THE EXPECTED VALUES OF SUM-CONNECTIVITY, HARMONIC AND SYMMETRIC DIVISION INDICES IN RANDOM PHENYLENE CHAINS

ZAHID RAZA

Department of Mathematics, College of Sciences
University of Sharjah, UAE
zraza@sharjah.ac.ae

Abstract. A special class of conjugated hydrocarbons known as phenylenes, which is composed of a special arrangement of six- and four-membered rings. In particular, any two six-membered rings (hexagons) are not adjacent, and every four-membered ring(square) is adjacent to a pair of nonadjacent hexagons. If each hexagon of phenylene is adjacent only to two squares, then the obtained chain is called the phenylene chain.

The main object of this paper is to determine the expected values of the sum-connectivity, harmonic, and symmetric division indices for this class of conjugated hydrocarbons. The comparisons between the expected values of these indices with respect to the random phenylene chains, have been determined explicitly. The graphical illustrations have been given in terms of the differences between the expected values of these indices.

Keywords: sum-connectivity index; harmonic index; symmetric division index; random phenylene chain; expected values; comparison.
Subjclass[2010]Primary 05C09 ; 05C92 ; 05C90.

1. Introduction

There are lot of topological indices in the literature of chemical graph theory. The first of it kind is the Wiener index [36]. After that most important topological index is a class of the Zagreb indices [19], molecular connectivity [27, 10].Suppose $\Gamma = \Gamma(V, E)$ is a graph of order n with vertex set V and edge set E. Then the sum-connectivity(S)[41], harmonic(H)[39] and symmetric division(SDI)[18] indices are defined as:

$$S(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{d_u + d_v}} \tag{1.1}$$

$$H(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{2}{d_u + d_v} \tag{1.2}$$

$$SDI(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{d_u^2 + d_v^2}{d_u d_v} \tag{1.3}$$

There are plenty of papers outlined the mathematical properties of these indices, for example one can consults the papers ([2]-[9], [13]) and the references therein.

The phenylenes are a class of conjugated hydrocarbons composed of a special arrangement of six- and four-membered rings. In particular, any two six-membered rings (hexagons) are not adjacent, and every four-membered ring(square) is adjacent to a pair of nonadjacent hexagons. If each hexagon of a phenylene is adjacent only to two squares, then the obtained chain is called phenylene chain.

The phenylenes exhibit unique physicochemical properties due to their aromatic and antiaromatic rings. 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).

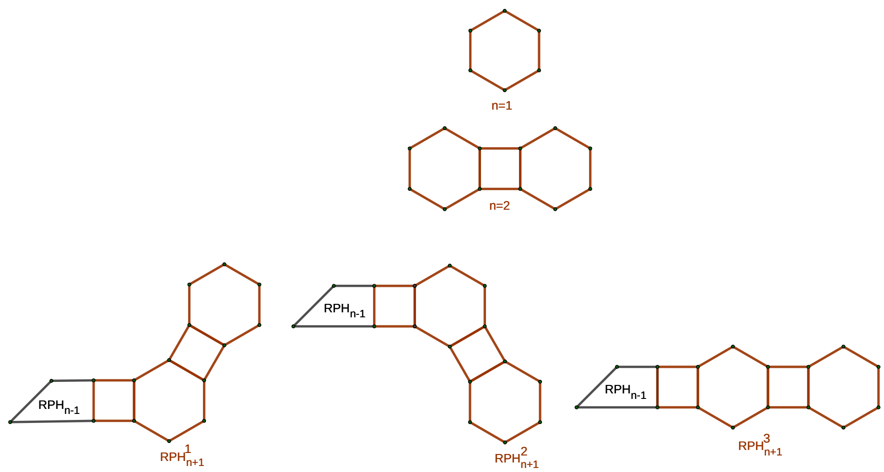

FIGURE 1. The three types of local arrangements in phenylene

There are unique phenylene chains for $n = 1$ and $n = 2$ as shown in Fig.1. More generally, a phenylene chain with n hexagons can be regarded as a phenylene chain $\mathcal{RPH}_n$, with $n-1$ hexagons to which a new terminal hexagon n-th has been adjoined by a square. But, 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 n hexagons as a phenylene chain obtained by stepwise addition of terminal hexagons with probability ρ, as shown in Fig. 1. A random phenylene chain $\mathcal{RPH}(n, \rho)$ with n hexagons as a phenylene chain can be obtained by stepwise addition of terminal hexagons. At each step $k(= 3, 4, \ldots, n)$ 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 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 [22, 28, 33] and references therein. It was discovered that the algebraic structure count of a phenylene is equal

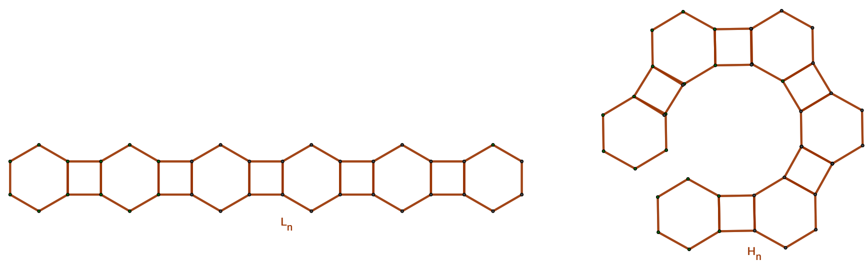

FIGURE 2. The linear chain and kicks

to the number of Kekule structures of the associated hexagonal squeeze [20, 21]. The energy and Estrada index of phenylenes has been determined in [16].

This unexpected connection between the two classes of polycyclic conjugated molecules, a lot of study has been carried out in this direction, for example, for the total π-electron energy[21], Narumi-Katayama index[32], and PI index [14], Merrifild-Simmons index [11], anti-Kekul and antiforceing number [40], Omega index and related polynomials [1, 25] The problem of the calculation of the Wiener index of phenylenes was solved in [26].

Peng and Li [31] obtained the explicit closed formula of the Kirchhoff index and the number of spanning trees of linear phenylene chains. Chen and Zhang [12] obtained an explicit analytical expression for the expected value of the Wiener index (resp. the number of perfect matchings) of a random phenylene chain. Very recently, Li, and Shuchao[34] obtained the extremal phenylene chains with respect to the coefficients sum of the permanently polynomial, the spectral radius, the Hosoya index and the MerrifieldSimmons index. In [38] the extremal phrnylene chains with respect to Kirchhoff index and degree based topological indices has been characterized. For more details one may see [15, 17, 23, 24, 29, 30, 35, 37].

In this paper, we extent the study of this class of hydrocarbon for sum-connectivity, harmonic and symmetric division indices and give their expected values and comparison between them.

2. The sum-connectivity, harmonic and symmetric division indices in random phenylene chains

In this section, the sum-connectivity, harmonic and symmetric division indices in a random phenylene 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 exits only $(2,2)$, $(2,3)$, and $(3,3)$-type of edges in $\mathcal{RPH}_n$. Thus, in order to compute the sum-connectivity, harmonic and symmetric division 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} Hence, the sum-connectivity, harmonic and symmetric division indices can be written as:

$$S(\mathcal{RPH}_n) = \frac{1}{2}x_{22}(\mathcal{RPH}_n) + \frac{1}{\sqrt{5}}x_{23}(\mathcal{RPH}_n) + \frac{1}{\sqrt{6}}x_{33}(\mathbb{RS}C_n). \tag{2.1}$$

$$H(\mathcal{RPH}_n) = (\frac{1}{2})m_{22}(\mathcal{RPH}_n) + (\frac{2}{5})x_{23}(\mathcal{RPH}_n) + (\frac{1}{3})x_{33}(\mathcal{RPH}_n). \tag{2.2}$$

$$SDI(\mathcal{RPH}_n) = 2x_{22}(\mathcal{RPH}_n) + \frac{13}{6}x_{23}(\mathcal{RPH}_n) + 2x_{33}(\mathbb{RS}C_n). \tag{2.3}$$

As due to the local arrangements, it is clear $\mathcal{RPH}(n;\rho)$ is a random phenylene chains. So, $S(\mathcal{RPH}(n;\rho))$, $H(\mathcal{RPH}(n;\rho))$ and $SDI(\mathcal{RPH}(n;\rho))$ are random variables. Let us denote by $E_n^S = E[S(\mathcal{RPH}(n;\rho))]$, $E_n^H = E[H(\mathcal{RPH}(n;\rho))]$ and $E_n^{SDI} = E[S(\mathcal{RPH}(n;\rho))]$ the expected values of these indices, respectively.

Theorem 2.1. *Let $\mathcal{RPH}(n;\rho)$ be a random phenylene chain of length $n(\geq 2)$. Then*

$$E_n^S = n\big[2\rho(\frac{1}{2} - \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{6}}) + \frac{4}{\sqrt{5}} + \frac{4}{\sqrt{6}}\big] - 4\rho(\frac{1}{2} - \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{6}}) - \frac{4}{\sqrt{5}} - \frac{4}{\sqrt{6}} + 3.$$

Proof. Since $E_2 = 3 + \frac{4}{\sqrt{5}} + \frac{4}{\sqrt{6}}$ 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 2.1, we have
$S(\mathcal{RPH}_n^1) = S(\mathcal{RPH}_{n-1}) + \frac{1}{2} + \frac{2}{\sqrt{5}} + \frac{5}{\sqrt{6}}$.

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 2.1, we have
$S(\mathcal{RPH}_n^1) = S(\mathcal{RPH}_{n-1}) + \frac{1}{2} + \frac{2}{\sqrt{5}} + \frac{5}{\sqrt{6}}$.

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 2.1, we have
$S(\mathcal{RPH}_n^1) = S(\mathcal{RPH}_{n-1}) + \frac{4}{\sqrt{5}} + \frac{4}{\sqrt{6}}$.

Thus, we obtain

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

$$E_n^S = S(\mathcal{RPH}_{n-1}) + 2\rho(\frac{1}{2} - \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{6}}) + 4(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}}). \tag{2.4}$$

But $E[E_n^S] = E_n^S$, so apply the operator E on 2.4, we get

$$E_n^S = E_{n-1}^S + 2\rho(\frac{1}{2} - \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{6}}) + 4(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}}). \quad n > 2 \tag{2.5}$$

and after solving the recurrence relation 2.5 with initial condition, we get

$$E_n^S = n\big[2\rho(\frac{1}{2} - \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{6}}) + \frac{4}{\sqrt{5}} + \frac{4}{\sqrt{6}}\big] - 4\rho(\frac{1}{2} - \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{6}}) - \frac{4}{\sqrt{5}} - \frac{4}{\sqrt{6}} + 3.$$

□

Theorem 2.2. *Let $\mathcal{RPH}(n;\rho)$ be a random phenylene chain of length $n(\geq 2)$. Then*

$$E_n^H = \frac{n}{15}(\rho + 44) - \frac{2}{15}(\rho - \frac{1}{2}).$$

Proof. Since $E_2^a = \frac{89}{15}$ 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 2.2, we have $H(\mathcal{RPH}_n^1) = H(\mathcal{RPH}_{n-1}) + \frac{89}{30}$.
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 2.2, we have $H(\mathcal{RPH}_n^1) = H(\mathcal{RPH}_{n-1}) + \frac{89}{30}$.
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 2.2, we have $H(\mathcal{RPH}_n^3) = H(\mathcal{RPH}_{n-1}) + \frac{44}{15}$.

Thus, we obtain

$$\begin{aligned} E_n^H &= \rho H(\mathcal{RPH}_n^1) + \rho H(\mathcal{RPH}_n^2) + (1-2\rho)H(\mathcal{RPH}_n^3) \\ &= 2\rho[H(\mathcal{RPH}_{n-1}) + \frac{89}{30}] + (1-2\rho)[H(\mathcal{RPH}_{n-1}) + \frac{44}{15}] \end{aligned}$$

$$E_n^H = H(\mathcal{RPH}_{n-1}) + \rho\frac{1}{15} + \frac{44}{15}. \tag{2.6}$$

But $E[E_n]^H = E_n^H$, so apply the operator E on 2.6, we get

$$E_n^H = E_{n-1}^H + \rho\frac{1}{15} + \frac{44}{15}. \quad n > 2 \tag{2.7}$$

and after solving the recurrence relation 2.7 with initial condition, we get

$$E_n^H = \frac{n}{15}(\rho + 44) - \frac{2}{15}(\rho - \frac{1}{2}).$$

□

Theorem 2.3. *Let $\mathcal{RPH}(n;\rho)$ be a random phenylene chain of length $n(\geq 2)$. Then*

$$E_n^{SDI} = n\big[\frac{50}{3} - \frac{2\rho}{3}\big] + \frac{4\rho}{3} - \frac{14}{3}.$$

Proof. Since $E_2 = \frac{86}{3}$ 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 2.3, we have
$SDI(\mathcal{RPH}_n^1) = SDI(\mathcal{RPH}_{n-1}) + \frac{49}{3}$.

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 2.3, we have
$SDI(\mathcal{RPH}_n^2) = SDI(\mathcal{RPH}_{n-1}) + \frac{49}{3}$

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 2.3, we have
$SDI(\mathcal{RPH}_n^3) = SDI(\mathcal{RPH}_{n-1}) + \frac{50}{3}$.

Thus, we obtain

$$\begin{aligned} E_n^S &= \rho SDI(\mathcal{RPH}_n^1) + \rho SDI(\mathcal{RPH}_n^2) + (1-2\rho)SDI(\mathcal{RPH}_n^3) \\ &= 2\rho[SDI(\mathcal{RPH}_{n-1}) + \frac{49}{3}] + (1-2\rho)[SDI(\mathcal{RPH}_{n-1}) + \frac{50}{3}] \end{aligned}$$

$$E_n^{SDI} = SDI(\mathcal{RPH}_{n-1}) - \frac{2\rho}{3} + \frac{50}{3}. \tag{2.8}$$

But $E[E_n^{SDI}] = E_n^{SDI}$, so apply the operator E on 2.8, we get

$$E_n^{SDI} = E_{n-1}^{SDI} - \frac{2\rho}{3} + \frac{50}{3}. \quad n > 2 \tag{2.9}$$

and after solving the recurrence relation 2.9 with initial condition, we get

$$E_n^{SDI} = n\left[\frac{50}{3} - \frac{2\rho}{3}\right] + \frac{4\rho}{3} - \frac{14}{3}.$$

□

We know that the phenylene linear and all-kinks-chains can be obtained for special value of the probability as $L_n = \mathcal{RPH}(n; 1/2)$ phenylene all-kinks-chains $H_n = \mathcal{RPH}(n; 0)$, respectively(see Fig. 2). We can obtain the sum-connectivity, harmonic and symmetric division indices of these special chains from Theorems 2.1, 2.2 and 2.3 as Corollary, which were computed in [38] as extremal graphs with respect to these topological indices.

Corollary 2.4. *For $n \geq 2$, we have*

(1)
- $S(L_n) = (\frac{4}{\sqrt{5}} + \frac{4}{\sqrt{6}})(n-1) + 3$.
- $S(H_n) = (\frac{1}{2} + \frac{2}{\sqrt{5}} + \frac{5}{\sqrt{6}})(n-1) + \frac{5}{2} + \frac{2}{\sqrt{5}} - \frac{1}{\sqrt{6}}$.

(2)
- $H(L_n) = \frac{44}{15}(n-1) + 3$
- $H(H_n) = \frac{44}{15}(n-1) + \frac{n}{30} + \frac{44}{15}$.

(3)
- $SDI(L_n) = \frac{50}{3}(n-1) + 12$
- $SDI(H_n) = \frac{49}{3}(n-1) + \frac{37}{3}$.

3. A comparison between the expected values degree-based topological indices for random phenylene chains

In this section, we will give analytic comparison between the expected values for the sum-connectivity, harmonic and symmetric division indices for a random phenylene chains with the same probabilities ρ. The the comparison between the expected values of these indices for different values of the probability ρ has been given in the following tables 1, 2 and 3. It is clear that symmetric difference index index is always greater that the other two indices namely, the harmonic index and sum-connectivity index.

Table 1. Expected values of indices for $\rho = 1/3$

n	E^H	E^S	E^{SID}
3	8.8889	9.8523	45.1111
4	11.8444	13.2840	61.5556
5	14.8000	16.7150	78.0000
6	17.7556	20.1461	94.4444
7	20.7111	23.5772	110.8889
8	23.6667	27.0082	127.3333
9	26.6222	30.4393	143.7778
10	29.5778	33.8703	160.2222

Table 2. Expected values of indices for $\rho = 1/5$

n	E^H	E^S	E^{SID}
3	8.8800	9.8492	45.2000
4	11.8267	13.2766	61.7333
5	14.7733	16.7040	78.2667
6	17.7200	20.1314	94.8000
7	20.6667	23.5587	111.3333
8	23.6133	26.9861	127.8667
9	26.5600	30.4135	144.4000
10	29.5067	33.84086	160.9333

TABLE 3. Expected values of indices for $\rho = 1/100$

n	E^H	E^S	E^{SID}
10	29.4053	33.7988	161.9467
20	58.7453	68.0200	328.5467
30	88.0853	102.2413	495.1467
40	117.4253	136.4626	661.7467
50	146.7653	170.68380	828.3467
60	176.1053	204.9050	994.9467
70	205.4453	239.1263	1161.5467
80	234.7853	273.3475	1328.1467
90	264.1253	307.5688	1494.7467
100	293.4653	341.7899	1661.3467

The graphical profile of the comparison is given in Fig.3 and Fig. 4 which suggests that symmetric division index is always grater than the harmonic index and sum-connectivity index for any n.

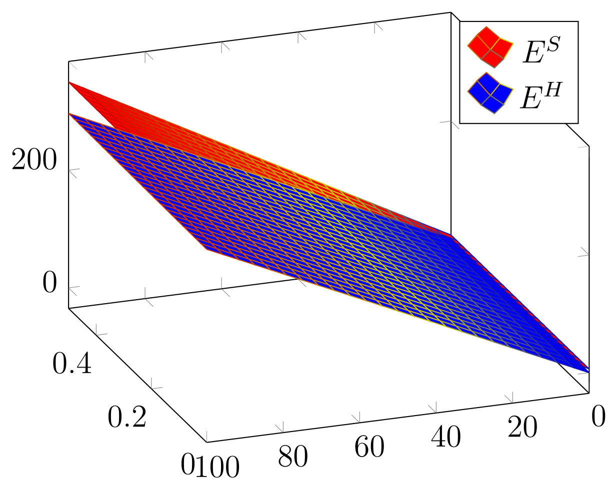

FIGURE 3. Comparison between expected values of S and H indices

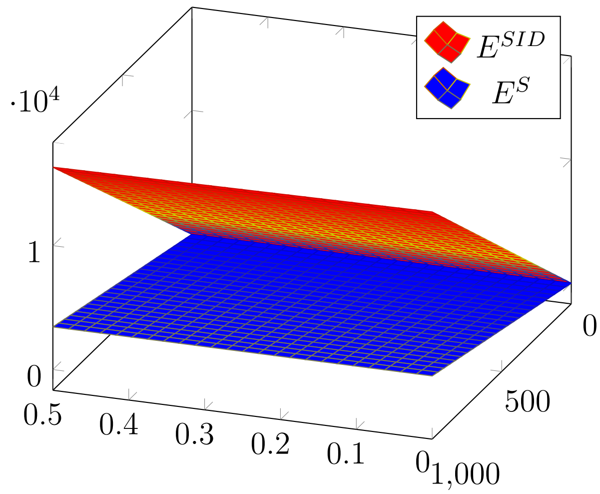

FIGURE 4. Difference between expected values of SDI and S indices

Now, we give the analytic proof that symmetric division index is always grater than the harmonic index and sum-connectivity index for any n with the same probability ρ.

Theorem 3.1.

$$E[S(\mathcal{RPH}(n;\rho))] > E[H(\mathcal{RPH}(n;\rho))] \qquad \forall \ \ n \geq 2$$

Proof. It is easy to see that the statement is true for $n = 2$. Thus, for $n > 2$, Let us denote $a = \frac{1}{2} - \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{6}}$ and $b = 4(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}})$, so, by applying the Theorems 2.1 and 2.2, we get

$$E[S(\mathcal{RPH}(n;\rho))] - E[H(\mathcal{RPH}(n;\rho))]$$

$$\begin{aligned}
&= \Big\{n(2a\rho + b) - 4a\rho - b + 3\Big\} - \Big\{\frac{n}{15}(\rho + 44) - \frac{2}{15}(\rho - \frac{1}{2})\Big\}. \\
&= \big[2a\rho + b - \frac{\rho}{15} - \frac{44}{15}\big]n + \frac{2\rho}{15} - 4a\rho + 3 - b - \frac{1}{15} \\
&= \frac{1}{15}[\rho(30a - 1)(n - 2) + (15b - 44)(n - 1)] \\
&> 0 \qquad\qquad \because n > 2,\ 30a - 1 > 0 \ and \ 15b - 44 > 0.
\end{aligned}$$

∎

Theorem 3.2.

$$E[SDI(\mathcal{RPH}(n;\rho))] > E[S(\mathcal{RPH}(n;\rho))] \qquad \forall \ \ n \geq 2$$

Proof. It is easy to see that the statement is true for $n = 2$. Thus, for $n > 2$, Let us denote $a = \frac{1}{2} - \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{6}}$ and $b = 4(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}})$, so, by applying the Theorems 2.1 and 2.3, we get

$$E[SDI(\mathcal{RPH}(n;\rho))] - E[S(\mathcal{RPH}(n;\rho))]$$

$$
\begin{aligned}
&= \Big\{\frac{n}{3}(50-2\rho)+\frac{4\rho}{3}-\frac{14}{3}\Big\}-\Big\{n(2a\rho+b)-4a\rho-b+3\Big\}.\\
&= \frac{1}{3}\big[(50-2\rho-6a\rho-3b)n+4\rho-14+12a\rho+3b-9\big]\\
&= \frac{1}{3}[(50-3b)(n-1)-2\rho(1+3a)(n-2)]\\
&> 0 \qquad\qquad \because n>2,\ 50-3b>2\rho(1+3a)\ \ \forall\ \ 0\le\rho\le 1/2.
\end{aligned}
$$

□

From Theorems 3.1 and 3.2, we have the following corollary:

Corollary 3.3. *For $n \geq 2$, we have*

$$E[SDI(\mathcal{RPH}(n;\rho))] > E[S(\mathcal{RPH}(n;\rho))] > E[H(\mathcal{RPH}(n;\rho))] \quad \forall\ n \geq 2$$

Acknowledgement

This research work is funded by the University of Sharjah under the Project #1802144068 and MASEP Research Group.

References

[1] M. Alaeiyan, R. Mojarad, J. Asadpour, The Omega Index of Polyomino Chain, Phenylene Graphs and Carbon Nanocones, Fuller. Nanotub. Car. N., 22, (2014), 316-321.
[2] S. Akhter, M. Imran, Z. Raza, Bounds for the general sum-connectivity index of composite graphs, Journal of Inequalities and Applications, 2017, 76(2017), DOI 10.1186/s13660-017-1350-y.
[3] S. Akhter, M. Imran, Z. Raza, On the general sum-connectivity index and general Randic index of cacti Journal of Inequalities and Applications, 2016, 300(2016), DOI 10.1186/s13660-016-1250-6.
[4] A. Ali, Z. Raza, A. A. Bhatti, Some vertex-degree-based topological indices of cacti, Ars Combinatoria, 144, (2019), 195-206.
[5] A. Ali, Z. Raza, A. A. Bhatti, Extremal pentagonal chains with respect to degree-based topological indices, Canadian Journal of Chemistry, 94(10), (2016), 870-876.
[6] A. Ali, Z. Raza, A. A. Bhatti, bond incident degree (BID) indices for some nanostructures , Optoelectronics Adv. Materials-Rapid Commun, Vol. 10, no. 1-2, 108-112(2016).
[7] A. Ali, Z. Raza, A. A. Bhatti, Bond Incident Degree (BID) Indices of Polyomino Chains: A Unified Approach, Applied Mathematics and Computation, 287(9),(2016), 28-37.
[8] A. Ali, A. A. Bhatti, Z. Raza, Topological study of tree-like polyphenylene systems, spiro hexagonal systems and polyphenylene dendrimer nanostars, Quantum Matter, 5(4), (2016), 534-538.
[9] A. Ali, L. Zhong, I. Gutman, Harmonic index and its generalizations: Extremal results and bounds, MATCH Commun. Math. Comput. Chem., 81 (2019), 249-311.
[10] D. Bonchev, Information Theoretic Indices for Characterization of Molecular Structure, Research Studies Press Wiley, Chichester, 1983.
[11] A. Chen, Merrifild-Simmons index in random phenylene chains and random hexagon chains, Discrete Dynamics in Nature and socisty, (2015), 1-7.
[12] A. Chen and F. Zhang, Wiener index and perfect matchings in random phenylene chains, MATCH Commun. Math. Comput. Chem., 61, (2009), 623-630.
[13] K.C. Das, Trinajstic, Comparison between first geometric-arithmetic index and atom-bond connectivity index, Chem. Phys. Lett., 497 (2010), 149-151.
[14] H. Deng, S. Chen and J. Zhang, The PI index of phenylenes, J. Math. Chem., 41(1), (2007), 63-69.

[15] H. Deng, J. Yang, F. Xia, A general modeling of some vertexdegree based topological indices in benzenoid systems and phenylenes, Comput. Math. Appl., 61(10), (2011), 3017-3023.

[16] B. Furtula, I. Gutman, Energy and Estrada index of phenylenes, Indian Journal of Chemistry, 47A, (2008), 220-224.

[17] T. Ghosh, S. Mondal and B. Mandal, Matching polynomial coefficients and the Hosoya indices of poly(p-phenylene) graphs, Mol. Phys., 116, (2018), 1-17.

[18] V.K. Gupta, V. Lokesha, S.B. Shwetha and P.S. Ranjini, On the symmetric division degree index of graph, Southeast Asian Bull. Math., vol. 40, pp. 59-80, 2016.

[19] I. Gutman, K. Das, The first Zagreb index 30 years after, MATCH Commun. Math. Comput. Chem. 50 (2004), 83-92.

[20] I. Gutman, B. Furtula, A Kekule structure basis for phenylenes, Journal of Molecular Structure, 770, (2006), 67-71.

[21] I. Gutman, A. Vodopivec, S. Radenkovic, B. Furtula, On π-electron excess of rings of benzenoid molecules, Indian Journal of Chemistry 45A, (2006,) 347-351.

[22] G. Huang, M. Kuang, H. Deng. The expected values of Hosoya index and Merrifield-Simmons index in a random polyphenylene chain, J. Comb. Optim., 32 (2016), 550-562.

[23] S. Markovic, A. Stajkovic, The evaluation of spectral moments for molecular graphs of phenylenes, Theor. Chem. Acc., 96(4) (1997), 256-260.

[24] S. Markovic, Z. Markovic, R.I. Mccrindle, Spectral moments of phenylenes, J. Chem. Inform. Comput. Sci., 41(1), (2001), 112-119.

[25] R. Mojarad, B. Daneshian, J. Asadpour, Omega and related Polynomials of phenylenes and their hexagonal squeezes, Optoelectron. Adv. Mat., 10(1),(2016), 113-116.

[26] J. Rada, O. Araujo, I. Gutman, Randic Index of Benzenoid Systems and Phenylenes, Croat. Chem. Acta., 74(2), (2001), 225-235.

[27] M. Randic, Characterization of molecular branching. J. Am. Chem. Soc. 97(1975), 660-661.

[28] Z. Raza, The harmoic and second Zagerb Indices of random polyphenyl and spiro chains, Polycyclic Aromatic Compounds, https://doi.org/10.1080/10406638.2020.1749089

[29] Z. Raza, The edge version of geometric arithmetic index of polyomino chains of 8-cycles and arbitrary carbon nanocones, Journal of Computational and Theoretical Nanoscience, Vol. 13, 1-5, 2016

[30] Z. Raza, A. A. Bhatti, A. Ali, More on Comparison Between First Geometric-Arithmetic Index and Atom-Bond Connectivity Index, Miskolc Mathematical Notes, Vol. 17, no. 1, 561-570(2016).

[31] Y. J. Peng, S. C. Li, On the Kirchhoff index and the number of spanning trees of linear phenylenes, MATCH Commun. Math. Comput. Chem., 77(3) (2017), 765-780.

[32] Z. Tomovic, I. Gutman, Narumi-Katayama index of phenylenes, J. Serb. Chem. Soc., 66(4) ,(2001), 1031-1036.

[33] S. Wei, X. Ke, G. Hao. Comparing the excepted values of the atom-bond connectivity and geometric-arithmetic indices in random spiro chains, J Inequal Appl 2018, 45 (2018). DOI.org/10.1186/s13660-018-1628-8.

[34] W. Wei, L. Shuchao, Extremal phenylene chains with respect to the coefficients sum of the permanental polynomial, the spectral radius, the Hosoya index and the MerrifieldSimmons index, Discrete Applied Mathematics, 271(1), (2019), 205-217.

[35] R. Wu and H. Deng, The General Connectivity Indices of Benzenoid Systems and Phenylenes, MATCH Commun. Math. Comput. Chem., 64, (2010), 459-470.

[36] H. Wiener, Structure determination of paraffin boiling points. J. Am. Chem. Soc. 69(1947), 17-20.

[37] T. Wu, Two Classes of Topological Indices of Phenylene Molecule Graphs, Math. Probel. Eng., 2016, 42-56.

[38] Y. Yang, D. Wang, Extremal phenylene chains with respect to the Kirchhoff index and degree-based topological indices, IAENG Int. J. Applied Math. 49(3), (2019), 274-280.

[39] L. Zhong, The harmonic index for graphs, Appl. Math. Lett., 25, (2012), 561-566.

[40] Q. Zhang, H. Bian, E. Vumar, On the anti-Kekul and antiforcing number of cata-condensed phenylenes, MATCH Commun. Math. Comput. Chem., 65(3), (2011), 799-806.
[41] B. Zhou, N. Trinajstic, On a novel connectivity index, J. Math.Chem., 46, (2009), 1252-2170.

Department of Mathematics,College of Sciences, University of Sharjah, UAE.
E-mail address: zraza@sharjah.ac.ae