در این مقاله، شاخص‌های نارومی- کاتایامای ev- درجه و ve-درجه را تعریف می‌کنیم، نیروی پیش‌بینی شدۀ این شاخص‌های جدید و گراف‌های اکسترمال را با توجه به این شاخص‌های توپولوژیکی جدید، بررسی می‌کنیم. همچنین برخی ویژگی‌های پایه‌ای ریاضی شاخص‌های نارومی- کاتایاما و زاگرب ev- درجه و ve- درجه را ارائه می‌کنیم.

لغات کلیدی: ev- درجه ، ve- درجه، شاخص توپولوژیکی ev- درجه، شاخص توپولوژیکی ve- درجه

The Second Geometric–Arithmetic Index for Trees and Unicyclic Graphs

NASRIN DEHGARDI[a], HAMIDEH ARAM[b] AND ABDOLLAH KHODKAR[c]

[a]Department of Mathematics and Computer Science, Sirjan University of Technology, Sirjan, Iran
[b]Department of Mathematics, Gareziaeddin Center, Khoy Branch, Islamic Azad University, Khoy, Iran
[c]Department of Mathematics, University of West Georgia, Carrollton, GA 30118, USA

دومین شاخص هندسی–ریاضی برای درختها و گرافهای تک‌دور

ادیتور رابط : حمیدرضا میمنی

چکیده

فرض کنید G یک گراف متناهی ساده با مجموعهٔ یالهای E(G) باشد. دومین شاخص هندسی–ریاضی بصورت زیر تعریف می‌شود:

$$GA_2(G) = \sum_{uv \in E(G)} \frac{2\sqrt{n_u n_v}}{n_u + n_v},$$

که در آن n_u تعداد رئوس G است که به u نزدیکتر از v هستند. ما در این مقاله برای درخت T، کران بالای دقیق $GA_2(T)$ را بر حسب مرتبه و بیشترین درجهٔ درخت محاسبه می‌کنیم. همچنین برای گراف تک‌دور G، کران بالای دقیق $GA_2(G)$ را بر حسب مرتبه و بیشترین درجهٔ گراف محاسبه می‌کنیم. بعلاوه، درختها و گرافهای تک‌دوری که به این کرانهای بالا رسیده‌اند را دسته بندی می‌کنیم.

لغات کلیدی: دومین شاخص هندسی– ریاضی، درخت، گراف تک‌دور

On the saturation number of graphs

SAEID ALIKHANI AND NEDA SOLTANI

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

عدد اشباع گراف‌ها

ادیتور رابط : ایوان گوتمن

چکیده

فرض کنید $G = (V, E)$ یک گراف همبند ساده است. یک جورسازی M در گراف G، مجموعه‌ای از یال‌های G است به‌طوری‌که هیچ دو یالی در M رأس مشترک نداشته باشند. جورسازی M ماکسیمال نامیده می‌شود اگر نتوانیم آن را به یک جورسازی با اندازهٔ بزرگ‌تر گسترش دهیم. اندازهٔ کوچک‌ترین جورسازی ماکسیمال گراف G را عدد اشباع G نامیده و آن را با $s(G)$ نشان می‌دهیم. در این مقاله، علاوه بر محاسبهٔ عدد اشباع ضرب کرونای برخی گراف‌ها، گراف‌های خاصی که در شیمی اهمیت دارند را درنظر گرفته و عدد اشباع آنها را مطالعه خواهیم کرد.

لغات کلیدی: جورسازی ماکسیمال، عدد اشباع، ضرب کرونا

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.

MATHEMATICAL CHEMISTRY

IRANIAN JOURNAL OF

CONTENTS

December 2018

ISSN

2228-6489 (Print Version)

2008-9015 (Online Version)