Extremal Phenylene Chains with Respect to the Kirchhoff Index and Degree-based Topological Indices

Yujun Yang *Member, IAENG*, and Dayong Wang

***Abstract*—The resistance distance between any two vertices of a graph G is defined as the net effective resistance between them in the network construct from G by replacing each edge of G with a unit resistor. The Kirchhoff index of G is defined as the sum of resistance distances between all pairs of vertices. Let L_n (resp. H_n) be the linear phenylene chain (resp. helicene phenylene chain) containing n hexagons and $n-1$ squares. In this paper, firstly, it is shown that among all phenylene chains with n hexagons and $n-1$ squares, L_n attains the maximum value of the Kirchhoff index. Moreover, it is demonstrated that the minimum Kirchhoff index is attained only when the phenylene chain is an "all-kink" chain, which leads to the conjecture that H_n has the minimum Kirchhoff index. Secondly, exact expressions for some degree-based topological indices, namely, the general Randić index, the Harmonic index, the first Zagreb index, the Sum-Connnectivity index, the Geometric-Arirthmetic index, the Atom-Bond connectivity index, and the Symmetric-Division index of phenylene chains are obtained, with extremal phenylene chains with respect to these degree-based topological indices being characterized.**

***Index Terms*—resistance distance, Kirchhoff index, phenylene chain, S, T-isomers**

I. Introduction

In 1993, the novel concept of *resistance distance* was proposed by Klein and Randić [1]. The term resistance distance was used because of the physical interpretation: one imagines unit resistors on each edge of a connected graph $G = (V(G), E(G))$ and takes the resistance distance between vertices i and j of G to be the net effective resistance between them, denoted by $\Omega_G(i,j)$. Recall the traditional (shortest path) distance between any two vertices i and j, denoted by $d_G(i,j)$, is known to be the length of a shortest path connecting them. It has been shown that [1]

$$\Omega_G(i,j) \leq d_G(i,j),$$

with equality if and only if i and j are connected by a unique path. The *Kirchhoff index* [1] of G is defined as the sum of resistance distances between all pairs of vertices,

$$Kf(G) = \sum_{\{u,v\}\subseteq V(G)} \Omega_G(u,v) = \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} \Omega_G(u,v).$$

The Kirchhoff index is not only an important graph invariant, but also an elegant structure descriptor, which plays essential roles in the study of QSAR/QSPR in chemistry. For this reason, the Kirchhoff index has extensively studied in mathematical and chemical literatures. The readers are referred to most recent papers [2]–[8] and references therein for more information on the Kirchhoff index.

Besides the Kirchhoff index, we also consider some interesting degree-based topological indices, namely, the general Randić index, the Harmonic index, the first Zagreb index, the Sum-Connnectivity index, the Geometric-Arirthmetic index, the Atom-Bond connectivity index, and the Symmetric-Division index.

In 1975, to study the properties of alkane, Randić [9] proposed a novel structure descriptor, which is called the *Randić index* $R(G)$ and defined as the sum over all edges of the (molecular) graph of the terms $[d_u d_v]^{-\frac{1}{2}}$, where d_u is the degree of u, i.e.

$$R(G) = \sum_{uv\in E(G)} [d_u d_v]^{-\frac{1}{2}}. \tag{1}$$

From then on, this topological index has been extensively studied. Then, in 2006, the Li and Gutman [10] extended the ordinary Randić index to *general Randić index* $R_\alpha(G)$ by replacing $-\frac{1}{2}$ to arbitrarily real number α, i.e.

$$R_\alpha(G) = \sum_{uv\in E(G)} [d_u d_v]^{\alpha}. \tag{2}$$

For more information on the general Randić index, the readers are refered to [11]–[14] and references therein.

An variant of the Randić index is the *Harmonic index* $H(G)$ [15], which is defined as the sum of the weights $\frac{2}{d(u)+d(v)}$ of all edges uv, i.e.

$$H(G) = \sum_{uv\in E(G)} \frac{2}{d(u)+d(v)}. \tag{3}$$

The *first Zagreb index* $M_1(G)$ [16] is defined as the sum over all vertices of the graph of the terms d_i^2, i.e.

$$M_1(G) = \sum_{i\in V(G)} d_i^2. \tag{4}$$

The first Zagreb index can also expressed as [16]

$$M_1(G) = \sum_{uv\in E(G)} [d(u)+d(v)]. \tag{5}$$

The *Sum-Connectivity index* $S(G)$ [17] is defined as the sum of the weights $\frac{1}{\sqrt{d(u)+d(v)}}$ of all edges uv, i.e.

$$S(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d(u)+d(v)}}. \tag{6}$$

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The *Geometric-Arithmetic index* $GA(G)$ [18] is defined as the sum of the weights $\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$ of all edges uv, i.e.

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}. \quad (7)$$

The *Atom-Bond connectivity index* $ABC(G)$ [19] is defined as the sum of the weights $\sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$ of all edges uv, i.e.

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}. \quad (8)$$

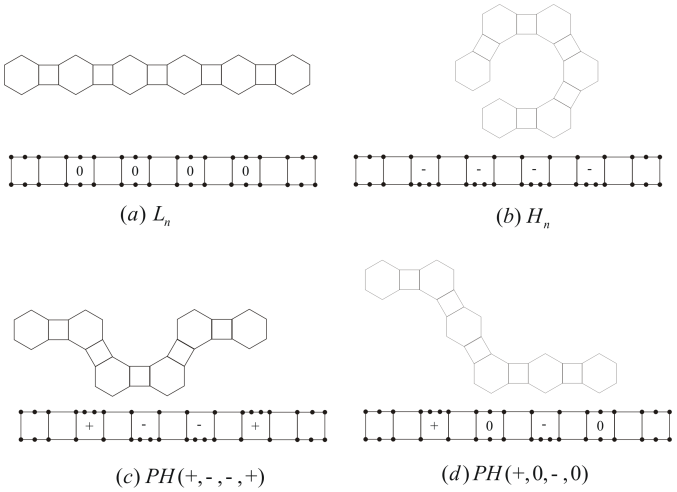
The *Symmetric-Division index* $SD(G)$ [20] is defined as the sum of the weights $\frac{d^2(u)+d^2(v)}{d(u)d(v)}$ of all edges uv, i.e.

$$SD(G) = \sum_{uv\in E(G)} \frac{d^2(u)+d^2(v)}{d(u)d(v)}. \quad (9)$$

Phenylenes are a class of conjugated hydrocarbons composed of six- and four-membered rings, where the six-membered rings (hexagons) are adjacent only to four-membered rings, and every four-membered ring is adjacent to a pair of nonadjacent hexagons. If each six-membered ring of a phenylene is adjacent only to two four-membered rings (squares), we say that is a *phenylene chain*. Due to their aromatic and antiaromatic rings, phenylenes exhibit unique physicochemical properties. Phenylenes, especially phenylene chains have attracted much attention due to excellent properties. For more details, the readers are referred to papers [21]–[37] and references therein.

In what follows, we focus only on phenylene chains. For convenience, we introduce notations to describe a phenylene chain. Actually, a phenylene chain with n hexagons ($n \geq 2$) and $n-1$ squares can be obtained in the following way: first take a linear polymino chain with $2n+1$ squares, then add two vertices to each of the 1st, 3rd, 5th, ..., $(2n+1)$-th square making it into a hexagon in one of the following three different ways: the first way is to add two vertices on the top row, the second way is to add two vertices on the bottom row, and the third way is to add one vertex on the top row and one vertex on the bottom row. For convenience, we always assume that the first and the last hexagons are obtained by the third way. For each of the remaining $(n-2)$-hexagons, we give a $+$ (resp. $-$, or 0) sign to the hexagon if the hexagon is obtained by the first (resp. second, or third) way. In this viewpoint, we are able to represent a phenylene chain with n hexagons ($n \geq 2$) and $n-1$ square by a $(n-2)$-vector $(S_1, S_2, \ldots, S_{n-2})$ such that $S_i \in \{+, -, 0\}$. We denote the phenylene chain which are represented by vector $\mathbf{V}$ by $PH(\mathbf{V})$. In particular, the phenylene chain $\underbrace{(0, 0, \ldots, 0)}_{n-2}$ is called a linear (phenylene) chain, which is denoted by L_n, and the phenylene chain $\underbrace{(-, -, \ldots, -)}_{n-2}$ is called a helicene (phenylene) chain, which is denoted by H_n. For example, some phenylene chains with six hexagons and five squares are given in Figure 1.

In this paper, we characterize extremal phenylene chains with respect to the Kirchhoff index and various degree-based indices. Firstly, It is shown that among all phenylene chains with n hexagons and $n-1$ squares, L_n attains the maximum value of the Kirchhoff index. Moreover, it is demonstrated that the minimum Kirchhoff index is attained only when the phenylene chain is an "all-kink" chain, which leads to the conjecture that H_n has the minimum Kirchhoff index. Secondly, for the degree-based indices including the general Randić index, the Harmonic index, the first Zagred index, the sum-connectivity index, the Geometric-Arithmetic index, the Atom-Bond index and the Symmetric-Division index, it is shown that among all phenylene chains with n hexagons and $n-1$ squares, L_n attains the minimum values of these indices, whereas the maximum values are attained if and only if the phenylene chain is an "all-kink" chain.



(a) L_n (b) H_n (c) $PH(+,-,-,+)$ (d) $PH(+,0,-,0)$

Fig. 1. Some phenylene chains with six hexagons and five squares.

II. Extremal phenylene chains with respect to the Kirchhoff index

In this section, we aim to characterize extremal phenylene chains with respect to the Kirchhoff index. In the characterization of extremal phenylene chains, the comparison theorem on the Kirchhoff index of S- & T-isomers, which is obtained in [38], plays an essential rule. It is well known that isomers (or more precisely structural isomers) are compounds with the same molecular formula but different structural formulas. That is, different isomers of a common molecular formula correspond to nonisomorphic (connected) graphs (of the same numbers of vertices & edges). The concept of S- & T-isomers was introduced by Polansky and Zander [39] in 1982, which entails a pair of graphical moieties A, B doubly interconnected in two different ways as in Figure 2. It is

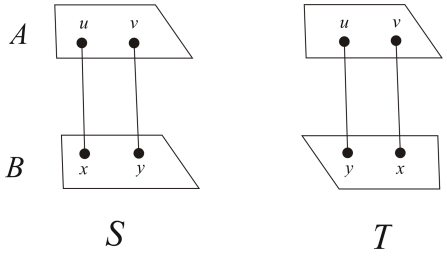


Fig. 2. A pair of vertices (pi-centers) u & v in moiety A are connected to vertices x & y in B, in one way in the S-isomer, and in the other way in the T-isomer.

easily seen that many pairs of phenylene chains can be viewed as S- & T-isomers. For example, some S- & T-isomers of phenylene chains are given in Figure 3.

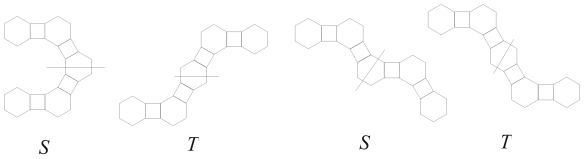


Fig. 3. Some S- & T-isomers of phenylene chains.

For a connected graph G and $k \in V(G)$, the *resistive eccentricity index* of k, denoted by $\Omega_G(k)$, is defined in [38] as the sum of resistance distances between k and all the other vertices of G, that is

$$\Omega_G(k) = \sum_{i \in V(G)}^{i \neq k} \Omega_G(k,i).$$

Then the comparison result on Kirchhoff indices of S, T-isomers is given in the following theorem.

Theorem II.1. *[1] Let S, T, A, B, u, v, x, y be defined as above. Then*

$$Kf(S) - Kf(T) = \frac{[\Omega_A(u) - \Omega_A(v)][\Omega_B(y) - \Omega_B(x)]}{2 + \Omega_A(u,v) + \Omega_B(x,y)}. \tag{10}$$

Using the comparison theorem, we are able to single out the unique phenylene chain with maximal Kirchhoff index among all phenylene chains containing n hexagons. For convenience, for $S_i \in \{+, -, 0\}$, we define

$$-S_i = \begin{cases} -, & \text{if } S_i = +; \\ +, & \text{if } S_i = -; \\ 0, & \text{otherwise.} \end{cases}$$

Theorem II.2. *Let $PH(\mathbf{V})$ be a phenylene chain containing $n+2$ hexagons and $n+1$ squares with $\mathbf{V} = (S_1, S_2, \ldots, S_n)$. If there exists some integer $i \in \{1, 2, \ldots, n\}$ such that $S_i \neq 0$, then let $\mathbf{V}' = (S_1, \ldots, S_{i-1}, 0, -S_{i+1}, \ldots, -S_n)$ and we have*

$$Kf(PH(\mathbf{V})) < Kf(PH(\mathbf{V}')).$$

Proof: Since $S_i \neq 0$, we know that $S_i = +$ or $S_i = -$. Here we prove that the assertion holds for $S_i = +$. The remaining case could be proved in the same way.

Now suppose that $PH(\mathbf{V})$ is a phenylene chain with $\mathbf{V} = (S_1, S_2, \ldots, S_n)$ such that $S_i = +$. Choose vertices u, v, x, and y in the $(i+1)$-th hexagon of $PH(\mathbf{V})$ as shown in Figure 4. First delete edges ux and vy from $PH(\mathbf{V})$, and then add two new edges uy and vx. Then a new phenylene chain $PH(\mathbf{V}')$ with $\mathbf{V}' = (S_1, \ldots, S_{i-1}, 0, -S_{i+1}, \ldots, -S_n)$ is obtained (see Figure 4). We proceed to show that $Kf(PH(\mathbf{V})) < Kf(PH(\mathbf{V}'))$. By the construction of $PH(\mathbf{V}')$, we know that $PH(\mathbf{V})$ and $PH(\mathbf{V}')$ are a pairs of S- & T-isomers. Suppose that the two components of $PH(\mathbf{V}) - \{ux, vy\}$ (also $PH(\mathbf{V}') - \{uy, vx\}$) are A and B such that the component containing u and v is A. Then by Theorem II.1, we have

$$\begin{aligned} &Kf(PH(\mathbf{V})) - Kf(PH(\mathbf{V}')) \\ &= \frac{[\Omega_A(u) - \Omega_A(v)][\Omega_B(y) - \Omega_B(x)]}{2 + \Omega_A(u,v) + \Omega_B(x,y)}. \end{aligned} \tag{11}$$

By the definitions of $\Omega_A(u)$ and $\Omega_A(v)$, we have

$$\begin{aligned} \Omega_A(u) - \Omega_A(v) &= \sum_{k \in V(A)} \Omega_A(u,k) - \sum_{k \in V(A)} \Omega_A(v,k) \\ &= \sum_{k \in V(A) \setminus \{u,v\}} [\Omega_A(u,k) - \Omega_A(v,k)]. \end{aligned} \tag{12}$$

Let w be the unique neighbor of u in A. Then for any $k \in V(A) \setminus \{u, v\}$, we have

$$\Omega_A(u,k) = 1 + \Omega_A(w,k). \tag{13}$$

On the other hand, since $d_A(v,w) = 1$ and v and w are connected by more than one path in A, we have $\Omega_A(v,w) < d_A(v,w) = 1$. Consequently, for any $k \in V(A) \setminus \{u, v\}$, we get

$$\Omega_A(v,k) \leq \Omega_A(v,w) + \Omega_A(w,k) < 1 + \Omega_A(w,k). \tag{14}$$

By (12), (13) and (14), it follows that

$$\Omega_A(u) - \Omega_A(v) > 0. \tag{15}$$

Using the same argument, we can get that

$$\Omega_B(y) - \Omega_B(x) < 0. \tag{16}$$

By (11), (15) and (16), we have $Kf(H(\mathbf{V})) - Kf(H(\mathbf{V}')) < 0$, which completes the proof.

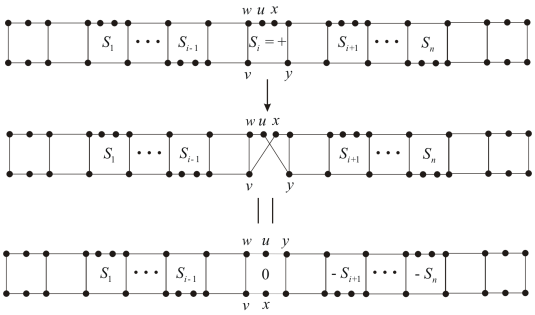


Fig. 4. Illustration of phenylene chains $PH(\mathbf{V})$ and $PH(\mathbf{V}')$ in the proof of Theorem 2.2.

In fact, by the proof of Theorem II.2, we know that if a phenylene chain is not straight (i.e. the linear chain), then the process of removing "kinks" in the phenylene chain may be iterated, each time increasing the Kirchhoff index, till finally arriving at the straight "unkinked" chain. Hence, as an immediate consequence of Theorem II.2, we have

Theorem II.3. *Among all phenylene chains with n hexagons and $n-1$ squares, the linear chain L_n has the maximum Kirchhoff index.*

Since the exact values of the Kirchhoff index of the linear chain L_n has been computed in [40] as follows:

$$Kf(L_n) = 9n^3 + \frac{29\sqrt{30}}{20} \frac{(11 + 2\sqrt{30})^{2n} + 1}{(11 + 2\sqrt{30})^{2n} - 1} n^2 + \frac{21}{40} n. \tag{17}$$

Theorem II.3 directly leads to

Corollary II.4. *Let PH_n be a phenylene chain with n hexagons and $n-1$ squares. Then*

$$Kf(PH_n) \leq 9n^3 + \frac{29\sqrt{30}}{20}\frac{(11+2\sqrt{30})^{2n}+1}{(11+2\sqrt{30})^{2n}-1}n^2 + \frac{21}{40}n, \tag{18}$$

with equality if and only if PH_n is the linear chain L_n.

It is natural to ask which phenylene chain has the minimum Kirchhoff index. This problem turns out to be much more complicated. Similar to the proof of Theorem 2.2, we can prove that if $PH(\mathbf{V})$ is a phenylene chain with $\mathbf{V} = (S_1, S_2, \ldots, S_n)$ such that there exists some integer $i \in \{1, 2, \ldots, n\}$ with $S_i = 0$, then the phenylene chain $PH(\mathbf{V}')$ with $\mathbf{V}' = (S_1, \ldots, S_{i-1}, -, -S_{i+1}, \ldots, -S_n)$ or $\mathbf{V}' = (S_1, \ldots, S_{i-1}, +, -S_{i+1}, \ldots, -S_n)$ has larger Kirchhoff index than $PH(\mathbf{V})$. For convenience, we call a phenylene chain $PH(\mathbf{V})$ an *"all-kink" chain* if $\mathbf{V}$ does not contain 0. In view of the above argument, if a phenylene chain is not an "all-kink" chain, then the process of adding "kinks" in the phenylene chain may be iterated, each time reducing the Kirchhoff index, till finally arriving at an "all-kink" chain. Hence we have

Theorem II.5. *Among all phenylene chains, the minimum Kirchhoff index is attained only when the phenylene chain is an "all-kink" chain.*

However, there are many different types of "all-kink" phenylene chains. So it still remain unsolved which "all-kink" phenylene chain has the minimum Kirchhoff index. For this problem, we only have some intuitive feelings. Among all "all kink" phenylene chains, as the helicene chain seems to be the most "compact", we believe that the minimum Kirchhoff index is attained at the helicene chain. For this reason, we propose the following conjecture.

Conjecture II.6. *Among all phenylene chains with n hexagons and $n-1$ squares, the helicene chain H_n has the minimum Kirchhoff index.*

III. Extremal phenylene chains with respect degree-based topological indices

In this section, we characterize extremal phenylene chains with respect to degree-based topological indices. To this end, we first divide the edge set of G into three different classes and compute the cardinality of each class.

Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ squares. It is clear that every vertex of $PH(\mathbf{V})$ has degree 2 or 3. In what follows, a j-vertex denotes a vertex of degree j, and a (j,k)-edge stands for an edge connecting a j-vertex with a k-vertex. For convenience, the number of j-vertices and (j,k)-edges are denoted by n_j and m_{jk}, respectively. We use h to denote the number of nonzero components of $\mathbf{V}$, i.e. the number of kinks in $PH(\mathbf{V})$. It is obvious that $PH(\mathbf{V})$ have $6n$ vertices and $8n-2$ edges. The edge set of $PH(\mathbf{V})$ can be partitioned into 3 classes according to the 3 different types of edges. In addition, the precise number of $(2,2)$-edges, $(2,3)$-edges and $(3,3)$-edges could be given in the following result.

Lemma III.1. *Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ square. Let h be the number of nonzero components of $\mathbf{V}$. Then we have*

$$m_{22} = 6 + h, \tag{19}$$

$$m_{23} = 4(n-1) - 2h, \tag{20}$$

$$m_{33} = 4(n-1) + h. \tag{21}$$

Proof: Let H_1, H_2, ..., H_n be the n consecutive hexagons of $PH(\mathbf{V})$. Since all the vertices of squares have degree 3, the $(2,2)$ edges must belong to hexagons. It is readily seen that both H_1 and H_n have 3 $(2,2)$-edges. For the remaining hexagons H_2, H_3, ..., H_{n-1}, we know that H_i has a $(2,2)$-edge if and only if H_i have two degree 2 vertices on the top or H_i have two degree 2 vertices on the bottom, which implies that H_i has a $(2,2)$-edge if and only if the corresponding component of $\mathbf{V}$ is nonzero. As $\mathbf{V}$ has h nonzero components, it follows that $m_{22} = 3+3+h = 6+h$.

We proceed to compute m_{33}. Note first that each square have four $(3,3)$-edges. Then, for an edge e not belonging to any square, it is easily verified that e is an $(3,3)$-edge if and only if the unique hexagon containing e corresponds to a nonzero component of $\mathbf{V}$. Bearing in mind that $PH(\mathbf{V})$ have $n-1$ squares, we conclude that $m_{33} = 4(n-1)+h$. Finally, note that $PH(\mathbf{V})$ has $8n-2$ edges, thus

$$\begin{aligned} m_{23} &= 8n - 2 - m_{22} - m_{23} \\ &= 8n - 2 - (6+h) - [4(n-1)+h] = 4(n-1) - 2h. \end{aligned}$$

■

According to Lemma III.1 and the definition of the general Randić index, the exact value of the general Randić index of $PH(\mathbf{V})$ is obtained.

Theorem III.2. *Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ square. Suppose that $\mathbf{V}$ have h nonzero components. Then*

$$R_\alpha(PH(\mathbf{V})) = 6\cdot 4^\alpha + 4(n-1)(6^\alpha + 9^\alpha) + h(3^\alpha - 2^\alpha)^2. \tag{22}$$

Proof: By the definition of the general Randić index, we have

$$\begin{aligned} R_\alpha(PH(\mathbf{V})) &= \sum_{e=uv\in E(PH(\mathbf{V}))} [d_u d_v]^\alpha \\ &= m_{22}[2\cdot 2]^\alpha + m_{23}[2\cdot 3]^\alpha + m_{33}[3\cdot 3]^\alpha \\ &= (6+h)4^\alpha + [4(n-1)-2h]6^\alpha + [4(n-1)+h]9^\alpha \\ &= 6\cdot 4^\alpha + 4(n-1)(6^\alpha + 9^\alpha) + h(4^\alpha - 2\cdot 6^\alpha + 9^\alpha) \\ &= 6\cdot 4^\alpha + 4(n-1)(6^\alpha + 9^\alpha) + h(3^\alpha - 2^\alpha)^2. \end{aligned}$$

■

Notice that $0 \leq h \leq n-2$, $h = 0$ if and only if $PH(\mathbf{V}) = L_n$, and $h = n-2$ if and only if $PH(\mathbf{V})$ is an "all-kink" chain. As a consequence of Theorem III.7, extremal phenylene chains with respect to the general Randić index could be characterized, as given in the following result.

Theorem III.3. *Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ square.*

(1) If $\alpha \neq 0$, then

$$\begin{aligned} &6\cdot 4^\alpha + 4(n-1)(6^\alpha + 9^\alpha) \leq R_\alpha(PH(\mathbf{V})) \\ &\leq n(5\cdot 9^\alpha + 2\cdot 6^\alpha + 4^\alpha) - 6\cdot 9^\alpha + 4^{\alpha+1}, \end{aligned} \tag{23}$$

with left equality if and only if $PH(\mathbf{V}) = L_n$, and right equality if and only if $PH(\mathbf{V})$ is an "all-kink" chain.

(2) If $\alpha = 0$, then

$$R_\alpha(PH(\mathbf{V})) = 4^\alpha + 4(n-1)(6^\alpha + 9^\alpha). \quad (24)$$

■

Next, we will characterize extremal phenylene chains with respect to the Harmonic index, first Zagreb index, sum-connectivity index, Geometric-Arithmetic index, Atom-Bond connectivity index and Symmetric Division index. Specifically, the second Zagreb index is for $\alpha = 1$ to the general Randić index, so we don't have to give the characterization.

According to Lemma III.1 and the definition of the Harmonic index, the exact value of the Harmonic index of $PH(\mathbf{V})$ is obtained.

Theorem III.4. *Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ square. Suppose that $\mathbf{V}$ have h nonzero components. Then*

$$H(PH(\mathbf{V})) = \frac{44}{15}(n-1) + \frac{1}{30}h + 3. \quad (25)$$

Proof: By the definition of the Harmonic index, we have

$$\begin{aligned} H(PH(\mathbf{V})) &= \sum_{e=uv\in E(PH(\mathbf{V}))} \frac{2}{d_u + d_v} \\ &= m_{22}[\frac{2}{2+2}] + m_{23}[\frac{2}{2+3}] + m_{33}[\frac{2}{3+3}] \\ &= (6+h)\frac{1}{2} + [4(n-1) - 2h]\frac{2}{5} + [4(n-1)+h]\frac{1}{3} \\ &= 3 + \frac{h}{2} + \frac{8}{5}(n-1) - \frac{4}{5}h + \frac{4}{3}(n-1) + \frac{h}{3} \\ &= \frac{44}{15}(n-1) + \frac{1}{30}h + 3. \end{aligned}$$

■

Notice that $0 \le h \le n-2$, $h = 0$ if and only if $PH(\mathbf{V}) = L_n$, and $h = n-2$ if and only if $PH(\mathbf{V})$ is an "all-kink" chain. As a consequence of Theorem III.4, extremal phenylene chains with respect to the Harmonic index could be characterized, as given in the following result.

Theorem III.5. *Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ square. we have*

$$\begin{aligned} &\frac{44}{15}(n-1) + 3 \le H(PH(V)) \le \\ &\frac{44}{15}(n-1) + \frac{n}{30} + \frac{44}{15}, \end{aligned} \quad (26)$$

with left equality if and only if $PH(\mathbf{V}) = L_n$, and right equality if and only if $PH(\mathbf{V})$ is an "all-kink" chain.

According to Lemma III.1 and the definition of the first Zagreb index, the exact value of the the first Zagreb index of $PH(\mathbf{V})$ is obtained.

Theorem III.6. *Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ square. Suppose that $\mathbf{V}$ have h nonzero components. Then*

$$M_1(PH(\mathbf{V})) = 44n - 20. \quad (27)$$

Proof: By the definition of the first Zagreb index, we have

$$\begin{aligned} M_1(PH(\mathbf{V})) &= \sum_{e=uv\in E(PH(\mathbf{V}))} [d_u + d_v] \\ &= m_{22}[2+2] + m_{23}[2+3] + m_{33}[3+3] \\ &= (6+h)4 + [4(n-1) - 2h]5 + [4(n-1)+h]6 \\ &= 24 + 4h + 20(n-1) - 10h + 24(n-1) + 6h \\ &= 44n - 20. \end{aligned}$$

■

It is interesting to note that all the first Zagreb index of the phenylene chain depends only on the number of hexagons, which is independent of the number of "kinks".

According to Lemma III.1 and the definition of the Sum-Connectivity index, the exact value of the the sum-connectivity index of $PH(\mathbf{V})$ is obtained.

Theorem III.7. *Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ square. Suppose that $\mathbf{V}$ have h nonzero components. Then*

$$S(PH(\mathbf{V})) = (\frac{4}{\sqrt{5}} + \frac{4}{\sqrt{6}})(n-1) + (\frac{1}{2} - \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{6}})h + 3. \quad (28)$$

Proof: By the definition of the Sum-Connectivity index, we have

$$\begin{aligned} S(PH(\mathbf{V})) &= \sum_{e=uv\in E(PH(\mathbf{V}))} \frac{1}{\sqrt{d_u + d_v}} \\ &= m_{22}[\frac{1}{\sqrt{2+2}}] + m_{23}[\frac{1}{\sqrt{2+3}}] + m_{33}[\frac{1}{\sqrt{3+3}}] \\ &= (6+h)\frac{1}{2} + [4(n-1) - 2h]\frac{1}{\sqrt{5}} + [4(n-1)+h]\frac{1}{\sqrt{6}} \\ &= 3 + \frac{h}{2} + \frac{4}{\sqrt{5}}(n-1) - \frac{2}{\sqrt{5}}h + \frac{4}{\sqrt{6}}(n-1) + \frac{h}{\sqrt{6}} \\ &= (\frac{4}{\sqrt{5}} + \frac{4}{\sqrt{6}})(n-1) + (\frac{1}{2} - \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{6}})h + 3. \end{aligned}$$

■

Notice that $0 \le h \le n-2$, $h = 0$ if and only if $PH(\mathbf{V}) = L_n$, and $h = n-2$ if and only if $PH(\mathbf{V})$ is an "all-kink" chain. As a consequence of Theorem III.7, extremal phenylene chains with respect to the Sum-Connectivity index could be characterized, as given in the following result.

Theorem III.8. *Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ square. we have*

$$\begin{aligned} &(\frac{4}{\sqrt{5}} + \frac{4}{\sqrt{6}})(n-1) + 3 \le S(PH(V)) \le \\ &(\frac{1}{2} + \frac{2}{\sqrt{5}} + \frac{5}{\sqrt{6}})(n-1) + (\frac{5}{2} + \frac{2}{\sqrt{5}} - \frac{1}{\sqrt{6}}), \end{aligned} \quad (29)$$

with left equality if and only if $PH(\mathbf{V}) = L_n$, and right equality if and only if $PH(\mathbf{V})$ is an "all-kink" chain.

According to Lemma III.1 and the definition of the Geometric-Arithmetic index, the exact value of the the Geometric-Arithmetic index of $PH(\mathbf{V})$ is obtained.

Theorem III.9. *Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ square. Suppose that $\mathbf{V}$ have h nonzero components. Then*

$$GA(PH(\mathbf{V})) = \frac{8\sqrt{6} + 20}{5}(n-1) + (2 - \frac{4\sqrt{6}}{5})h + 6. \quad (30)$$

Proof: By the definition of the Geometric-Arithmetic index, we have

$$\begin{aligned}GA(PH(\mathbf{V})) &= \sum_{e=uv\in E(PH(\mathbf{V}))}\frac{2\sqrt{d_u d_v}}{d_u+d_v}\\ &= m_{22}[\frac{2\sqrt{2\cdot 2}}{2+2}]+m_{23}[\frac{2\sqrt{2\cdot 3}}{2+3}]+m_{33}[\frac{2\sqrt{3\cdot 3}}{3+3}]\\ &= (6+h)+[4(n-1)-2h]\frac{2\sqrt{6}}{5}+[4(n-1)+h]\\ &= 6+h+\frac{8\sqrt{6}}{5}(n-1)-\frac{4\sqrt{6}}{5}h+4(n-1)+h\\ &= \frac{8\sqrt{6}+20}{5}(n-1)+(2-\frac{4\sqrt{6}}{5})h+6.\end{aligned}$$

■

Notice that $0 \leq h \leq n-2$, $h=0$ if and only if $PH(\mathbf{V}) = L_n$, and $h = n-2$ if and only if $PH(\mathbf{V})$ is an "all-kink" chain. As a consequence of Theorem III.9, extremal phenylene chains with respect to the Geometric-Arithmetic index could be characterized, as given in the following result.

Theorem III.10. *Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ square. we have*

$$\begin{aligned}&\frac{8\sqrt{6}+20}{5}(n-1)+6 \leq GA(PH(V)) \leq\\ &\frac{4\sqrt{6}+30}{5}(n-1)+\frac{4\sqrt{6}}{5}+4,\end{aligned} \tag{31}$$

with left equality if and only if $PH(\mathbf{V}) = L_n$, and right equality if and only if $PH(\mathbf{V})$ is an "all-kink" chain.

According to Lemma III.1 and the definition of the Atom-Bond connectivity index, the exact value of the the Atom-Bond connectivity index of $PH(\mathbf{V})$ is obtained.

Theorem III.11. *Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ square. Suppose that $\mathbf{V}$ have h nonzero components. Then*

$$ABC(PH(\mathbf{V})) = \frac{8+6\sqrt{2}}{3}(n-1)-(\frac{\sqrt{2}}{2}-\frac{2}{3})h+3\sqrt{2}. \tag{32}$$

Proof: By the definition of the Atom-Bond connectivity index, we have

$$\begin{aligned}ABC(PH(\mathbf{V})) &= \sum_{e=uv\in E(PH(\mathbf{V}))}\sqrt{\frac{d_u+d_v-2}{d_u d_v}}\\ &= m_{22}[\sqrt{\frac{2+2-2}{2\cdot 2}}]+m_{23}[\sqrt{\frac{2+3-2}{2\cdot 3}}]\\ &\quad +m_{33}[\sqrt{\frac{3+3-2}{3\cdot 3}}]\\ &= (6+h)\frac{\sqrt{2}}{2}+[4(n-1)-2h]\frac{\sqrt{2}}{2}+[4(n-1)+h]\frac{2}{3}\\ &= 3\sqrt{2}+\frac{\sqrt{2}}{2}h+2\sqrt{2}(n-1)-\sqrt{2}h+\frac{8}{3}(n-1)+\frac{2}{3}h\\ &= \frac{8+6\sqrt{2}}{3}(n-1)-(\frac{\sqrt{2}}{2}-\frac{2}{3})h+3\sqrt{2}.\end{aligned}$$

■

Notice that $0 \leq h \leq n-2$, $h=0$ if and only if $PH(\mathbf{V}) = L_n$, and $h = n-2$ if and only if $PH(\mathbf{V})$ is an "all-kink" chain. As a consequence of Theorem III.11, extremal phenylene chains with respect to the Atom-Bond connectivity index could be characterized, as given in the following result.

Theorem III.12. *Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ square. we have*

$$\begin{aligned}&\frac{8+6\sqrt{2}}{3}(n-1)+3\sqrt{2} \leq ABC(PH(V)) \leq\\ &(\frac{10}{3}+\frac{3\sqrt{2}}{2})(n-1)+\frac{7\sqrt{2}}{2}-\frac{2}{3},\end{aligned} \tag{33}$$

with left equality if and only if $PH(\mathbf{V}) = L_n$, and right equality if and only if $PH(\mathbf{V})$ is an "all-kink" chain.

According to Lemma III.1 and the definition of the Symmetric-Division index, the exact value of the the Symmetric Division index of $PH(\mathbf{V})$ is obtained.

Theorem III.13. *Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ square. Suppose that $\mathbf{V}$ have h nonzero components. Then*

$$SD(PH(\mathbf{V})) = \frac{50}{3}(n-1)-\frac{1}{3}h+12. \tag{34}$$

Proof: By the definition of the Symmetric-Division index, we have

$$\begin{aligned}SD(PH(\mathbf{V})) &= \sum_{e=uv\in E(PH(\mathbf{V}))}\frac{d_u^2+d_v^2}{d_u d_v}\\ &= m_{22}[\frac{2^2+2^2}{2\cdot 2}]+m_{23}[\frac{2^2+3^2}{2\cdot 3}]+m_{33}[\frac{3^2+3^2}{3\cdot 3}]\\ &= (6+h)2+[4(n-1)-2h]\frac{13}{6}+[4(n-1)+h]2\\ &= 12+2h+\frac{26}{3}(n-1)-\frac{13}{3}h+8(n-1)+2h\\ &= \frac{50}{3}(n-1)-\frac{1}{3}h+12.\end{aligned}$$

■

Notice that $0 \leq h \leq n-2$, $h=0$ if and only if $PH(\mathbf{V}) = L_n$, and $h = n-2$ if and only if $PH(\mathbf{V})$ is an "all-kink" chain. As a consequence of Theorem III.13, extremal phenylene chains with respect to the Symmetric-Division index could be characterized, as given in the following result.

Theorem III.14. *Let $PH(\mathbf{V})$ be a phenylene chain with n hexagons and $n-1$ square. we have*

$$\begin{aligned}&\frac{50}{3}(n-1)+12 \leq SD(PH(V)) \leq\\ &\frac{49}{3}(n-1)+\frac{37}{3},\end{aligned} \tag{35}$$

with left equality if and only if $PH(\mathbf{V}) = L_n$, and right equality if and only if $PH(\mathbf{V})$ is an "all-kink" chain.

IV. Conclusion

The Kirchhoff index and the degree-based topological indices considered in this paper are important topological indices, which have significant applications in chemistry. For this reason, they have been extensively studied. In this paper, extremal phenylene chains with maximum Kirchhoff index, minimum and maximum generalized Randić index, Harmonic index, first Zagreb index, Sum-Connectivity index, Geometric-Arithmetic index, Atom-Bond connectivity index

and Symmetric-Division index been singled out. However, the problem which phenylene chain attains minimum Kirchhoff index is still open, which deserves further study.

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