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Research Article

Two Classes of Topological Indices of Phenylene Molecule Graphs

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A phenylene is a conjugated hydrocarbons molecule composed of six- and four-membered rings. The matching energy of a graph G is equal to the sum of the absolute values of the zeros of the matching polynomial of G, while the Hosoya index is defined as the total number of the independent edge sets of G. In this paper, we determine the extremal graph with respect to the matching energy and Hosoya index for all phenylene chains.

1. Introduction

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 hexagons. They are nanostructures that can be precisely designed and manufactured for a wide variety of applications; see [1–3] and the references therein.

A topological index is a numerical quantity derived in an unambiguous manner from the structure graph of a molecule, as a graph structural invariant; that is, it does not depend on the labeling or the pictorial representation of a graph. Various topological indices usually reflect molecular size and shape. One topological index is Hosoya index, which was first introduced by Hosoya [4]. It plays an important role in the so-called inverse structure-property relationship problems. For details of Hosoya index and its applications, the readers are suggested to refer to [5, 6]. A new topological index in chemistry, matching energy, is first introduced by Gutman and Wagner [7] in 2012 to study topological resonance energy of conjugated molecules, which has received a lot of attention from researchers in recent years. For more background and applications about matching energy, see [8–16].

In this paper, our aim is to determine the phenylenes with minimum and maximum matching energy (Hosoya index) among all the phenylenes with n hexagons.

In the following we present some definitions and notations.

Let $G = (V, E)$ be a graph with the vertex set $V(G)$ and the edge set $E(G)$. Let e and v be an edge and a vertex in G, respectively. We denote by $G - e$ the graph obtained from G by removing edge e and by $G - v$ the graph obtained from G by deleting vertex v.

By $m(G, k)$ we denote the number of k-matchings of a graph G. The matching polynomial of a graph G with n vertices is fined as

$$\alpha(G, x) = \sum_{k\geq 0} (-1)^k m(G, k) x^{n-2k}, \quad (1)$$

where $m(G, 0) = 1$ and $m(G, k) \geq 0$ for all $k = 1, 2, \dots, [n/2]$. This expression $\alpha(G, x)$ induces a quasi-order relation (i.e., reflexive and transitive relation) on the set of all graphs with n vertices. If G and H are two graphs with matching polynomial in the form (1), then the quasi-order $\succeq$ is defined by

$$G \succeq H \Longleftrightarrow m(G, k) \geq m(H, k) \quad \forall k = 0, 1, \dots, \lfloor n/2 \rfloor. \quad (2)$$

Particularly, if $G \succeq H$ and there exists some k such that $m(G, k) > m(H, k)$, then we write $G \succ H$.

Gutman and Wagner in [7] first proposed the concept of the *matching energy* of a graph, denoted by ME(G), as

$$\mathrm{ME} = \mathrm{ME}(G) = \frac{2}{\pi}\int_0^{\infty} x^{-2}\ln\left[\sum_{k\geq 0} m(G,k)\,x^{2k}\right]dx. \quad (3)$$

Meanwhile, they gave also another form of definition of matching energy of a graph. That is,

$$\mathrm{ME}(G) = \sum_{i=1}^{n}\left|\mu_i\right|, \quad (4)$$

where μ_i denotes the root of matching polynomial of G. By (2) and (3), we easily obtain the fact as follows:

$$\begin{gathered} G \succeq H \Longrightarrow \mathrm{ME}(G) \geq \mathrm{ME}(H), \\ G \succ H \Longrightarrow \mathrm{ME}(G) > \mathrm{ME}(H). \end{gathered} \quad (5)$$

The Z-counting polynomial was defined by Hosoya [4] as

$$Z(G) = Z(G,x) = \sum_k m(G,k)\,x^k. \quad (6)$$

Particularly, set $x = 1$; then $Z(G,1) = \sum_k m(G,k)$ is called *Hosoya index* of G. Furthermore, The Z-counting polynomial of graphs has the property as follows.

Lemma 1 (see [4]). *(a) Let G be a graph consisting of two components G_1 and G_2. Then $Z(G) = Z(G_1)Z(G_2)$.*

(b) Let $uv \in E(G)$ be an edge of G. Then $Z(G) = Z(G - uv) + xZ(G - u - v)$.

A *phenylene chain* containing n ($n \geq 2$) hexagons, denoted by PHB_n, is a phenylene with the properties that (a) no vertex is incident with two hexagons or squares and (b) no hexagon is adjacent to more than two squares. We denote by $\mathscr{B}_n$ the set of all phenylene chains with n hexagons. Let $\mathrm{PHB}_n \in \mathscr{B}_n$. If the subgraph PHB_n induced by the vertices with degree 3 is the union of $n-1$ disjoint copies of a square, then PHB_n is called a *linear phenylene chain* and denoted by PHL_n (see Figure 1). If the subgraph $\mathrm{PHB}_n$of induced by the vertices with degree 3 is isomorphic to the graph S_{n-1} having $n-1$ squares (see Figure 1), then PHB_n is called a *zigzag phenylene chain* and is denoted by PHZ_n (see Figure 1). It is easy to see that $\mathscr{B}_2 = \{\mathrm{PHL}_2\} = \{\mathrm{PHZ}_2\}$ and $\mathscr{B}_3 = \{\mathrm{PHL}_3, \mathrm{PHZ}_3\}$. Finally, by the definition of a phenylene chain, any element PHB_n in $\mathscr{B}_n$ can be obtained from an appropriately chosen graph $\mathrm{PHB}_{n-1} \in \mathscr{B}_{n-1}$ by attaching to it a new graph θ, where θ is obtained from an edge of a square attaching an edge of a hexagon; see Figure 2.

2. Main Results

Theorem 2. *Let $\mathscr{B}_n$ be the set of all phenylene chains with n hexagons. For any $PHB_n \in \mathscr{B}_n$, then*

$$ME(PHL_n) \leq ME(PHB_n) \leq ME(PHZ_n), \quad (7)$$

where the equalities on the left side hold only if $PHB_n \cong PHL_n$, and the equalities on the right side hold only if $PHB_n \cong PHZ_n$.

By (2) and (5), we know that Theorem 2 holding only needs to prove the following result.

Theorem 3. *For any $PHB_n \in \mathscr{B}_n$ and for each $k \geq 0$,*

$$m(PHL_n,k) \leq m(PHB_n,k) \leq m(PHZ_n,k), \quad (8)$$

where the equalities on the left side hold only if $PHB_n \cong PHL_n$ and the equalities on the right side hold only if $PHB_n \cong PHZ_n$.

Let $f(x) = \sum_{k=0}^{n} a_k x^k$ and $g(x) = \sum_{k=0}^{n} b_k x^k$ be two polynomials of x. We say $f(x) \preceq g(x)$ if $a_k \leq b_k$ for all k. If $f(x) \preceq g(x)$ and there exists some k such that $a_k < b_k$, then we say $f(x) \prec g(x)$. By (6), it is easy to obtain the following result which is equivalent to Theorem 3.

Theorem 4. *For any $PHB_n \in \mathscr{B}_n$ ($n \geq 2$),*

(I) *if $PHL_n \neq PHB_n$, then $Z(PHL_n) \prec Z(PHB_n)$,*

(II) *if $PHZ_n \neq PHB_n$, then $Z(PHB_n) \prec Z(PHZ_n)$.*

In the following we will use the notation G for $Z(G)$, when it would lead to no confusion.

Proof. Checking Figure 2, by Lemma 1, we obtained that

$$\mathrm{PHB}_n = \left(1+6x+9x^2+2x^3\right)\mathrm{PHB}_{n-1} + \left(x+4x^2+3x^3\right)\left[\left(\mathrm{PHB}_{n-1}-s_{2n-3}\right)+\left(\mathrm{PHB}_{n-1}-t_{2n-3}\right)\right] + \left(x^2+3x^3+x^4\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}-t_{2n-3}\right), \quad (9)$$

$$\mathrm{PHB}_n - y = \begin{cases} \left(1+4x+3x^2\right)\mathrm{PHB}_{n-1} + \left(x+2x^2\right)\left(\mathrm{PHB}_{n-1}-t_{2n-3}\right) + \left(x+3x^2+x^3\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}\right) + \left(x^2+2x^3\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}-t_{2n-3}\right) & \text{if } y = b_1^n, \\ \left(1+4x+3x^2\right)\mathrm{PHB}_{n-1} + \left(x+2x^2+x^3\right)\left(\mathrm{PHB}_{n-1}-t_{2n-3}\right) + \left(x+2x^2\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}\right) + \left(x^2+x^3\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}-t_{2n-3}\right) & \text{if } y = b_2^n, \\ \left(1+4x+3x^2\right)\mathrm{PHB}_{n-1} + \left(x+2x^2+x^3\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}\right) + \left(x+2x^2\right)\left(\mathrm{PHB}_{n-1}-t_{2n-3}\right) + \left(x^2+x^3\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}-t_{2n-3}\right) & \text{if } y = b_3^n, \\ \left(1+4x+3x^2\right)\mathrm{PHB}_{n-1} + \left(x+2x^2\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}\right) + \left(x+3x^2+x^3\right)\left(\mathrm{PHB}_{n-1}-t_{2n-3}\right) + \left(x^2+2x^3\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}-t_{2n-3}\right) & \text{if } y = b_4^n, \end{cases} \quad (10)$$

$$\mathrm{PHB}_n - y - z = \begin{cases} \left(1+3x+x^2\right)\mathrm{PHB}_{n-1} + \left(x+x^2\right)\left(\mathrm{PHB}_{n-1}-t_{2n-3}\right) + \left(x+2x^2\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}\right) + \left(x^2+x^3\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}-t_{2n-3}\right) & \text{if } y = b_1^n,\ z = b_2^n; \\ \left(1+3x+x^2\right)\mathrm{PHB}_{n-1} + \left(x+x^2\right)\left(\mathrm{PHB}_{n-1}-t_{2n-3}\right) + \left(x+x^2\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}\right) + x\left(\mathrm{PHB}_{n-1}-s_{2n-3}-t_{2n-3}\right) & \text{if } y = b_2^n,\ z = b_3^n; \\ \left(1+3x+x^2\right)\mathrm{PHB}_{n-1} + \left(x+x^2\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}\right) + \left(x+2x^2\right)\left(\mathrm{PHB}_{n-1}-t_{2n-3}\right) + \left(x^2+x^3\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}-t_{2n-3}\right) & \text{if } y = b_3^n,\ z = b_4^n. \end{cases} \quad (11)$$

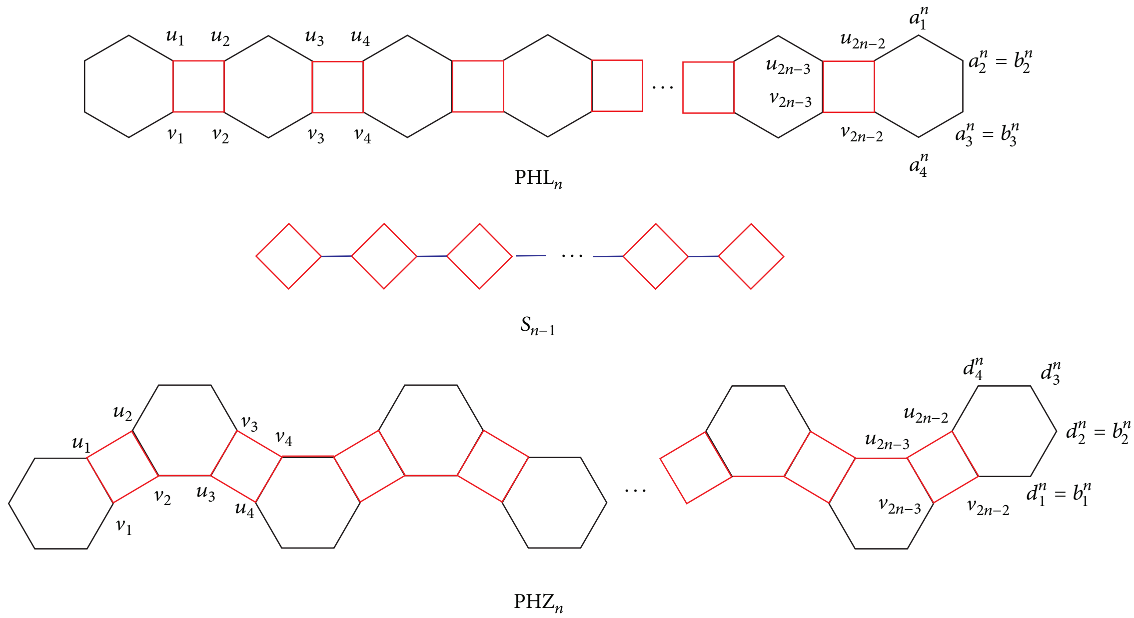

Figure 1: A linear phenylene chain PHL_n and a zigzag phenylene chain PHZ_n.

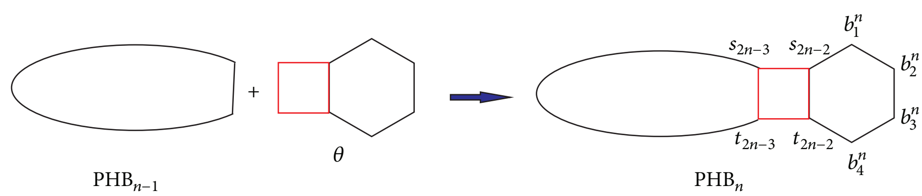

Figure 2: A phenylene chain PHB_n.

By (10) and (11), we have

(i) $\mathrm{PHB}_n - b_3^n \prec \mathrm{PHB}_n - b_1^n$ and $\mathrm{PHB}_n - b_2^n \prec \mathrm{PHB}_n - b_4^n$;

(ii) $\mathrm{PHB}_n - b_2^n - b_3^n \prec \mathrm{PHB}_n - b_1^n - b_2^n$ and $\mathrm{PHB}_n - b_2^n - b_3^n \prec \mathrm{PHB}_n - b_3^n - b_4^n$.

Particularly, if $\mathrm{PHB}_n = \mathrm{PHL}_n$, then

(i′) $\mathrm{PHL}_n - a_2^n = \mathrm{PHL}_n - a_3^n \prec \mathrm{PHL}_n - a_1^n = \mathrm{PHL}_n - a_4^n$,

(ii′) $\mathrm{PHL}_n - a_2^n - a_3^n \prec \mathrm{PHL}_n - a_1^n - a_2^n = \mathrm{PHL}_n - a_3^n - a_4^n$,

(iii′) $(\mathrm{PHL}_n - a_2^n) + (\mathrm{PHL}_n - a_3^n) \prec (\mathrm{PHL}_n - a_2^n) + (\mathrm{PHL}_n - a_1^n) = (\mathrm{PHL}_n - a_3^n) + (\mathrm{PHL}_n - a_4^n)$.

We prove Theorem 4(I) by mathematical induction. First we consider $n = 3$. In this case, $\mathscr{B}_n = \{\mathrm{PHL}_3, \mathrm{PHZ}_3\}$. By (9), we have

$$\begin{aligned}\mathrm{PHL}_3 &= \left(1 + 6x + 9x^2 + 2x^3\right)\mathrm{PHL}_2 \\ &\quad + \left(x + 4x^2 + 3x^3\right)\left[\left(\mathrm{PHL}_2 - a_2^2\right) + \left(\mathrm{PHL}_2 - a_3^2\right)\right] \\ &\quad + \left(x^2 + 3x^3 + x^4\right)\left(\mathrm{PHL}_2 - a_2^2 - a_3^2\right),\end{aligned}$$

$$\begin{aligned}\mathrm{PHZ}_3 &= \left(1 + 6x + 9x^2 + 2x^3\right)\mathrm{PHZ}_2 \\ &\quad + \left(x + 4x^2 + 3x^3\right)\left[\left(\mathrm{PHZ}_2 - d_1^2\right) + \left(\mathrm{PHZ}_2 - d_2^2\right)\right] \\ &\quad + \left(x^2 + 3x^3 + x^4\right)\left(\mathrm{PHZ}_2 - d_1^2 - d_2^2\right) \\ &= \left(1 + 6x + 9x^2 + 2x^3\right)\mathrm{PHL}_2 \\ &\quad + \left(x + 4x^2 + 3x^3\right)\left[\left(\mathrm{PHL}_2 - a_4^2\right) + \left(\mathrm{PHL}_2 - a_3^2\right)\right] \\ &\quad + \left(x^2 + 3x^3 + x^4\right)\left(\mathrm{PHL}_2 - a_3^2 - a_4^2\right).\end{aligned} \tag{12}$$

By (i′)–(iii′), we have $\mathrm{PHL}_3 \prec \mathrm{PHZ}_3$.

Suppose that Theorem 4(I) is right for all phenylene chains with few n hexagons. Let PHB_n be a phenylene chain with $n \geq 4$ hexagons, which is obtained from $\mathrm{PHB}_{n-1} \in \mathscr{B}_{n-1}$ by attaching to it a new θ (see Figure 2). We show that if $\mathrm{PHL}_n \neq \mathrm{PHB}_n$, then $\mathrm{PHL}_n \prec \mathrm{PHB}_n$. By (9) we obtain that

$$\begin{aligned}\mathrm{PHL}_n &= \left(1 + 6x + 9x^2 + 2x^3\right)\mathrm{PHL}_{n-1} \\ &\quad + \left(x + 4x^2 + 3x^3\right)\end{aligned}$$

$$\cdot\left[\left(\mathrm{PHL}_{n-1}-u_{2n-3}\right)+\left(\mathrm{PHL}_{n-1}-v_{2n-3}\right)\right]$$
$$+\left(x^2+3x^3+x^4\right)\left(\mathrm{PHL}_{n-1}-u_{2n-3}-v_{2n-3}\right),$$
$$\mathrm{PHB}_n=\left(1+6x+9x^2+2x^3\right)\mathrm{PHB}_{n-1}$$
$$+\left(x+4x^2+3x^3\right)$$
$$\cdot\left[\left(\mathrm{PHB}_{n-1}-s_{2n-3}\right)+\left(\mathrm{PHB}_{n-1}-t_{2n-3}\right)\right]$$
$$+\left(x^2+3x^3+x^4\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}-t_{2n-3}\right). \quad (13)$$

By the inductive hypotheses we have $\mathrm{PHL}_{n-1} \preceq \mathrm{PHB}_{n-1}$, $(\mathrm{PHL}_{n-1}-u_{2n-3})+(\mathrm{PHL}_{n-1}-v_{2n-3}) \preceq (\mathrm{PHB}_{n-1}-s_{2n-3})+(\mathrm{PHB}_{n-1}-t_{2n-3})$, and $(\mathrm{PHL}_{n-1}-u_{2n-3}-v_{2n-3}) \preceq (\mathrm{PHB}_{n-1}-s_{2n-3}-t_{2n-3})$. Since $\mathrm{PHL}_n \neq \mathrm{PHB}_n$, either $\mathrm{PHL}_{n-1} \neq \mathrm{PHB}_{n-1}$ or $\{s_{n-1}, t_{n-1}\} \neq \{u_{2n-3}, v_{2n-3}\}$, and hence at least one of the three inequalities is strict. Therefore, we get that $\mathrm{PHL}_n \prec \mathrm{PHB}_n$.

In the following we prove Theorem 4(II) by induction.

By the proof of Theorem 4(I), we know that $\mathrm{PHB}_3 \prec \mathrm{PHZ}_3$.

Similarly, suppose that Theorem 4(II) is right for all phenylene chains with few n hexagons. Let PHB_n be a phenylene chain with $n \geq 4$ hexagons, which is obtained from $\mathrm{PHB}_{n-1} \in \mathscr{B}_{n-1}$ by attaching to it a new θ (see Figure 2). We show that if $\mathrm{PHB}_n \neq \mathrm{PHZ}_n$, then $\mathrm{PHB}_n \prec \mathrm{PHZ}_n$. By (9) we have

$$\mathrm{PHB}_n=\left(1+6x+9x^2+2x^3\right)\mathrm{PHB}_{n-1}$$
$$+\left(x+4x^2+3x^3\right)$$
$$\cdot\left[\left(\mathrm{PHB}_{n-1}-s_{2n-3}\right)+\left(\mathrm{PHB}_{n-1}-t_{2n-3}\right)\right]$$
$$+\left(x^2+3x^3+x^4\right)\left(\mathrm{PHB}_{n-1}-s_{2n-3}-t_{2n-3}\right) \quad (14)$$
$$\mathrm{PHZ}_n=\left(1+6x+9x^2+2x^3\right)\mathrm{PHZ}_{n-1}$$
$$+\left(x+4x^2+3x^3\right)$$
$$\cdot\left[\left(\mathrm{PHZ}_{n-1}-u_{2n-3}\right)+\left(\mathrm{PHZ}_{n-1}-v_{2n-3}\right)\right]$$
$$+\left(x^2+3x^3+x^4\right)\left(\mathrm{PHZ}_{n-1}-u_{2n-3}-v_{2n-3}\right).$$

By the inductive hypotheses we have $\mathrm{PHB}_{n-1} \preceq \mathrm{PHZ}_{n-1}$, $(\mathrm{PHB}_{n-1}-s_{2n-3})+(\mathrm{PHB}_{n-1}-t_{2n-3}) \preceq (\mathrm{PHZ}_{n-1}-u_{2n-3})+(\mathrm{PHZ}_{n-1}-v_{2n-3})$, and $(\mathrm{PHB}_{n-1}-s_{2n-3}-t_{2n-3}) \preceq (\mathrm{PHZ}_{n-1}-u_{2n-3}-v_{2n-3})$. Since $\mathrm{PHB}_n \neq \mathrm{PHZ}_n$, either $\mathrm{PHB}_{n-1} \neq \mathrm{PHZ}_{n-1}$ or $\{s_{n-1}, t_{n-1}\} \neq \{u_{2n-3}, v_{2n-3}\}$, and hence at least one of the three inequalities is strict. Therefore, we get that $\mathrm{PHB}_n \prec \mathrm{PHZ}_n$.

The proof is complete. □

By the definition of Hosoya index and Theorem 4, we can obtain the following result.

Theorem 5. *Let $\mathscr{B}_n$ be the set of all phenylene chains with n hexagons. For any $PHB_n \in \mathscr{B}_n$, then*

$$Z\left(PHL_n, 1\right) \leq Z\left(PHB_n, 1\right) \leq Z\left(PHZ_n, 1\right), \quad (15)$$

where the equalities on the left side hold only if $PHB_n \cong PHL_n$ and the equalities on the right side hold only if $PHB_n \cong PHZ_n$.

Competing Interests

The author declares that there are no competing interests regarding the publication of this paper.

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