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Research article

The expected values of arithmetic bond connectivity and geometric indices in random phenylene chains

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ABSTRACT

Phenylenes are a class of conjugated hydrocarbons composed of a special arrangement of six- and four-membered rings. In this paper, the expected values of the atom-bond connectivity (ABC), geometric-arithmetic (GA), and Zagreb indices of this class of conjugated hydrocarbons have been determined. At the end, the comparisons with respect to the random phenylene chains among the expected values of these indices, have been determined explicitly. The graphical profiles of these indices have been shown in order to support our results.

1. Introduction

There are lot of topological indices in the literature of chemical graph theory. The first of it kind is the Wiener index [1]. After that most important topological index is a class of the Zagreb indices [2], molecular connectivity [3, 4, 5]. The first and second Zagreb indices are defined as:

$$M_1(G) = \sum_{uv \in E(G)} d_u + d_v \tag{1}$$

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v \tag{2}$$

A new index named atom-bond connectivity (ABC) index was introduced by Estrada et al. in 1998 and defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \tag{3}$$

In the same paper [6], the authors used this index to model thermodynamic properties of organic chemical compounds. In 2008, Estrada [7], proved that ABC-index can be used as a tool to explain the stability of branched alkanes. This new idea has attracted many Mathematicians which gave lot of mathematical properties of ABC-index.

In 2009, Vukicevic and Furtula [8] introduced a new topological index of a graph G, named the geometric-arithmetic(GA) index and is defined as follows:

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \tag{4}$$

It is proved in [8] that some physico-chemical properties of a compound can be well correlated with GA index and predict more accurate that than Randic index. There are lot of research papers related to the GA index of a graph G which can be found in literature, see for example [9, 10, 11]. There are plenty of papers outlined the mathematical properties of these four indices, for example one can consults the papers [10, 12, 13, 14, 15, 16, 17, 18] and the references therein.

The phenylenes exhibit unique physicochemical properties due to their aromatic and antiaromatic rings. The phenylenes composed of a special arrangement of six- and four-membered rings. More precisely, any two six-membered rings are not adjacent, and every four-membered ring is adjacent to a pair of nonadjacent six-membered rings (hexagons).

In general, phenylenes, especially phenylene chains have attracted much attention due to excellent properties. For example it was a great discovery in the theory of phenylenes that many π-electron properties of a phenylene are closely related to the analogous properties of a benzenoid molecule, called its hexagonal squeeze (HS).

There are unique phenylene chains for $n = 1$ and $n = 2$ as shown in Fig. 1. More generally, for $n \geq 3$, the terminal hexagon can be attached in three different ways, which results in a random phenylene chain $\mathcal{RPH}(n, \rho)$ with probability ρ, as shown in Fig. 1. Thus $\mathcal{RPH}(n, \rho)$ can be obtained by stepwise addition of terminal hexagons. At each step

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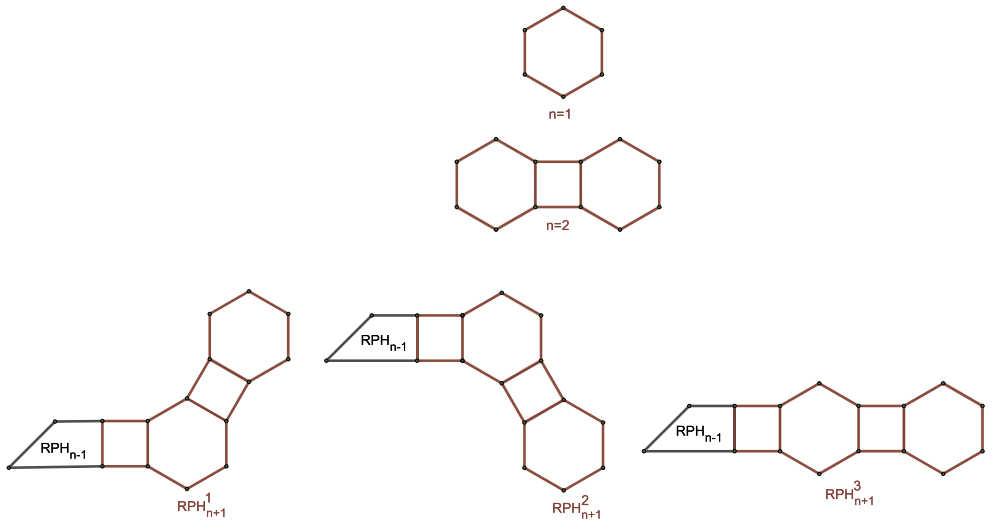

Fig. 1. The three types of local arrangements in phenylene.

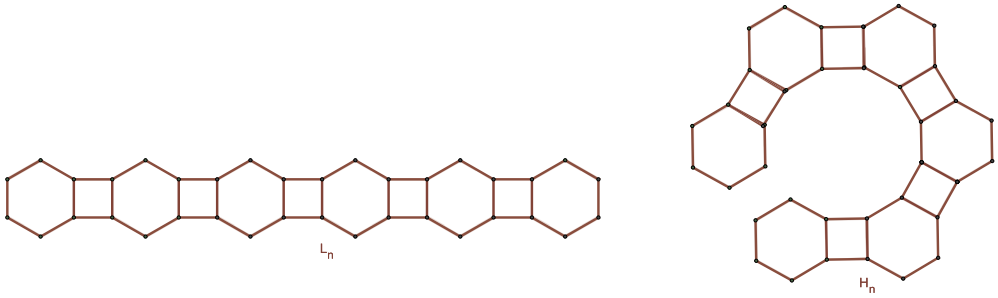

Fig. 2. The linear and kicks chains.

$k(=3,4,\ldots,n)$ a random selection is made from one of the three possible constructions:

(a) $\mathcal{RPH}_{k-1} \to \mathcal{RPH}_k^1$ with probability ρ,
(b) $\mathcal{RPH}_{k-1} \to \mathcal{RPH}_k^2$ with probability ρ, or
(c) $\mathcal{RPH}_{k-1} \to \mathcal{RPH}_k^3$ with probability $q = 1 - 2\rho$, with probability.

If, we consider the probability is invariant to the step parameter and constant, then this process is a zeroth-order Markov process. If we obtained a random phenylene chains which involved only the first or second types of arrangements, then such a chain will be called all-kinks chains, denoted by H_n and if we obtained a chain from only third type of arrangements, then such a chain will be called linear and denoted by L_n for example see Fig. 2. There are few papers which focused on the random structure of a chemical graphs, see for example [19, 20] and references therein. It was discovered that the algebraic structure count of a phenylene is equal to the number of Kekule structures of the associated hexagonal squeeze [21, 22]. The energy and Estrada index of phenylenes has been determined in [23]. A lot of papers have been published related to the topological indices of this class of hydrocarbons, for example, the total π-electron energy [22], Narumi-Katayama index [24], and PI index [25], Merrifild-Simmons index [26], anti-Kekul and antiforceing number [27], Omega index and related polynomials [28, 29]. The Wiener index of phenylenes has been calculated in [30].

Peng and Li [31] obtained the Kirchhoff index and the number of spanning trees of linear phenylene chains.

Chen and Zhang [32] obtained expected value of Wiener index of a random phenylene chain. Very recently, Li, and Shuchao [33] obtained the extremal phenylene chains with respect to the coefficients sum of the permanently polynomial, the spectral radius, the Hosoya index and the Merrifield–Simmons index. In [34] the extremal phenylene chains with respect to Kirchhoff index and degree based topological indices have been characterized. For more details one may see [35, 36, 37, 38, 39, 40, 41, 42]. In this paper, we extend the study of this class of hydrocarbon for four different types of indices namely, ABC, GA and the Zagreb indices and give their expected values for the same probability and outlines a details comparison between these indices with respect to the random phenylene chains. More precisely, we have proved that ABC index is always less than the GA index and first Zagreb index is less than the second Zagreb index for any value of n and ρ.

2. The ABC and GA indices in random phenylene chains

In this section, the ABC and GA indices in a random polyphenyl chain $\mathcal{RPH}_n$ with n hexagons will be considered. For that, let $\mathcal{RPH}_n$ be the chain obtained from $\mathcal{RPH}_{n-1}$ as shown in Fig. 1. From the structure of the $\mathcal{RPH}_n$ chain, it is easy to see that there exist only three types of edge in $\mathcal{RPH}_n$ namely $(2,2),(2,3)$, and $(3,3)$, thus, one can obtain following forms of these two indices:

$$ABC(\mathcal{RPH}_n) = \frac{1}{\sqrt{2}}x_{22}(\mathcal{RPH}_n) + \frac{1}{\sqrt{2}}x_{23}(\mathcal{RPH}_n) + \frac{2}{3}x_{33}(\mathcal{RPH}_n). \tag{5}$$

$$GA(\mathcal{RPH}_n) = x_{22}(\mathcal{RPH}_n) + \frac{2\sqrt{6}}{5}x_{23}(\mathcal{RPH}_n) + x_{33}(\mathcal{RPH}_n). \tag{6}$$

Hence in order to compute ABC and GA indices of $\mathcal{RPH}_n$, one has to determine $x_{22}(\mathcal{RPH}_n)$, $x_{23}(\mathcal{RPH}_n)$ and $x_{33}(\mathcal{RPH}_n)$ type of edges and

for simplicity, we denote $x_{ij}(\mathcal{RPH}_n)$ just by x_{ij}. As due to the local arrangements, it is clear $\mathcal{RPH}(n;\rho,\rho)$ is a random phenylene chains. So, $ABC(\mathcal{RPH}(n;\rho))$ and $GA(\mathcal{RPH}(n;\rho))$ are random variables. Let us denote by $E_n = E[ABC(\mathcal{RPH}(n;\rho))]$ and $E_n^a = E[GA(\mathcal{RPH}(n;\rho))]$, the expected values of these indices, respectively.

Theorem 1. *If $n \geq 2$ and $\mathcal{RPH}(n;\rho)$ is a random phenylene chain of length n, then*

$$E_n^a = \left[(4 - \frac{8\sqrt{6}}{5})\rho + 4 + \frac{8\sqrt{6}}{5}\right]n + (\frac{16\sqrt{6}}{5} - 8)\rho + \sqrt{2} - \frac{8\sqrt{6}}{5}.$$

Proof. Since $E_2^a = 10 + \frac{8\sqrt{6}}{5}$ which is true, thus for $n \geq 3$, there are three possibilities to be considered as shown in Fig. 1.

1. If $\mathcal{RPH}_{n-1} \to \mathcal{RPH}_n^1$ with probability ρ, then
   $x_{22}(\mathcal{RPH}_n^1) = x_{22}(\mathcal{RPH}_{n-1}) + 1, x_{23}(\mathcal{RPH}_n^1) = x_{23}(\mathcal{RPH}_{n-1}) + 2$ and
   $x_{33}(\mathcal{RPH}_n^1) = x_{33}(\mathcal{RPH}_{n-1}) + 5$ and from (6), we have
   $GA(\mathcal{RPH}_n^1) = GA(\mathcal{RPH}_{n-1}) + \frac{4\sqrt{6}}{5} + 6.$
2. If $\mathcal{RPH}_{n-1} \to \mathcal{RPH}_n^2$ with probability ρ, then
   $x_{22}(\mathcal{RPH}_n^1) = x_{22}(\mathcal{RPH}_{n-1}) + 1, x_{23}(\mathcal{RPH}_n^1) = x_{23}(\mathcal{RPH}_{n-1}) + 2$ and
   $x_{33}(\mathcal{RPH}_n^1) = x_{33}(\mathcal{RPH}_{n-1}) + 5$ and from (6), we have
   $GA(\mathcal{RPH}_n^1) = GA(\mathcal{RPH}_{n-1}) + \frac{4\sqrt{6}}{5} + 6.$
3. If $\mathcal{RPH}_{n-1} \to \mathcal{RPH}_n^3$ with probability $1 - 2\rho$, then
   $x_{22}(\mathcal{RPH}_n^3) = x_{22}(\mathcal{RPH}_{n-1}), x_{23}(\mathcal{RPH}_n^3) = x_{23}(\mathcal{RPH}_{n-1}) + 4$ and
   $x_{33}(\mathcal{RPH}_n^3) = x_{33}(\mathcal{RPH}_{n-1}) + 4$ and from (6), we have
   $GA(\mathcal{RPH}_n^3) = GA(\mathcal{RPH}_{n-1}) + 4 + \frac{8\sqrt{6}}{5}.$

Thus, we obtain

$$\begin{aligned} E_n^a &= \rho GA(\mathcal{RPH}_n^1) \\ &\quad + \rho GA(\mathcal{RPH}_n^2) + (1-2\rho)GA(\mathcal{RPH}_n^3) \\ &= 2\rho[GA(\mathcal{RPH}_{n-1}) + \frac{4\sqrt{6}}{5} + 6] \\ &\quad + (1-2\rho)[ABC(\mathcal{RPH}_{n-1}) + 4 + \frac{8\sqrt{6}}{5}] \end{aligned}$$

$$E_n^a = GA(\mathcal{RPH}_{n-1}) + \rho[4 - \frac{8\sqrt{6}}{5}] + [4 + \frac{8\sqrt{6}}{5}]. \tag{7}$$

But $E[E_n]^a = E_n^a$, so apply the operator E on (7), we get

$$E_n^a = E_{n-1}^a + \rho[4 - \frac{8\sqrt{6}}{5}] + [4 + \frac{8\sqrt{6}}{5}]. \quad n > 2 \tag{8}$$

and after solving the recurrence relation (8) with initial condition, we get

$$E_n^a = \left[(4 - \frac{8\sqrt{6}}{5})\rho + 4 + \frac{8\sqrt{6}}{5}\right]n + (\frac{16\sqrt{6}}{5} - 8)\rho + \sqrt{2} - \frac{8\sqrt{6}}{5}. \quad \square$$

Theorem 2. *If $n \geq 2$ and $\mathcal{RPH}(n;\rho)$ is a random phenylene chain of length n, then*

$$E_n = \left[(\frac{4}{3} - \sqrt{2})\rho + 2\sqrt{2} + \frac{8}{3}\right]n + (2\sqrt{2} - \frac{8}{3})\rho + \sqrt{2} - \frac{8}{3}.$$

Proof. Since $E_2 = \frac{8}{3} + 5\sqrt{2}$ which is true, thus for $n \geq 3$, there are three possibilities to be considered as shown in Fig. 1.

a. If $\mathcal{RPH}_{n-1} \to \mathcal{RPH}_n^1$ with probability ρ, then
   $x_{22}(\mathcal{RPH}_n^1) = x_{22}(\mathcal{RPH}_{n-1}) + 1, x_{23}(\mathcal{RPH}_n^1) = x_{23}(\mathcal{RPH}_{n-1}) + 2$ and
   $x_{33}(\mathcal{RPH}_n^1) = x_{33}(\mathcal{RPH}_{n-1}) + 5$ and from (5), we have
   $ABC(\mathcal{RPH}_n^1) = ABC(\mathcal{RPH}_{n-1}) + \frac{3\sqrt{2}}{2} + \frac{10}{3}.$
b. If $\mathcal{RPH}_{n-1} \to \mathcal{RPH}_n^2$ with probability ρ, then
   $x_{22}(\mathcal{RPH}_n^1) = x_{22}(\mathcal{RPH}_{n-1}) + 1, x_{23}(\mathcal{RPH}_n^1) = x_{23}(\mathcal{RPH}_{n-1}) + 2$ and
   $x_{33}(\mathcal{RPH}_n^1) = x_{33}(\mathcal{RPH}_{n-1}) + 5$ and from (5), we have
   $ABC(\mathcal{RPH}_n^1) = ABC(\mathcal{RPH}_{n-1}) + \frac{3\sqrt{2}}{2} + \frac{10}{3}.$
c. If $\mathcal{RPH}_{n-1} \to \mathcal{RPH}_n^3$ with probability $1 - 2\rho$, then
   $x_{22}(\mathcal{RPH}_n^3) = x_{22}(\mathcal{RPH}_{n-1}), x_{23}(\mathcal{RPH}_n^3) = x_{23}(\mathcal{RPH}_{n-1}) + 4$ and
   $x_{33}(\mathcal{RPH}_n^3) = x_{33}(\mathcal{RPH}_{n-1}) + 4$ and from (5), we have
   $ABC(\mathcal{RPH}_n^3) = ABC(\mathcal{RPH}_{n-1}) + 2\sqrt{2} + \frac{8}{3}.$

Thus, we obtain

$$\begin{aligned} E_n &= \rho ABC(\mathcal{RPH}_n^1) \\ &\quad + \rho ABC(\mathcal{RPH}_n^2) + (1-2\rho)ABC(\mathcal{RPH}_n^3) \\ &= 2\rho[ABC(\mathcal{RPH}_{n-1}) + \frac{3\sqrt{2}}{2} + \frac{10}{3}] \\ &\quad + (1-2\rho)[ABC(\mathcal{RPH}_{n-1}) + 2\sqrt{2} + \frac{8}{3}] \end{aligned}$$

$$E_n = ABC(\mathcal{RPH}_{n-1}) + \rho[\frac{4}{3} - \sqrt{2}] + [2\sqrt{2} + \frac{8}{3}]. \tag{9}$$

But $E[E_n] = E_n$, so apply the operator E on (9), we get

$$E_n = E_{n-1} + \rho[\frac{4}{3} - \sqrt{2}] + [2\sqrt{2} + \frac{8}{3}]. \quad n > 2 \tag{10}$$

and after solving the recurrence relation (10) with initial condition, we get

$$E_n = \left[(\frac{4}{3} - \sqrt{2})\rho + 2\sqrt{2} + \frac{8}{3}\right]n + (2\sqrt{2} - \frac{8}{3})\rho + \sqrt{2} - \frac{8}{3}. \quad \square$$

We know that the phenylene linear and all-kinks-chains can be obtained for special value of the probability as $L_n = \mathcal{RPH}(n;\frac{1}{2})$ phenylene all-kinks-chains $H_n = \mathcal{RPH}(n;0)$, respectively (see Fig. 2). We can obtain the ABC and GA indices of these special chains from Theorems 2 and 1 as corollary, which were computed in [34] as extremal graphs with respect to these two indices.

Corollary 3. *For $n \geq 2$, we have*

1. • $ABC(L_n) = (\frac{10}{3} + 3\sqrt{2})n + 2\sqrt{2} - 4.$
   • $ABC(H_n) = (\frac{8}{3} + 2\sqrt{2})n + \sqrt{2} - \frac{8}{3}.$
2. • $GA(L_n) = (6 + \frac{4\sqrt{6}}{5})n - 2.$
   • $GA(H_n) = (4 + \frac{8\sqrt{6}}{5})n + 2 - \frac{8\sqrt{6}}{5}.$

2.1. A comparison between the expected values of ABC and GA indices for random phenylene chains

In this subsection, we will give analytic comparison between the expected values for the ABC and GA indices for a random phenylene chains with same ρ probability. The graphical profile of the comparison is given in Fig. 3 which suggests that GA index is always greater than the ABC index for any n.

Theorem 4. *If $n \geq 2$, then*

$$E[GA(\mathcal{RPH}(n;\rho))] > E[ABC(\mathcal{RPH}(n;\rho))].$$

Proof. It is easy to see that the statement is true for $n = 2$. Thus, for $n > 2$, by applying the Theorems 2 and 1, we get

$$E[GA(\mathcal{RPH}(n;\rho))] - E[ABC(\mathcal{RPH}(n;\rho))]$$

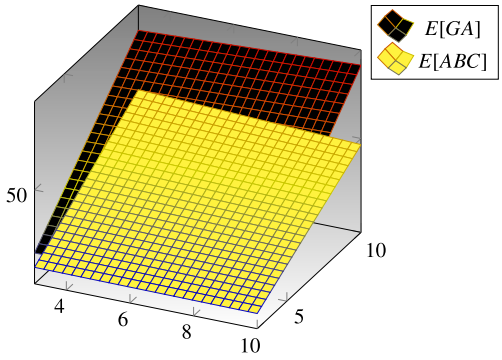

Fig. 3. Comparison between $E[ABC]$ and $E[GA]$.

$$= \Big\{[(4-\frac{8\sqrt{6}}{5})\rho+4+\frac{8\sqrt{6}}{5}]n + (\frac{16\sqrt{6}}{5}-8)\rho+\sqrt{2}-\frac{8\sqrt{6}}{5}\Big\} - \Big\{[(\frac{4}{3}-\sqrt{2})\rho+2\sqrt{2}+\frac{8}{3}]n + (2\sqrt{2}-\frac{8}{3})\rho+\sqrt{2}-\frac{8}{3}\Big\}.$$

$$= [(4-\frac{8\sqrt{6}}{5}-\frac{4}{3}+\sqrt{2})\rho+4+\frac{8\sqrt{6}}{5}-2\sqrt{2}-\frac{8}{3}]n + (\frac{16\sqrt{6}}{5}-8-2\sqrt{2}+\frac{8}{3})\rho+2-\sqrt{2}+\frac{8}{3}-\frac{8\sqrt{6}}{5}$$

where $\alpha = 4-\frac{8\sqrt{6}}{5}-\frac{4}{3}+\sqrt{2}>0$

$$= \rho\alpha(n-2)+(2-\sqrt{2})(2n+1)+8(n-1)[\frac{\sqrt{6}}{5}-\frac{1}{3}]$$

>0 $\because n>2$ *and* $0\le\rho\le 1/2$. □

3. The Zagreb indices in random phenylene chains

This section is devoted to compute the expected values of the first and second Zagreb indices for a phenylene chain $\mathcal{RPH}_n$. From equations (1) and (2) and the structure of the chain $\mathcal{RPH}_n$, we have the followings:

$$M_1(\mathcal{RPH}_n) = 4x_{22}(\mathcal{RPH}_n)+5x_{23}(\mathcal{RPH}_n)+6x_{33}(\mathcal{RPH}_n). \quad (11)$$

$$M_2(\mathcal{RPH}_n) = 4x_{22}(\mathcal{RPH}_n)+6x_{23}(\mathcal{RPH}_n)+9x_{33}(\mathcal{RPH}_n). \quad (12)$$

Thus, to compute the Zagreb indices of $\mathcal{RPH}_n$, one has to determine $x_{22}(\mathcal{RPH}_n)$, $x_{23}(\mathcal{RPH}_n)$ and $x_{33}(\mathcal{RPH}_n)$ type of edges and for simplicity we denote $x_{ij}(\mathcal{RPH}_n)$ by x_{ij}. Due to the local arrangement, it is clear that $\mathcal{RPH}(n;\rho)$ is a random phenylene chain. So are $M_1(\mathcal{RPH}(n;\rho))$ and $M_2(\mathcal{RPH}(n;\rho))$. Let us denote by $E_n^1 = E[M_1(\mathcal{RPH}(n;\rho))]$ and $E_n^2 = E[M_2(\mathcal{RPH}(n;\rho))]$, the expected values of these indices, respectively.

Theorem 5. *If $n\ge 2$ and $\mathcal{RPH}(n;\rho)$ is a random phenylene chain of length n, then*

$$E_n^1 = 44n-20.$$

Proof. Since $E_2^1 = 68$ which is true, thus for $n\ge 3$, there are three possibilities to be considered as shown in Fig. 1.

1. If $\mathcal{RPH}_{n-1}\to\mathcal{RPH}_n^1$ with probability ρ, then $x_{22}(\mathcal{RPH}_n^1) = x_{22}(\mathcal{RPH}_{n-1})+1, x_{23}(\mathcal{RPH}_n^1) = x_{23}(\mathcal{RPH}_{n-1})+2$ and $x_{33}(\mathcal{RPH}_n^1) = x_{33}(\mathcal{RPH}_{n-1})+5$ and from (11), we have $M_1(\mathcal{RPH}_n^1) = M_1(\mathcal{RPH}_{n-1})+44$.
2. If $\mathcal{RPH}_{n-1}\to\mathcal{RPH}_n^2$ with probability ρ, then $x_{22}(\mathcal{RPH}_n^1) = x_{22}(\mathcal{RPH}_{n-1})+1, x_{23}(\mathcal{RPH}_n^1) = x_{23}(\mathcal{RPH}_{n-1})+2$ and $x_{33}(\mathcal{RPH}_n^1) = x_{33}(\mathcal{RPH}_{n-1})+5$ and from (11), we have $M_1(\mathcal{RPH}_n^1) = M_1(\mathcal{RPH}_{n-1})+44$.
3. If $\mathcal{RPH}_{n-1}\to\mathcal{RPH}_n^3$ with probability $1-2\rho$, then $x_{22}(\mathcal{RPH}_n^3) = x_{22}(\mathcal{RPH}_{n-1}), x_{23}(\mathcal{RPH}_n^3) = x_{23}(\mathcal{RPH}_{n-1})+4$ and $x_{33}(\mathcal{RPH}_n^3) = x_{33}(\mathcal{RPH}_{n-1})+4$ and from (11), we have $M_1(\mathcal{RPH}_n^1) = M_1(\mathcal{RPH}_{n-1})+44$.

Thus, we obtain

$$E_n^1 = \rho M_1(\mathcal{RPH}_n^1)+\rho M_1(\mathcal{RPH}_n^2) + (1-2\rho)M_1(\mathcal{RPH}_n^3)$$
$$= 2\rho[M_1(\mathcal{RPH}_{n-1})+44] + (1-2\rho)[M_1(\mathcal{RPH}_{n-1})+44].$$
$$E_n^1 = M_1(\mathcal{RPH}_{n-1})+44. \quad (13)$$

But $E[E_n^1] = E_n^1$, so apply the operator E to (13), we get

$$E_n^1 = E_{n-1}^1+44. \quad n>2 \quad (14)$$

and after solving the recurrence relation (14) with initial condition, we get

$E_n^1 = 44n-20$. □

It is interesting to note that the expected value of first Zagreb index does not depend upon the probability ρ.

Theorem 6. *If $n\ge 2$ and $\mathcal{RPH}(n;\rho)$ is a random phenylene chain of length n, then*

$$E_n^2 = (60+2\rho)n-4(\rho+9).$$

Proof. Since $E_2^2 = 84$ which is true, thus for $n\ge 3$, there are three possibilities to be considered as shown in Fig. 1.

1. If $\mathcal{RPH}_{n-1}\to\mathcal{RPH}_n^1$ with probability ρ, then $x_{22}(\mathcal{RPH}_n^1) = x_{22}(\mathcal{RPH}_{n-1})+1, x_{32}(\mathcal{RPH}_n^1) = x_{23}(\mathcal{RPH}_{n-1})+2$ and $x_{33}(\mathcal{RPH}_n^1) = x_{33}(\mathcal{RPH}_{n-1})+5$ and from (12), we have $M_2(\mathcal{RPH}_n^1) = M_2(\mathcal{RPH}_{n-1})+61$.
2. If $\mathcal{RPH}_{n-1}\to\mathcal{RPH}_n^2$ with probability ρ, then $x_{22}(\mathcal{RPH}_n^1) = x_{22}(\mathcal{RPH}_{n-1})+1, x_{23}(\mathcal{RPH}_n^1) = x_{23}(\mathcal{RPH}_{n-1})+2$ and $x_{33}(\mathcal{RPH}_n^1) = x_{33}(\mathcal{RPH}_{n-1})+5$ and from (12), we have $M_2(\mathcal{RPH}_n^1) = M_2(\mathcal{RPH}_{n-1})+61$.
3. If $\mathcal{RPH}_{n-1}\to\mathcal{RPH}_n^3$ with probability $1-2\rho$, then $x_{22}(\mathcal{RPH}_n^3) = x_{22}(\mathcal{RPH}_{n-1}), x_{23}(\mathcal{RPH}_n^3) = x_{23}(\mathcal{RPH}_{n-1})+4$ and $x_{33}(\mathcal{RPH}_n^3) = x_{33}(\mathcal{RPH}_{n-1})+4$ and from (12), we have $M_2(\mathcal{RPH}_n^3) = M_2(\mathcal{RPH}_{n-1})+60$.

Thus, we get

$$E_n^2 = \rho M_2(\mathcal{RPH}_n^1) + \rho M_2(\mathcal{RPH}_n^2)+(1-2\rho)M_2(\mathcal{RPH}_n^3)$$
$$= 2\rho[M_2(\mathcal{RPH}_{n-1})+61] + (1-2\rho)[M_2(\mathcal{RPH}_{n-1})+60]$$
$$E_n^2 = M_2(\mathcal{RPH}_{n-1})+2\rho+60. \quad (15)$$

But $E[E_n]^2 = E_n^2$, so apply the operator E on (15), we get

$$E_n^2 = E_{n-1}^2+2\rho+60. \quad n>2 \quad (16)$$

and after solving the recurrence relation of (16) with initial condition, we get

$E_n^2 = (60+2\rho)n-4(\rho+9)$. □

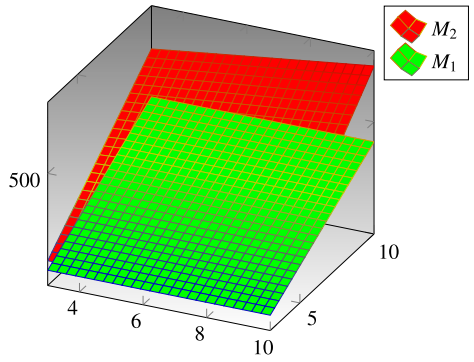

Fig. 4. Comparison between $E[M_2]$ and $E[M_1]$.

The phenylene linear chain $L_n = \mathcal{RPH}(n; \frac{1}{2})$, phenylene alkicks-chain $H_n = \mathcal{RPH}(n; 0)$ were characterized as the extremal phenylene chains with respect to the Zagreb indices in [34]. It is easy to obtain the Zagreb indices of these special chains as corollary of Theorems 5 and 6.

Corollary 7. *For $n \geq 2$, we have*

1. • $M_1(L_n) = M_1(H_n) = 44n - 20$.
2. • $M_2(L_n) = 61n - 38$.
   • $M_2(H_n) = 60n - 36$.

3.1. A comparison between the expected values of Zagreb indices for random phenylene chains

In this subsection, we will give analytic comparison between the expected values of the Zagreb indices for a random phenylene chains. The graphical profile of the comparison is given in Fig. 4 which suggests that second Zagreb index is always greater than the first Zagreb index for any n.

Theorem 8. *If $n \geq 2$, then*

$$E[M_2(\mathcal{RPH}(n;\rho))] > EM_1(\mathcal{RPH}(n;\rho))].$$

Proof. It is easy to see that the statement is true for $n = 2$. Thus, if $n > 2$, then by Theorems 5 and 6, one can have the followings

$$\begin{aligned} &E[M_2(\mathcal{RPH}(n;\rho))] - E[M_1(\mathcal{RPH}(n;\rho))] \\ &= (60 + 2\rho)n - 4(\rho + 9) - 44n + 20 \\ &= 16n + 2n\rho - 4\rho - 16 \\ &= 16(n-1) + 2\rho(n-2) \\ &> 0 \qquad \because n > 2 \text{ and } 0 \leq \rho \leq 1/2. \end{aligned}$$ □

Declarations

Author contribution statement

Zahid Raza: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

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Competing interest statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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