THE COMPARATIVE ANALYSIS OF THE MULTIPLICATIVE ATOM-BOND CONNECTIVITY AND GEOMETRIC-ARITHMETIC INDICES IN RANDOM POLYPHENYL AND SPIRO CHAINS

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Abstract. The polyphenyl chains with n hexagons are the special graphs of unbranched polycyclic aromatic hydrocarbons. The objective of this study is to find the expected values of the multiplicative version of the atomic-bond connectivity index and geometric-arithmetic index of this class of special hydrocarbons. The average values of these two indices with respect to the set of all polyphenyl chains have been determined. Finally, the comparisons between the expected values of aforementioned indices in the random polyphenyl and spiro chains, have been outlined.

Keywords: multiplicative ABC and GA index; random polyphenyl chain; random spiro chain; expected value.

1. Introduction

Topological indices (TIs) are digital counterparts of chemical structures and therefore represent these discrete molecular constitutional formulas by numerical functions. Some of their main uses are for quantitative structure-property or structure-activity relationships, QSPR and QSAR, respectively [20],[16]. Chemical graphs are connected non-directed graphs which are graph-theoretically planar.

The Wiener index [29], the Zagreb indices [15], or the Hosoya index [17], which are integers are the earliest TIs, have a high degeneracy. As compare to TIs, which are non-integer such as molecular connectivity (Randic [22]), higher-order molecular connectivity ([21]), or information-theoretic indices ([3], [25]) have lower degeneracy.

E. Estrada et al. [13] proposed atom-bond connectivity index of a graph G. The stability of alkanes and the strain energy of cycloalkanes has been study through the correlation with the ABC index in[13, 14].

Recently Kulli (2016b) introduce the multiplicative version of atomic-bond connectivity index defined as

$$ABC\prod(G) = \prod_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \tag{1.1}$$

The authors computed the multiplicative atom-bond connectivity index of some nanotubes. Since the multiplicative atom-bond connectivity index has not been widely studied until now, the results on the multiplicative atombond connectivity index are still limited, compared to the atom-bond connectivity index, for more recent work see [24]. In [26] geometric-arithmetic index has been defined and in

[26] it is proved that the GA index is well correlated with a lot of physico-chemical properties. The GA index predict better than the Randic index. More details related the mathematical properties of GA index can be found in [7, 8, 12, 23, 32, 33].

Recently Kulli (2016b) introduce the multiplicative version of geometric-arithmetic index defined as

$$GA\prod(G) = \prod_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \tag{1.2}$$

The polyphenyls will be considered as the molecular graphs which can be used in organic synthesis, drug synthesis, heat exchanger, etc., see for more details in [18,27,31]. Biphenyl compounds also have extensive industrial applications. For example, 4,4-bis (chloromethyl) biphenyl can be used for the synthesis of brightening agents. Especially, polychlorinated biphenyls, which are dangerous organic pollutants and lead to global pollution, can be applied in print and dyeing extensively [4].

Let us consider n hexagons $h_1, h_2, \ldots, h_n$. Then one can obtained a polyphenyl chain of length n by adding a bridge to each pair of consecutive hexagons, which is denoted by $\mathbb{RP}C_n$.

Since two consecutive hexagons can be bridged by three different ways. Thus, $\mathbb{RP}C_n$ may not be unique when $n > 2$. Thus there can be three types of local arrangements denoted by $\mathbb{RP}C_n^1$, $\mathbb{RP}C_n^2$, and $\mathbb{RP}C_n^3$ respectively (see Figure 1). So, to obtained $\mathbb{RP}C_n$ from a fixed $\mathbb{RP}C_{n-1}$ is a random process. Let us associate the probabilities ρ_1, ρ_2 and $1-\rho_1-\rho_2$ for obtaining $\mathbb{RP}C_n^1$, $\mathbb{RP}C_n^2$, and $\mathbb{RP}C_n^3$ from a fixed $\mathbb{RP}C_{n-1}$, respectively. If ρ_1 and ρ_2 are constants and independent of n, Then above is a zeroth-order Markov process. The above polyphenyl chain denoted by $\mathbb{RP}C(n;\rho_1,\rho_2)$ is known as a random polyphenyl chain.

If $n = 1, 2$ there are unique random polyphenyl chains and for $n > 2$ the general form of polyphenyl chains has been shown in Figure 1. Some results on matchings and independent sets, Wiener index, etc., of polyphenyl chains can be found in [1, 2, 9, 10, 11].

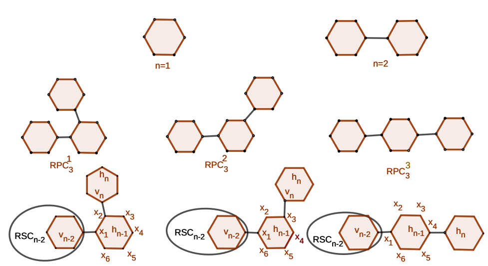

FIGURE 1. Random Polyphenyl Chains for $n = 1, 2, 3$ and $n > 3$

If we squeeze each cut edge between each consecutive hexagons in $\mathbb{RP}C_n$, then we will obtained a spiro chain, which is denoted by $\mathbb{RS}C_n$. Similarly, for $n > 2$ its is easy to see that $\mathbb{RS}C_n$ is not unique and has three types denoted by $\mathbb{RS}C_n^1$, $\mathbb{RS}C_n^2$, and $\mathbb{RS}C_n^3$ (see Figure 2), respectively. Thus, getting a $\mathbb{RS}C_n$ from a fixed $\mathbb{RS}C_{n-1}$ is a random process. Namely, the probability of getting $\mathbb{RS}C_n^1$, $\mathbb{RS}C_n^2$, and $\mathbb{RS}C_n^3$ from a fixed $\mathbb{RS}C_{n-1}$ are ρ_1, ρ_2 and $1-\rho_1-\rho_2$, respectively. Suppose that ρ_1 and ρ_2 are constants and independent of n, then this process is a zeroth-order Markov process. The the obtained polyphenyl chain denoted by $\mathbb{RS}C(n;\rho_1,\rho_2)$ is known to be a random sprio chain. The Wiener index of random polyphenyl chain has been

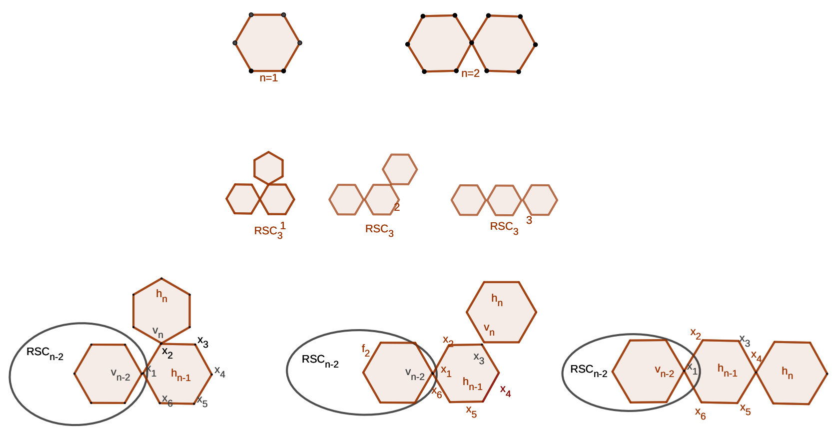

FIGURE 2. Random Sprio Chains for $n = 1, 2, 3$ and $n > 3$

computed in [32] . The Kirchhoff index in random polypheny and spiro chains has been determined by Huang et al. [18] . In 2016, Deng et al. [19] established exact formulas for the expected values of the Hosoya index and Merrifield-Simmons index of a random polyphenylene and spiro chain. The spiro and polypheny hexagonal chains with respect to the number of BC-subtrees has been consider in [31]. The comparison of excepted values of ABC and GA indices in random spiro chains has been given in [27]. For more details one may refer to [5, 6, 9, 10, 30].

2. Results and Discussion

In this section, we will give our main results related with the two types of chains.

2.1. **The multiplicative ABC and GA indices in random spiro chains.**

Let us consider randon spiro chain $\mathbb{RS}C_n$ obtained from $\mathbb{RS}C_{n-1}$ as described in Figure 2. It easy to see that we have only $(2,2), (2,4)$, and $(4,4)$-edges in $\mathbb{RS}C_n$ and by equations (1.1) and (1.2). We have the following expression for multiplicative ABC and GA indices:

$$ABC\prod(\mathbb{RS}C_n) = (\frac{\sqrt{2}}{2})^{m_{22}(\mathbb{RS}C_n)+m_{24}(\mathbb{RS}C_n)} * (\frac{\sqrt{6}}{4})^{m_{44}(\mathbb{RS}C_n)} \tag{2.1}$$

$$GA\prod(\mathbb{RS}C_n) = (1)^{m_{22}(\mathbb{RS}C_n)+m_{44}(\mathbb{RS}C_n)} * (\frac{2\sqrt{2}}{3})^{m_{24}(\mathbb{RS}C_n)} \tag{2.2}$$

Thus, to compute the multiplicative ABC and GA indices of $\mathbb{RS}C_n$, we just need to determine $m_{22}(\mathbb{RS}C_n), m_{24}(\mathbb{RS}C_n)$ and $m_{24}(\mathbb{RS}C_n)$ and for simplicity of the notation, we denote $m_{ij}(\mathbb{RS}C_n)$ just m_{ij} in the rest of the section.

Since $\mathbb{RS}C(n;\rho_1,\rho_2)$ is a random spiro chain. So, $ABC\prod\mathbb{RS}C(n;\rho_1,\rho_2)$ and $GA\prod\mathbb{RS}C(n;\rho_1,\rho_2)$ are random variables. For simplicity, we denote their expected values by $E_n = E[ABC\prod\mathbb{RS}C(n;\rho_1,\rho_2)]$ and $E_n = E[GA\prod\mathbb{RS}C(n;\rho_1,\rho_2)]$, respectively.

Theorem 2.1. *For $n > 1$, and a random spiro chains $\mathbb{RS}C(n;\rho_1,\rho_2)$, we have*

$$E_n^a = E[ABC\prod\mathbb{RS}C(n;\rho_1,\rho_2)] = \frac{(\rho_1(\sqrt{3}-2)+2)^{n-2}}{2^{4n-2}}.$$

Proof. From the definition of multiplicative ABC index, we have

$$ABC\prod(\mathbb{RS}C_n) = (\frac{1}{\sqrt{2}})^{m_{22}+m_{24}}(\frac{\sqrt{6}}{4})^{m_{44}} \tag{2.3}$$

It is easy to see that for $n = 2$, $E_1^a = (\frac{1}{2})^6$. Now when $n \geq 3$, it is obvious that then numbers of edges of type m_{22}, m_{24} and m_{44} depends on the three possibilities as described in Figure 2

i. If $\mathbb{RS}C_n^1$ is obtained from fixed $\mathbb{RS}C_{n-1}$ with probability ρ_1, then $m_{22}(\mathbb{RS}C_n^1) = m_{22}(\mathbb{RS}C_{n-1}) + 3$, $m_{24}(\mathbb{RS}C_n^1) = m_{24}(\mathbb{RS}C_{n-1}) + 2$ $m_{44}(\mathbb{RS}C_n^1) = m_{44}(\mathbb{RS}C_{n-1}) + 1$ and by 2.3 we have,

$$\begin{aligned} ABC\prod(\mathbb{RS}C_n^1) &= (\frac{1}{\sqrt{2}})^{m_{22}+m_{24}}(\frac{\sqrt{6}}{4})^{m_{44}}(\frac{1}{\sqrt{2}})^5(\frac{\sqrt{6}}{4}) \\ &= ABC\prod(\mathbb{RS}C_{n-1})(\frac{\sqrt{3}}{16}) \end{aligned}$$

ii. If ρ_2 is the probability to obtained $\mathbb{RS}C_n^2$ from a fixed $\mathbb{RS}C_{n-1}$, then $m_{22}(\mathbb{RS}C_n^2) = m_{22}(\mathbb{RS}C_{n-1})+2$, $m_{24}(\mathbb{RS}C_n^2) = m_{24}(\mathbb{RS}C_{n-1})+4$, $m_{44}(\mathbb{RS}C_n^2) = m_{44}(\mathbb{RS}C_{n-1})$, and by 2.3 we have

$$ABC\prod(\mathbb{RS}C_n^2) = ABC\prod(\mathbb{RS}C_{n-1})\frac{1}{8}$$

iii. If $\mathbb{RS}C_{n-1} \to \mathbb{RS}C_n^3$ with probability $1-\rho_1-\rho_2$, then $m_{22}(\mathbb{RS}C_n^3) = m_{22}(\mathbb{RS}C_{n-1})+2$, $m_{24}(\mathbb{RS}C_n^3) = m_{24}(\mathbb{RS}C_{n-1}) + 4$, $m_{44}(\mathbb{RS}C_n^3) = m_{44}(\mathbb{RS}C_{n-1})$, so

$$ABC\prod(\mathbb{RS}C_n^3) = ABC\prod(\mathbb{RS}C_{n-1})\frac{1}{8}$$

From above three types, we can obtain the followings:,

$$\begin{aligned}
& E_n^a \\
= \quad & E[ABC\prod(\mathbb{RSC}(n,\rho_1,\rho_2))] \\
= \quad & \rho_1 ABC\prod(\mathbb{RSC}_n^1) + \rho_2 ABC\prod(\mathbb{RSC}_n^2) \\
+ \quad & (1-\rho_1-\rho_2)ABC\prod(\mathbb{RSC}_n^3) \\
= \quad & \rho_1[ABC\prod(\mathbb{RSC}_{n-1})\frac{\sqrt{3}}{16}] + \rho_2[ABC\prod(\mathbb{RSC}_{n-1})\frac{1}{8}] \\
+ \quad & (1-\rho_1-\rho_2)ABC\prod(\mathbb{RSC}_{n-1}) \\
= \quad & ABC\prod(\mathbb{RSC}_{n-1})[\rho_1\frac{\sqrt{3}}{16} + \rho_2\frac{1}{8} + \frac{1}{8} - \rho_1\frac{1}{8} - \rho_2\frac{1}{8}] \\
= \quad & ABC\prod(\mathbb{RSC}_{n-1})[\frac{\sqrt{3}}{16}\rho_1 - \rho_1\frac{1}{8} + \frac{1}{8}]
\end{aligned}$$

Since $E[E_n^a] = E_n^a$ and apply the operator E to the above equation, we get

$$E_n^a = \quad E_{n-1}^a[\rho_1\frac{\sqrt{3}-2}{16} + \frac{1}{8}] \qquad n > 2 \tag{2.4}$$

Using the initial condition and the recurrence relation of equation 2.4, we get our result

$$E_n^a = \frac{(\rho_1(\sqrt{3}-2)+2)^{n-2}}{2^{4n-2}}.$$

□

Theorem 2.2. *Let $\mathbb{RSC}(n;\rho_1,\rho_2)$ be a spiro chains. Then*

$$E[GA\prod(\mathbb{RSC}(n;\rho_1,\rho_2))] = \frac{64}{81}(\frac{8\rho_1+64}{81})^{n-2}; \qquad n > 1$$

Proof. From the the formula in (2.2), we have $GA\prod(\mathbb{RSC}_n) = (1)^{m_{22}+m_{44}}(\frac{2\sqrt{2}}{3})^{m_{24}}$. It is easy to see that for $n = 2$, $E_2 = \frac{64}{91}$. Now when $n \geq 2$, it is easy to see that m_{22}, m_{24} and m_{44} depend on the three possibilities as described in Figure 2.

i. If $\mathbb{RSC}_{n-1} \to \mathbb{RSC}_n^1$ with probability ρ_1, then $m_{22}(\mathbb{RSC}_n^1) = m_{22}(\mathbb{RSC}_{n-1})+3$, $m_{24}(\mathbb{RSC}_n^1) = m_{24}(\mathbb{RSC}_{n-1}) + 2$, $m_{44}(\mathbb{RSC}_n^1) = m_{44}(\mathbb{RSC}_{n-1}) + 1$, thus

$$\begin{aligned}
GA\prod(\mathbb{RSC}_n^1) &= 1^{m_{22}+m_{44}}(\frac{2\sqrt{2}}{3})^{m_{24}+2} \\
&= (\frac{8}{9})GA\prod(\mathbb{RSC}_{n-1})
\end{aligned}$$

ii. If $\mathbb{RSC}_{n-1} \to \mathbb{RSC}_n^2$ with probability ρ_2, then $m_{22}(\mathbb{RSC}_n^2) = m_{22}(\mathbb{RSC}_{n-1})+2$, $m_{24}(\mathbb{RSC}_n^2) = m_{24}(\mathbb{RSC}_{n-1}) + 4$, $m_{44}(\mathbb{RSC}_n^2) = m_{44}(\mathbb{RSC}_{n-1})$, thus we have $GA\prod(\mathbb{RSC}_n^2) = GA(\mathbb{RSC}_{n-1})(\frac{2\sqrt{2}}{3})^4$

iii. If $\mathbb{RSC}_{n-1} \to \mathbb{RSC}_n^3$ with probability $1-\rho_1-\rho_2$, then $m_{22}(\mathbb{RSC}_n^3) = m_{22}(\mathbb{RSC}_{n-1})+2$, $m_{24}(\mathbb{RSC}_n^3) = m_{24}(\mathbb{RSC}_{n-1}) + 4$, $m_{44}(\mathbb{RSC}_n^3) = m_{44}(\mathbb{RSC}_{n-1})$ $GA\prod(\mathbb{RSC}_n^3) = GA(\mathbb{RSC}_{n-1})(\frac{2\sqrt{2}}{3})^4$.

$$\begin{aligned}
&E_n[GA\prod(\mathbb{RS}C_n)]\\
&= \rho_1 GA\prod(\mathbb{RS}C_n^1)+\rho_2 GA\prod(\mathbb{RS}C_n^2)\\
&+ (1-\rho_1-\rho_2)GA\prod(\mathbb{RS}C_n^3)\\
&= \rho_1[GA\prod(\mathbb{RS}C_{n-1})\frac{8}{9}]+\rho_2[GA\prod(\mathbb{RS}C_{n-1})(\frac{2\sqrt{2}}{3})^4]\\
&+ (1-\rho_1-\rho_2)GA\prod(\mathbb{RS}C_{n-1})(\frac{2\sqrt{2}}{3})^4\\
&= GA\prod(\mathbb{RS}C_{n-1})[\frac{8}{9}\rho_1-\rho_1(\frac{8}{9})^2+(\frac{8}{9})^2]\\
&= GA\prod(\mathbb{RS}C_{n-1})[\rho_1(1-\frac{8}{9})\frac{8}{9}+(\frac{8}{9})^2]\\
&= GA\prod(\mathbb{RS}C_{n-1})[\frac{8\rho_1+64}{81}]
\end{aligned}$$

Since $E[E_n]=E_n$ and apply the operator E to the above equation, we get

$$E_n = E_{n-1}[\frac{8\rho_1+64}{81}]. \tag{2.5}$$

Using the initial condition and the recurrence relation of equation 2.5, we get our result

$$E_n = \frac{64}{81}[\frac{8\rho_1+64}{81}]^{n-2} \qquad n>1$$

□

It is easy to notice from Theorems 2.1 and 2.2 that the expected valued functions $E[ABC\prod(\mathbb{RS}C(n;\rho_1,\rho_2))]$ and $E[ABC\prod(\mathbb{RS}C(n;\rho_1,\rho_2))]$ are linear in ρ_1 and asymptotic to n. In particular, we can obtain the multiplicative ABC and GA indices of polyphenyl orth-chain $M_n=\mathbb{RS}C(n;0,1)$, polyphenyl para-chain $P_n=\mathbb{RS}C(n;0,0)$, and polyphenyl meta-chain $O_n=\mathbb{RS}C(n;1,0)$.

Corollary 2.3. *For $n>1$, we have*

(1)
- $ABC\prod(P_n)=ABC\prod(M_n)=\frac{1}{2^{3n}}$.
- $ABC\prod(O_n)=\frac{(\sqrt{3})^{n-2}}{2^{4n-2}}$.

(2)
- $GA\prod(P_n)=GA\prod(M_n)=(\frac{64}{81})^{n-1}$.
- $GA\prod(O_n)=(\frac{8}{9})^n$.

2.2. **The average value of multiplicative ABC and GA for a random and spiro chains.** In this section, the average values of the multiplicative version of the ABC and GA indices with respect to the set of all spiro chains $\mathcal{SP}_n$ has been determined. The average values over the set $\mathcal{SP}_n$ are defined by

$$ABC_{ave}\prod(\mathcal{SP}_n) = \frac{1}{|\mathcal{SP}_n|}\sum_{G\in\mathcal{SP}_n} ABC\prod(G)$$

and

$$GA_{ave}\prod(\mathcal{SP}_n) = \frac{1}{|\mathcal{SP}_n|}\sum_{G\in\mathcal{SP}_n} GA\prod(G)$$

respectively. Actually, these are the population means of the ABC and GA indices of all elements in $\mathcal{SP}_n$. Since $\rho_1 = \rho_2 = 1-\rho_1-\rho_2$, thus, we may apply Theorems 2.1 and 2.2 by putting $\rho_1 = \rho_2 = 1-\rho_1-\rho_2 = 1/3$ and obtain the following result.

Theorem 2.4. *Let $\mathcal{SP}_n$ be the set of spiro chains, then*

$$\begin{aligned} ABC_{avg}\prod(\mathcal{SP}_n) &= \frac{(\frac{\sqrt{3}+4}{3})^{n-2}}{2^{4n-2}} \\ GA_{avg}\prod(\mathcal{SP}_n) &= 5^{2n-4} * \frac{2^{3n}}{3^{5n-1}} \end{aligned}$$

From Corollary 2.3, it is easy to see that

$$\begin{aligned} &\frac{ABC\prod(O_n) + ABC\prod(P_n) + ABC\prod(M_n)}{3} \\ &= \frac{\frac{\sqrt{3}^{n-2}}{2^{4n-2}} + \frac{1}{2^{3n}} + \frac{1}{2^{3n}}}{3} \\ &= \frac{(\sqrt{3})^{n-2} + 2 * 2^{n-2}}{2^{4n-2}3} \\ &= \frac{\frac{(\sqrt{3})^{n-2}+2^{n-1}}{3}}{2^{4n-2}}. \end{aligned}$$

and

$$\begin{aligned} &\frac{GA\prod(O_n) + GA\prod(P_n) + GA\prod(M_n)}{3} \\ &= \frac{1}{3}\left[(\frac{8}{9})^n + 2(\frac{64}{81})^{n-1}\right] \\ &= (\frac{8}{9})^n\left[\frac{9^{n-2} + 2 * 8^{n-2}}{9^{n-2}}\right] \\ &= \frac{2^{3n}(3^{2n-4} + 2^{3n-5})}{3^{4n-4}} \end{aligned}$$

Since $(\frac{\sqrt{3}+4}{3})^{n-2} \geq \frac{(\sqrt{3})^{n-2}+2^{n-1}}{3}$ $\forall\, n \geq 4$. Thus the average value of the $ABC\prod_{avg}(\mathbb{RSC}(n,\rho_1,\rho_2))$ or $GA\prod_{avg}(\mathbb{RSC}(n,\rho_1,\rho_2))$ is always greater or equal to the average value of the multiplicative ABC index over the set $\{O_n, P_n, M_n\}$.

2.3. **The multiplicative ABC and GA indices in random polyphenyl chain.** In this section, we consider the multiplicative version of ABC and GA indices in $\mathbb{RP}C_n$ a random polyphenyl chain. Let $\mathbb{RP}C_n$ be the polyphenyl chain obtained by from $\mathbb{RP}C_{n-1}$ as described in Figure 1. Clearly, there are only $(2,2),(2,3)$, and $(3,3)$-edges in $\mathbb{RP}C_n$. By the definitions of the multiplicative ABC and GA indices we can directly check that

$$ABC\prod(\mathbb{RP}C_n) = (\frac{\sqrt{2}}{2})^{m_{22}(\mathbb{RP}C_n)+m_{23}(\mathbb{RP}C_n)} * (\frac{2}{3})^{m_{33}(\mathbb{RS}C_n)} \tag{2.6}$$

$$GA\prod(\mathbb{RP}C_n) = (1)^{m_{22}(\mathbb{RP}C_n)+m_{33}(\mathbb{RP}C_n)} * (\frac{2\sqrt{6}}{5})^{m_{23}(\mathbb{RP}C_n)} \tag{2.7}$$

Thus, to compute the multiplicative ABC and GA indices of $\mathbb{RP}C_n$, we just need to determine $m_{22}(\mathbb{RP}C_n), m_{24}(\mathbb{RP}C_n)$ and $m_{24}(\mathbb{RP}C_n)$ and for simplicity of the notation, we denote $m_{ij}(\mathbb{RP}C_n)$ just m_{ij} in the rest of the section.

Since $\mathbb{RP}C(n;\rho_1,\rho_2)$ is a random polyphenyl chain. So, $ABC\prod\mathbb{RP}C(n;p_1,p_2)$ and $GA\prod\mathbb{RP}C(n;p_1,p_2)$ are random variables. For simplicity, we denote expected values by $E_n = E[ABC\prod\mathbb{RP}C(n;p_1,p_2)]$ and $E_n = E[GA\prod\mathbb{RP}C(n;p_1,p_2)]$, respectively.

Theorem 2.5. *Let $\mathbb{RP}C(n;\rho_1,\rho_2)$ be a random polyphenyl chain of length n, where $n \geq 1$. Then*

$$E_n^a = ABC\prod(\mathbb{RP}C_n) = \frac{[3+\rho_1(2\sqrt{2}-3)]^{n-2}}{2^{2n+1} * 3^{2n-3}}.$$

Proof. It is easy to see that for $n=2$, $E_2^a = \frac{1}{2^5*3}$. Now when $n \geq 2$, it is obvious that m_{22}, m_{23} and m_{33} depend on the three possibilities as shown in Figure 1.

1. If $\mathbb{RP}C_{n-1} \to \mathbb{RP}C_n^1$ with probability ρ_1, then
   $m_{22}(\mathbb{RP}C_n^1) = m_{22}(\mathbb{RP}C_{n-1})+3, m_{23}(\mathbb{RP}C_n^1) = m_{23}(\mathbb{RP}C_{n-1})+2$ and $m_{33}(\mathbb{RP}C_n^1) = m_{33}(\mathbb{RP}C_{n-1})+2$. Then from (2.6), we have
   $ABC\prod(\mathbb{RP}C_n^1) = ABC\prod(\mathbb{RP}C_{n-1})\frac{\sqrt{2}}{18}$
2. If $\mathbb{RP}C_{n-1} \to \mathbb{RP}C_n^2$ with probability ρ_2, then
   $m_{22}(\mathbb{RP}C_n^1) = m_{22}(\mathbb{RP}C_{n-1})+2, m_{23}(\mathbb{RP}C_n^1) = m_{23}(\mathbb{RP}C_{n-1})+4$ and $m_{33}(\mathbb{RP}C_n^1) = m_{33}(\mathbb{RP}C_{n-1})+1$. Then from (2.6), we have
   $ABC\prod(\mathbb{RP}C_n^2) = (\frac{\sqrt{2}}{2})^6(\frac{2}{3})ABC\prod(\mathbb{RP}C_{n-1}) = \frac{1}{12}ABC\prod(\mathbb{RP}C_{n-1})$
3. If $\mathbb{RP}C_{n-1} \to \mathbb{RP}C_n^3$ with probability $1-\rho_1-\rho_2$, then
   $m_{22}(\mathbb{RP}C_n^1) = m_{22}(\mathbb{RP}C_{n-1})+2, m_{23}(\mathbb{RP}C_n^1) = m_{23}(\mathbb{RP}C_{n-1})+4$ and $m_{33}(\mathbb{RP}C_n^1) = m_{33}(\mathbb{RP}C_{n-1})+1$.Then from (2.6), we have
   $ABC\prod(\mathbb{RP}C_n^3) = (\frac{\sqrt{2}}{2})^6(\frac{2}{3})ABC\prod(\mathbb{RP}C_{n-1}) = \frac{1}{12}ABC\prod(\mathbb{RP}C_{n-1})$

Thus, we obtain

$$\begin{aligned} E_n^a &= \rho_1 ABC\prod(\mathbb{RPC}_n^1) + \rho_2 ABC\prod(\mathbb{RPC}_n^2) \\ &+ (1-\rho_1-\rho_2)ABC\prod(\mathbb{RPC}_n^3) \\ &= \rho_1\frac{\sqrt{2}}{18}ABC\prod(\mathbb{RPC}_{n-1}) + \frac{\rho_2}{12}ABC\prod(\mathbb{RPC}_{n-1}) \\ &+ \frac{(1-\rho_1-\rho_2)}{12}ABC\prod(\mathbb{RPC}_{n-1}) \\ &= ABC\prod(\mathbb{RPC}_{n-1})\Big[\frac{3+\rho_1(2\sqrt{2}-3)}{36}\Big] \end{aligned}$$

Since $E[E_n]^a = {E_n}^a$ and apply the operator E to the above equation, we get

$$E_n^a = E_{n-1}^a\Big[\frac{3+\rho_1(2\sqrt{2}-3)}{36}\Big]. \tag{2.8}$$

Using the initial condition and the recurrence relation of equation (2.8), we get our result

$$E_n^a = \frac{[3+\rho_1(2\sqrt{2}-3)]^{n-2}}{2^{2n+1} * 3^{2n-3}} \qquad n > 1$$

□

Theorem 2.6. *Let $\mathbb{RPC}(n;\rho_1,\rho_2)$ be a random polyphenyl chain of length n, where $n \geq 2$. Then*

$$GA(\mathbb{RPC}_n) = (\frac{2\sqrt{6}}{5})^4\Big[(\frac{2\sqrt{6}}{5})^4 + \rho_1((\frac{2\sqrt{6}}{5})^2 - (\frac{2\sqrt{6}}{5})^4)\Big]^{n-2}.$$

Proof. It is easy to see that for $n = 2$, $E_2 = (\frac{24}{25})^2$. Now when $n \geq 3$, we have to consider the three possibilities as shown in Figure 1.

1. If $\mathbb{RPC}_{n-1} \to \mathbb{RPC}_n^1$ with probability ρ_1, then $m_{22}(\mathbb{RPC}_n^1) = m_{22}(\mathbb{RPC}_{n-1})+3, m_{23}(\mathbb{RPC}_n^1) = m_{23}(\mathbb{RPC}_{n-1})+2$ and $m_{33}(\mathbb{RPC}_n^1) = m_{33}(\mathbb{RPC}_{n-1}) + 2$. Then from (2.7), we have $GA\prod(\mathbb{RPC}_n^1) = GA\prod(\mathbb{RPC}_{n-1})(\frac{2\sqrt{6}}{5})^2$
2. If $\mathbb{RPC}_{n-1} \to \mathbb{RPC}_n^2$ with probability ρ_2, then $m_{22}(\mathbb{RPC}_n^1) = m_{22}(\mathbb{RPC}_{n-1})+2, m_{23}(\mathbb{RPC}_n^1) = m_{23}(\mathbb{RPC}_{n-1})+4$ and $m_{33}(\mathbb{RPC}_n^1) = m_{33}(\mathbb{RPC}_{n-1}) + 1$. Then from (2.7), we have $GA\prod(\mathbb{RPC}_n^2) = GA\prod(\mathbb{RPC}_{n-1})(\frac{2\sqrt{6}}{5})^4$
3. If $\mathbb{RPC}_{n-1} \to \mathbb{RPC}_n^3$ with probability $1-\rho_1-\rho_2$, then $m_{22}(\mathbb{RPC}_n^1) = m_{22}(\mathbb{RPC}_{n-1})+2, m_{23}(\mathbb{RPC}_n^1) = m_{23}(\mathbb{RPC}_{n-1})+4$ and $m_{33}(\mathbb{RPC}_n^1) = m_{33}(\mathbb{RPC}_{n-1}) + 1$.Then from (2.7), we have $GA\prod(\mathbb{RPC}_n^3) = GA\prod(\mathbb{RPC}_{n-1})(\frac{2\sqrt{6}}{5})^4$

Thus, we obtain

$$\begin{aligned} E_n &= \rho_1 GA\prod(\mathbb{RPC}_n^1) + \rho_2 GA\prod(\mathbb{RPC}_n^2) \\ &+ (1-\rho_1-\rho_2)GA\prod(\mathbb{RPC}_n^3) \end{aligned}$$

Since $E[E_n] = E_n$ and apply the operator E to the above equation, we get

$$E_n = E_{n-1}\Big[(\frac{2\sqrt{6}}{5})^4 + \rho_1((\frac{2\sqrt{6}}{5})^2 - (\frac{2\sqrt{6}}{5})^4)\Big] \tag{2.9}$$

Using the initial condition and the recurrence relation of equation (2.9), we get our result

$$E_n = \quad (\frac{2\sqrt{6}}{5})^4\Big[(\frac{2\sqrt{6}}{5})^4 + \rho_1((\frac{2\sqrt{6}}{5})^2 - (\frac{2\sqrt{6}}{5})^4)\Big]^{n-2} \quad n > 1$$

□

From Theorems 2.5 and 2.6, it is easy to obtain the multiplicative ABC and GA indices of polyphenyl meta-chain $\overline{O}_n = \mathbb{RPC}(n; 1, 0)$, polyphenyl orth-chain $\overline{M}_n = \mathbb{RPC}(n; 0, 1)$, and polyphenyl para-chain $\overline{P}_n = \mathbb{RPC}(n; 0, 0)$.

Corollary 2.7. *For $n > 1$, we have*

(1)
- $ABC\prod(\overline{P}_n) = ABC\prod(\overline{M}_n) = \frac{1}{2^{2n+1} * 3^{n-1}}$.
- $ABC\prod(\overline{O}_n) = \frac{(\sqrt{2})^{n-2}}{2^{n+3} * 3^{2n-3}}$.

(2)
- $GA\prod(\overline{P}_n) = GA\prod(\overline{M}_n) = (\frac{24}{25})^{2n-2}$.
- $GA\prod(\overline{O}_n) = (\frac{24}{25})^n$.

3. A comparison between the expected values of multiplicative ABC and GA indices

Recently, in [27] authors compared the expected values of the GA index and ABC index for a random polyphenyl chain. Now with the help of Theorems 2.1,2.2,2.5, and 2.6, we will make a comparison between the expected values for the multiplicative ABC and GA indices of a random spiro chain and random polyphenyl chain with the same probabilities $\rho_i (i = 1, 2)$. The following lemma is easy to prove by induction, we we omit its proof.

Lemma 3.1. *For all $m \geq 2$, we have*

$$f(m) = \frac{(\sqrt{3})^{m-2} 3^{2m}}{2^{7m-2}} < 1.$$

Theorem 3.2. *For $n \geq 2$, we have*

$$E[GA\prod(\mathbb{RSC}(n; \rho_1, \rho_2))] > E[ABC\prod(\mathbb{RSC}(n; \rho_1, \rho_2))].$$

Proof. Obviously for $n = 1$, the statement is true. So, when $n > 2$, by Theorems 2.1 and 2.2, we have

$$E[GA\prod(\mathbb{RSC}(n; \rho_1, \rho_2))] - E[ABC\prod(\mathbb{RSC}(n; \rho_1, \rho_2))]$$

$$
\begin{aligned}
&= \frac{64}{81}(\frac{8\rho_1+64}{81})^{n-2} - \frac{(\rho_1(\sqrt{3}-2)+2)^{n-2}}{2^{4n-2}} \\
&= (\frac{8}{9})^n - \frac{(\sqrt{3})^{n-2}}{2^{4n-2}} \quad \because 0 \leq \rho_1 \leq 1 \\
&= \frac{2^{3n}}{3^{2n}}\left[1 - \frac{(\sqrt{3})^{n-2} * 3^{2n}}{2^{7n-2}}\right] > 0
\end{aligned}
$$

□

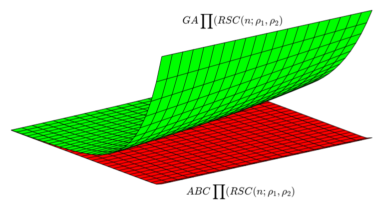

FIGURE 3. Difference between the Geometric index and ABC index with respect to the random chain

Figure 3 show that the expected value of the index $GA\prod(\mathbb{RS}C(n;\rho_1,\rho_2))$ is always greater than the expected value of the $ABC\prod(\mathbb{RS}C(n;\rho_1,\rho_2))$.

Theorem 3.3. *For $n \geq 1$, we have*

$$E[GA\prod(\mathbb{RP}C(n;\rho_1,\rho_2))] > E[ABC\prod(\mathbb{RP}C(n;\rho_1,\rho_2))].$$

Proof. When $n > 2$, by Theorems 2.5 and 2.6, we have

$$E[GA\prod(\mathbb{RP}C(n;\rho_1,\rho_2))] - E[ABC\prod(\mathbb{RP}C(n;\rho_1,\rho_2))]$$

$$
\begin{aligned}
&= (\frac{24}{25})^2\left[\frac{24}{25^2}(24+\rho_1)\right]^{n-2} - \frac{[3+\rho_1(2\sqrt{2}-3)]^{n-2}}{2^{2n+1} * 3^{2n-3}} \\
&= (\frac{24}{25})^n - \frac{(\sqrt{2})^{n-2}}{2^{n+3} * 3^{2n-3}} \quad \because 0 \leq \rho_1 \leq 1 \\
&= (\sqrt{2})^{n-2}\left[\frac{4^n * (\sqrt{2})^{n+2} * 3^n}{5^{2n}} - \frac{1}{2^{n+3} * 3^{2n-3}}\right] \\
&= (\sqrt{2})^{n-2}\left[2(\frac{12\sqrt{2}}{25})^n - \frac{1}{2^{n+3} * 3^{2n-3}}\right] > 0
\end{aligned}
$$

□

Figure 4 show that the expected value of the index $GA\prod(\mathbb{RS}C(n;\rho_1,\rho_2))$ is always greater than the expected value of the $ABC\prod(\mathbb{RS}C(n;\rho_1,\rho_2))$.

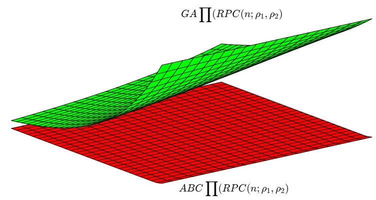

Figure 4. Difference between the Geometric index and ABC index with respect to the random chain

4. Conclusion

In this paper, we compute and compare the expected values of the multiplicative ABC and GA index over the set of all random and spiro polyphenyl chains. Firstly, the explicit formulae for the expected values of multiplicative ABC and GA indices in random polyphenyl and spiro chains are presented. Secondly, the average values of $ABC\prod$ and $GA\prod$ indices are presented with respect to the set of all polyphenyl chains with n hexagons. Finally, we compare the expected values of $ABC\prod$ and $GA\prod$ indices in random polyphenyl chains, the expected values of $ABC\prod$ and $GA\prod$ indices between random polyphenyl chains and spiro chains. In the aspect of research, there are still two problems considered. On one hand, one can continue to discuss the problem about other degree-based topological indices (such as Zagreb index and sum-connectivity index) for the polyphenyl and spiro chains. On the other, one may also calculating the $ABC\prod$ and $GA\prod$ indices in random polygonal chains and makes the same comparisons between them from pure graph theory.

5. Declarations

5.1. **Availability of data and materials.** Not applicable

5.2. **Funding.** This research work is funded by the University of Sharjah, UAE, under the Project #1802144068 and MASEP Research Group.

5.3. **Authors' contributions.** Not applicable

References

[1] Y. Bai, B. Zhao, P. Zhao, Extremal Merrifield-Simmons index and Hosoya index of polyphenyl chains, MATCH Commun. Math. Comput. Chem., 62 (2009), 649656.
[2] H. Bian, F. Zhang. Tree-like polyphenyl systems with extremal Wiener indices, MATCH Commun. Math. Comput. Chem., 61 (2009), 631642.
[3] D. Bonchev, Information Theoretic Indices for Characterization of Molecular Structure, Research Studies Press Wiley, Chichester, 1983.
[4] M. Burechecks, V. Pekarek, T. Ocelka, Thermochemical properties and relative stability of polychlorinated biphenyls, Environ. Tox. Pharm., 25 (2008), 26102617.

[5] A. Chen, F. Zhang. Wiener index and perfect matchings in random phenylene chains, MATCH. Commun. Math. Comput. Chem., 61 (2009), 623630.
[6] X. Chen, B. Zhao, P. Zhao, Six-membered ring spiro chains with extremal Merrifild-Simmons index and Hosaya index, MATCH Commun. Math. Comput. Chem., 62 (2009), 657665.
[7] K.C. Das, On geometric-arithmetic index of graphs, MATCH Commun. Math. Comput. Chem., 64 (2010) 3, 619630.
[8] K.C. Das, Trinajstic, Comparison between first geometric-arithmetic index and atom-bond connectivity index, Chem. Phys. Lett., 497 (2010), 149151.
[9] H. Deng, Wiener indices of spiro and polyphenyl hexagonal chains, Mathematical and Computer Modelling, 55 (2012), 634644.
[10] H. Deng, Z. Tang, Kirchhoff indices of spiro and polyphenyl hexagonal chains, Util. Math., 95 (2014), 113128.
[11] T. Doslic, M.S. Litz, Matchings and independent sets in polyphenylene chains, MATCH Commun. Math. Comput. Chem., 67 (2012), 313330.
[12] T. Divnic, M. Milivojevic, L. Pavlovic, Extremal graphs for the geometric-arithmetic index with given minimum degree, Discrete Appl. Math., 162 (2014), 386390.
[13] E. Estrada, L. Torres, L. Rodrguez, An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes, Indian J. Chem., 37A (1998), 849-855.
[14] E. Estrada, Atom-bond connectivity and the energetic of branched alkanes, Chem. Phys. Lett.463 (2008), 422425.
[15] I. Gutman, K. Das, The first Zagreb index 30 years after, MATCH Commun. Math. Comput. Chem. 50, 8392 (2004)
[16] H. Gonzales-Diaz (Ed.), Topological Indices for Medicinal Chemistry, Biology, Parasitology, Neurological and Social Networks, Transworld Researcg Network, 2010.
[17] H. Hosoya, A newly proposed quantity chracterizingthe topologcal nature of struuctural isomers of saturated hydrocarbons. Bull. Chem. Soc. Japan 44, 2332-2339 (1971).
[18] G. Huang, M. Kuang, H. Deng. The expected values of Kirchhoff indices in the random polyphenyl and spiro chains, Ars Math. Contemp., 9 (2015), 197207.
[19] 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), 550562.
[20] M. Karelson, Moledular Descriptors in QSR/QSPR, Wiley-Interscience, New York, 2000.
[21] L. B. Kier, L. H. Hall, Molecular Connectivity in Chemistry and Drug Research (Academic Press, New York, (1976)
[22] M. Randic, Characterization of molecular branching. J. Am. Chem. Soc. 97, 660-661 (1975).
[23] J. M. Rodrguez, J. M. Sigarreta, Spectral properties of geometric-arithmetic index, Appl. Math.Comput., 277 (2016), 142153.
[24] R. krekovski, D. Dimitrov, J. Zhong, H. Wu, W. Gao, Remarks on Multiplicative Atom-Bond Connectivity Index, IEEE Access, 7(2019),76806-76811.
[25] N. Trinajstii, Chemical Graph Theory, CRC Press, Boca Raton, 2nd Ed., 1992.
[26] D. Vukicevic, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, J. Math. Chem., 46 (2009), 13691376.
[27] 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.
[28] W. Yang, F. Zhang. Wiener index in random polyphenyl chains, MATCH. Commun. Math.Comput. Chem., 68 (2012), 371376.
[29] H. Wiener, Structure determination of paraffin boiling points. J. Am. Chem. Soc. 69, 17-20 (1947)
[30] Y. Yang, H. Liu, H. Wang, H. Fu, Subtrees of spiro and polypheny hexagonal chains, Appl. Math.Comput., 268 (2015), 547-560.
[31] Y. Yang, H. Liu, H. Wang, S. Sun, On spiro and polypheny hexagonal chains with respect to the number of BC-subtrees, Int. J. Comput. Math., 94 (2017) 4, 774-799.
[32] Y. Yuan, B. Zhou, N. Trinajstic, On geometric-arithmetic index, J. Math. Chem., 47 (2010), 833841.

[33] B. Zhou, I. Gutman, B. Furtula, Z. Du, On two types of geometric-arithmetic index, Chem.Phys. Lett., 482 (2009), 153155.