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.

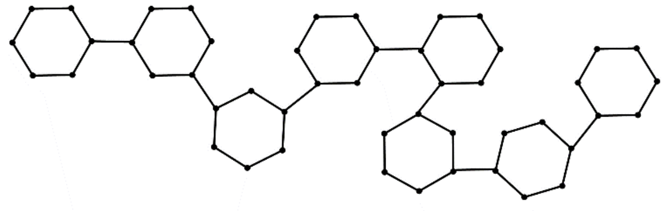

Figure 1: A polyphenyl hexagonal chain of length 8.

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.

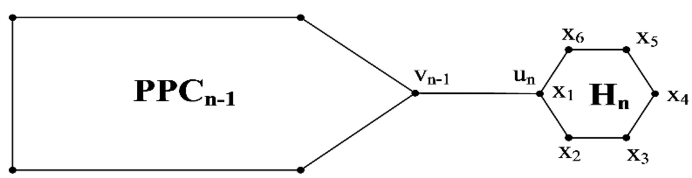

Figure 2: A polyphenyl hexagonal chain of length n.

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.

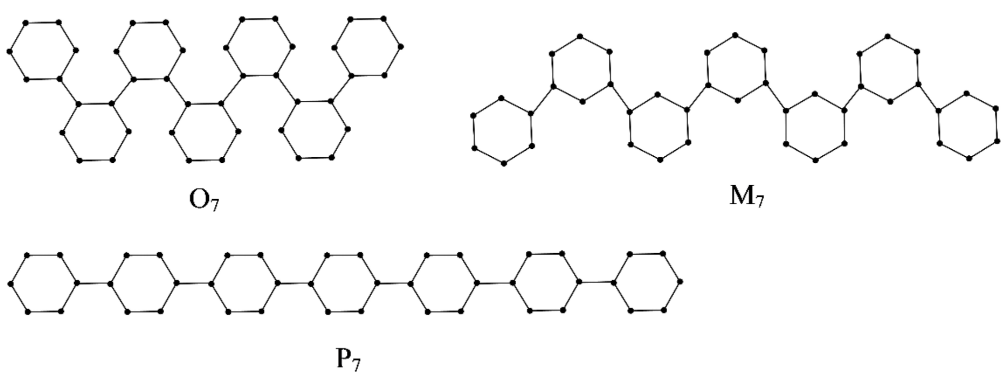

Figure 3: Polyphenyl hexagonal ortho-, meta-, and para-chains of length 7.

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.

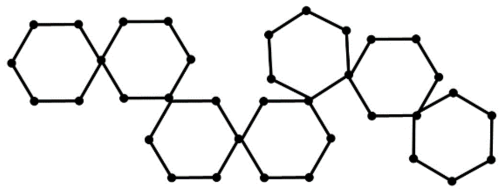

Figure 4: A spiro hexagonal chain of length 7.

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.

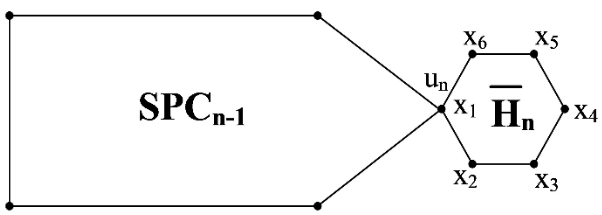

Figure 5: A spiro hexagonal chain of length n.

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 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.

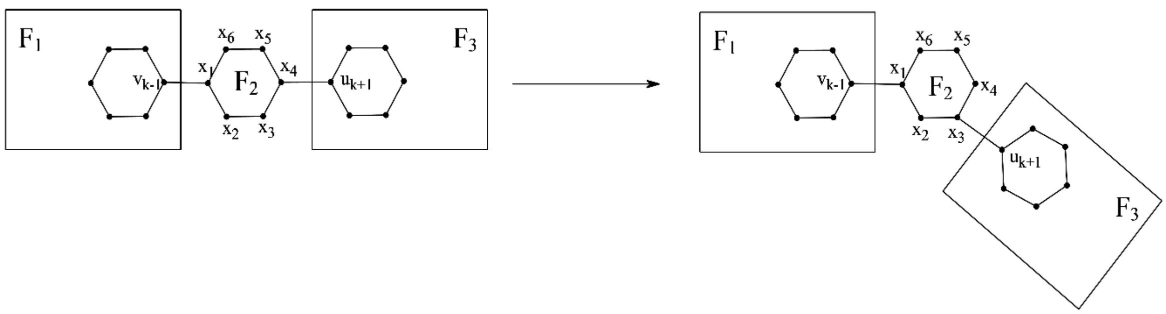

Figure 6: The first cut-edge transformation.

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

$$D_G(v_x) = \sum_{u\in F_1} d_G(v_x,u) + \sum_{u\in F_2} d_G(v_x,u) + \sum_{u\in F_3} d_G(v_x,u),$$
$$D_{G'}(v_x) = \sum_{u\in F_1} d_{G'}(v_x,u) + \sum_{u\in F_2} d_{G'}(v_x,u) + \sum_{u\in F_3} d_{G'}(v_x,u)$$
$$\sum_{u\in F_1} d_G(v_x,u) = \sum_{u\in F_1} d_{G'}(v_x,u),$$
$$\sum_{u\in F_2} d_G(v_x,u) = \sum_{u\in F_2} d_{G'}(v_x,u),$$
$$\sum_{u\in F_3} d_G(v_x,u) = \sum_{u\in F_3} d_{G'}(v_x,u) + 6b.$$

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

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

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 $F_1 = H_1H_2\cdots H_{k-1}$, $F_2 = H_k$, $F_3 = H_{k+1}H_{k+2}\cdots H_n$. 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 $a \geq b$.

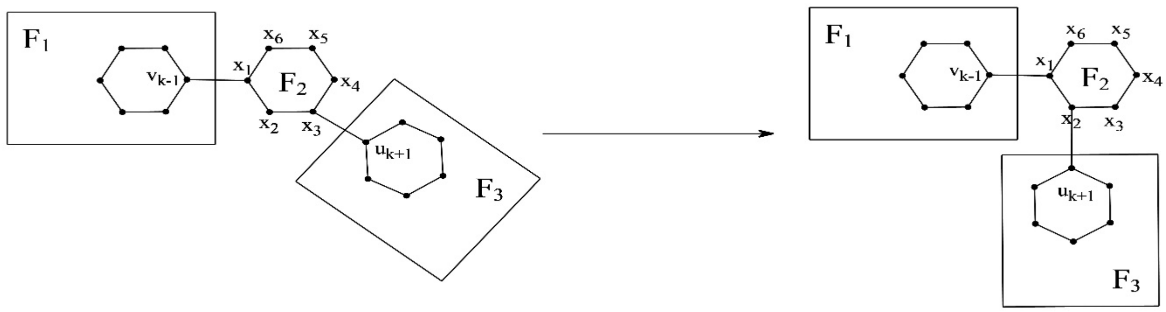

Figure 7: The second cut-edge transformation.

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 $v_xv_y \in E(F_1)\cup E(F_3)$, 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*

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

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

Proof. Suppose on the contrary that $G = H_1H_2\cdots H_n (n \ge 3)$, 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 $G = \overline{H}_1\overline{H}_2\cdots\overline{H}_n (n \ge 3)$ 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.

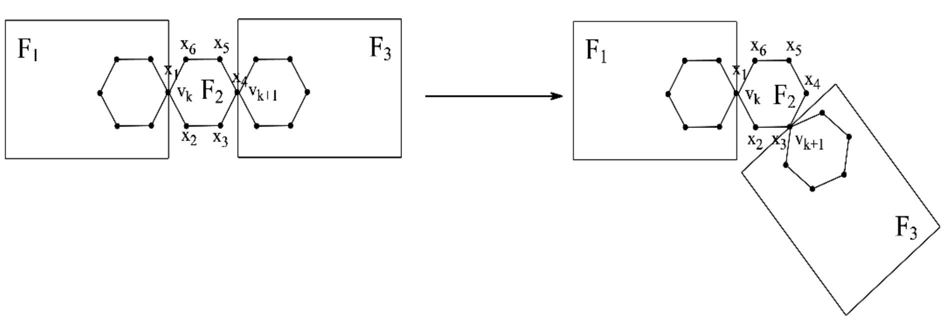

Figure 8: The first cut-vertex transformation.

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).

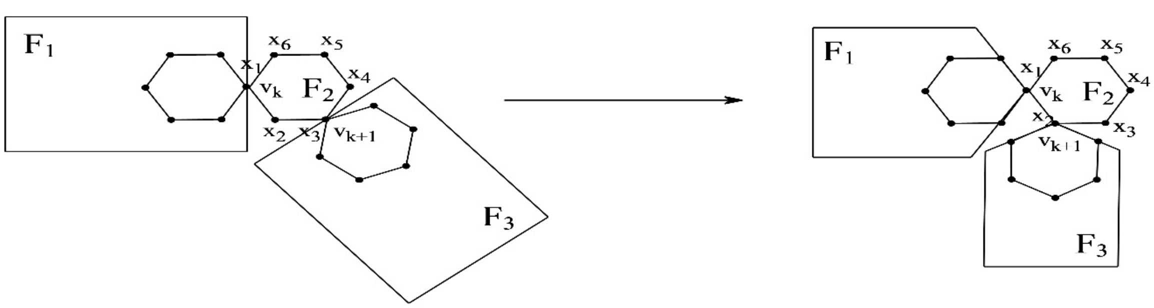

Figure 9: The second cut-vertex transformation.

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.