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Research article

The comparative analysis of two molecular indices in random polyphenyl and spiro chains

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Abstract: Zagreb indices are well-known and historical indices that are very useful to calculate the properties of compounds. In the last few years, various kinds of Zagreb and Randic indices are investigated and defined to fulfil the demands of various engineering applications. Phenylenes are a class of conjugated hydrocarbons composed of a special arrangement of six- and four-membered rings. This special chain, produced by zeroth-order Markov process has been commonly appeared in the field of pharmacology and materials. Here, we compute the expected values of a multiplicative versions of the geometric arithmetic and atomic bond connectivity indices for these special hydrocarbons. Moreover, we make comparisons in the form of explicit formulae and numerical tables between the expected values of these indices in the random polyphenyl $\mathbb{P}_n$ and spiro $\mathbb{S}_n$ chains.

Keywords: atomic bond connectivity index; geometric arithmetic index; expected values; random polyphenyl chain; spiro chains; comparisons

1. Introduction

Chemical graph theory, is a branch of mathematics, dealing with mathematical modelling of graphs that is also an essential branch of theoretical chemistry. Initial chemical research introduces the theory of chemical graph. Chemists confirm that the physicochemical properties of a compound have been associated with the molecular arrangement, resulting in derived from an enormous number of investigational data. Furthermore, the researchers considered the same topological index based on various chemical properties and applied it to QSR/ QSPR learning. Generally, the features of a compound derived by chemical experiments are not much authentic. Although, theoretical calculations assume a vital role in many extraordinary cases, e.g., the proportion of trace elements is very small and mass cannot be obtained, that makes it problematic to direct and inspect their properties. Consequently, the way utilizing chemical experimentation are less productive than chemical topological index computing. All through this research paper, we demonstrated the molecular structure as where an atom is communicated by every node and every edge indicates the chemical bond between two atoms of a graph. Here, the crystals, compounds, medications, or materials are shown by graphical structures and known as molecular graphs. The earliest integer topological indices such as $W(G)$ index in [1] have a high degeneracy, the $Z(G)$ index in [2], the Zagreb index in [3], compared to non-integer such as information theoretic indices explained in [4–6] or higher-order molecular connectivity index briefed in [7, 8]. The Atom Bond Connectivity (ABC) index is introduced by Estrada et al. [9] and the stability of alkanes is correlated by this and the strain energy of cycloalkanes, see [10, 11]. Zagreb index is the oldest index having a number of applications in the field of chemicals. To fit the different applications, researchers have made a few changes to various indices as of late, and have suggested some more versions. Next, a graph G has a node set $V(G)$ and an edge set $E(G), d(x)$ gives the degree of the node $x \in V(G)$. Recently, Kulli [12] introduced the multiplicative version of ABC index and described 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 ABC index of some nanotubes. Since the multiplicative ABC index is not yet studied widely, the results on the multiplicative ABC index are yet restricted, when contrasted with the ABC index, for more recent work see [13]. In [14] geometric arithmetic index (GA) has been defined and well correlated with a lot of properties of the compound and it predicts physio-chemical properties better than the Randic index. More details about the GA index can be found in [15–26]. Kulli [12] also introduced the multiplicative version of geometric arithmetic index

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

ABC and GA indices are shown to have an extensive scope of topological variables upheld by chemical experimental data. Since the variables mentioned above are described in the field of chemical for the fundamentals of additional applied applications having some potential application substance. About a similar application, the edge version topological indices with unique indices perform as corresponding associations that appropriate the different chemical data sets. The polyphenyls may be used in heat exchanger, drug synthesis, organic synthesis, etc. See [27] for further applications regarding the applications of polyphenyls.

In organic chemistry, spiro compounds are a significant class of cycloalkanes. In spiro compounds, a spiro association is a relationship between two rings in which the same atom joint consists of two rings. A free spiro association is a link having only one atom in common with two adjacent rings. Another name of normal atom is the spiro atom. According to the spiro atoms, monospiro, dispiro, trispiro are the compounds. We study a subclass of branchless multi-spiro particles where each ring has a hexagon and so, their graphs are named spiro hexagonal chains.

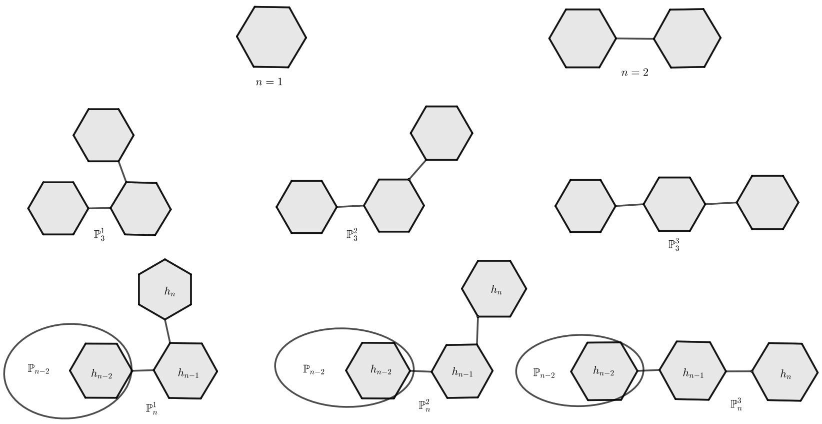

Figure 1. Random Polyphenyl Chains for $n = 1, 2, 3$ and $n > 3$.

A polyphenyl chain denoted by $\mathbb{P}_n$ is obtained from n hexagons h_1, h_2, h_n by joining two consecutive hexagons by an edge (see Figure 1). If $n = 1, 2$, chains as shown in Figure 1 are unique. There are three different ways to join two consecutive hexagons and hence $\mathbb{P}_n$ is not unique for $n > 2$. $\mathbb{P}_n^1$, $\mathbb{P}_n^2$, and $\mathbb{P}_n^3$ are the three local arrangements of $\mathbb{P}_n$ (see Figure 1). Hence, $\mathbb{P}_n$ is a random process obtained from a fixed $\mathbb{P}_{n-1}$ and $\mathbb{P}_n^1$, $\mathbb{P}_n^2$, and $\mathbb{P}_n^3$ can be obtained from $\mathbb{P}_{n-1}$, with ρ_1, ρ_2 and $1 - \rho_1 - \rho_2$ probabilities. If the probabilities $\rho_i; i = 1, 2$ are constants and do not pendent on n, then this procedure is a Markov process of order zero. The obtained chain $\mathbb{P}(n; \rho_1, \rho_2)$ is called random polyphenyl.

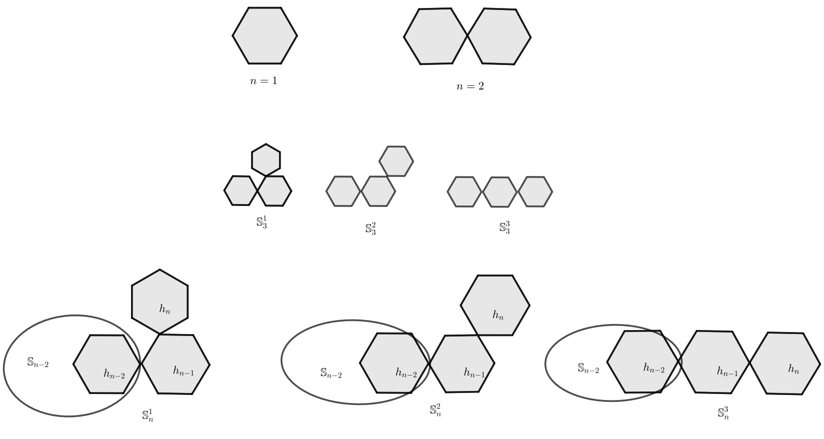

Figure 2. Random spiro Chains for $n = 1, 2, 3$ and $n > 3$.

If each consecutive hexagon in $\mathbb{P}_n$ joined directly to each other, then we have a spiro chain $\mathbb{S}_n$. Similarly, for $n > 2$, the chain $\mathbb{S}_n$ has three types of local arrangements denoted by $\mathbb{S}_n^1$, $\mathbb{S}_n^2$ and $\mathbb{S}_n^3$, respectively, and $\mathbb{S}_n$ is not unique (see Figure 2). The obtained chain $\mathbb{S}(n; \rho_1, \rho_2)$ is called random spiro.

Although, the mathematical theoretical model and the actual compound composition principle has a special gap (for example, the aromaticity of the structures give the stability of the polybenzene system that is additionally obtained through its final arrangement, and the steric effect (steric hindrance) plays an important part in defining the comparative constancy of orth, para and meta isomers). There are few advance contributions in these structures in the special topological indices due to random chain structural operation. In [28] we determined the Kirchhoff index for these two special chains and the W(G) index in [29]. The Z(G) index and F(G) index [30]. BC-subtrees characterized in [31]. H(G) and $M_2(G)$ indices in [19]. ABC and GA indices in [32]. Independent sets, matchings, and some other properties [4, 17, 33–39]. For more details, one may refer to [15, 40–51].

Markov process of various molecular structures has a critical importance of research implication in chemical studies in nature embedding. For instance, the thickness of water is changed at a lower temperature and so, the thickness is more likely to be empty. It is to a good judgment, the lower the temperature is, the less dynamic the atom, and the more modest the thickness vacillations ought to be. The researchers claim that water is another important point and so, water is always changing rapidly in both states. By nature, both states are distinct. Any transformation in any other will bring about an unexpected transformed thickness that is usually specified at that basic point. In this behalf, we can say that water consists of two liquids of various thickness, e.g., water is definitely not a liquid. However, the two liquids are the combination of a lower and higher thickness of liquid. Due to various thicknesses, lengths, association qualities, and hydrogen bonds between the two liquids are unique that converts their features like diffusion and thickness. The molecular structure is different in these two types of water, one of which is that the water particles are scattered and thick, and the other with a low thickness is a standard tetrahedral structure. At a typical temperature and pressing factor, low-thickness water particles are arbitrarily inserted in high-thickness water atoms. Furthermore, their mathematical theory depends on the Markov process and the mutual embedding of various molecular graphs. Besides, $\mathbb{P}_n$ and $\mathbb{S}_n$ chains show a typical method in regards to join molecule graphs.

In this paper, we study two important chains named as random spiro and random polyphenyl in detail. Consequently, there are countless commitments that have been discussed on different random properties and applications of ABC and GA indices. This inspires us to make an essential study on the multiplicative ABC and GA indices and makes theoretical support available for the future use of above-mentioned indices. So, the multiplicative ABC and multiplicative GA indices for random polyphenyl and random spiro chains has been computed in this paper.

2. Results and discussion

Our main results about these two types of chains have been discussed in this part. First, we consider the random spiro chain $\mathbb{S}(n; \rho_1, \rho_2)$ as shown in Figure 2, and there are only $(2, 2), (2, 4)$ and $(4, 4)$ edges in $\mathbb{S}_n$. As we know that the multiplicative ABC and GA indices for random spiro chains are random variables and their expected values are denoted by $E_n^{ABC} = E[ABC \prod(\mathbb{S}(n; \rho_1, \rho_2))]$ and $E_n^{GA} = E[GA \prod(\mathbb{S}(n; \rho_1, \rho_2))]$ respectively. From Eqs (1.1) and (1.2), we have:

$$ABC \prod(\mathbb{S}_n) = (\frac{\sqrt{2}}{2})^{x_{22}(\mathbb{S}_n)+x_{24}(\mathbb{S}_n)}(\frac{\sqrt{6}}{4})^{x_{44}(\mathbb{S}_n)} \tag{2.1}$$

$$GA \prod(\mathbb{S}_n) = (1)^{x_{22}(\mathbb{S}_n)+x_{44}(\mathbb{S}_n)}(\frac{2\sqrt{2}}{3})^{x_{24}(\mathbb{S}_n)} \tag{2.2}$$

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

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

2) $E_n^{GA} = E[GA \prod(\mathbb{S}(n;\rho_1,\rho_2))] = \frac{64}{81}(\frac{8\rho_1+64}{81})^{n-2}$.

Proof. For $n = 2$, we have $E_2^{ABC} = 1/64$ and $E_2^{GA} = 64/81$. If $n > 2$, then we have to consider three local arrangements (see Figure 2).

i. If $\mathbb{S}_{n-1} \to \mathbb{S}_n^1$ with probability ρ_1, then $x_{22}(\mathbb{S}_n^1) = x_{22}(\mathbb{S}_{n-1}) + 3$, $x_{24}(\mathbb{S}_n^1) = x_{24}(\mathbb{S}_{n-1}) + 2$, $x_{44}(\mathbb{S}_n^1) = x_{44}(\mathbb{S}_{n-1}) + 1$, and by Eqs (2.1) and (2.2), we have

$$\begin{aligned} ABC\prod(\mathbb{S}_n^1) &= (\frac{1}{\sqrt{2}})^{x_{22}+x_{24}}(\frac{\sqrt{6}}{4})^{x_{44}}(\frac{1}{\sqrt{2}})^5(\frac{\sqrt{6}}{4}) \\ &= \frac{\sqrt{3}}{16}ABC\prod(\mathbb{S}_{n-1}). \end{aligned}$$

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

ii. If ρ_2 is the probability to obtained $\mathbb{S}_n^2$ from a fixed $\mathbb{S}_{n-1}$, then $x_{22}(\mathbb{S}_n^2) = x_{22}(\mathbb{S}_{n-1}) + 2$, $x_{24}(\mathbb{S}_n^2) = x_{24}(\mathbb{S}_{n-1}) + 4$, $x_{44}(\mathbb{S}_n^2) = x_{44}(\mathbb{S}_{n-1})$, and by (2.1) we get

$$ABC\prod(\mathbb{S}_n^2) = \frac{1}{8}ABC\prod(\mathbb{S}_{n-1}).$$

$$GA\prod(\mathbb{S}_n^2) = (\frac{2\sqrt{2}}{3})^4 GA\prod(\mathbb{S}_{n-1})$$

iii. If $\mathbb{S}_{n-1} \to \mathbb{S}_n^3$ with probability $1-\rho_1-\rho_2$, then $x_{22}(\mathbb{S}_n^3) = x_{22}(\mathbb{S}_{n-1}) + 2$, $x_{24}(\mathbb{S}_n^3) = x_{24}(\mathbb{S}_{n-1}) + 4$, $x_{44}(\mathbb{S}_n^3) = x_{44}(\mathbb{S}_{n-1})$, so

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

$$GA\prod(\mathbb{RS}C_n^3) = (\frac{2\sqrt{2}}{3})^4 GA\prod(\mathbb{RS}C_{n-1}).$$

By the above three types of local arrangements, we have:,

$$\begin{aligned} E_n^{ABC} &= \rho_1 ABC\prod(\mathbb{S}_n^1) + \rho_2 ABC\prod(\mathbb{S}_n^2) + (1-\rho_1-\rho_2)ABC\prod(\mathbb{S}_n^3) \\ &= \rho_1[ABC\prod(\mathbb{S}_{n-1})\frac{\sqrt{3}}{16}] + \rho_2[ABC\prod(\mathbb{S}_{n-1})\frac{1}{8}] \\ &+ (1-\rho_1-\rho_2)ABC\prod(\mathbb{S}_{n-1}) \\ &= ABC\prod(\mathbb{S}_{n-1})[\rho_1\frac{\sqrt{3}}{16} + \rho_2\frac{1}{8} + \frac{1}{8} - \rho_1\frac{1}{8} - \rho_2\frac{1}{8}] \\ &= ABC\prod(\mathbb{S}_{n-1})[\frac{\sqrt{3}}{16}\rho_1 - \rho_1\frac{1}{8} + \frac{1}{8}] \end{aligned} \tag{2.3}$$

and also, we have

$$
\begin{aligned}
E_n^{GA} &= \rho_1 GA\prod(\mathbb{S}_n^1) + \rho_2 GA\prod(\mathbb{S}_n^2) + (1-\rho_1-\rho_2)GA\prod(\mathbb{S}_n^3) \\
&= \rho_1[GA\prod(\mathbb{S}_{n-1})\frac{8}{9}] + \rho_2[GA\prod(\mathbb{S}_{n-1})(\frac{2\sqrt{2}}{3})^4] \\
&+ (1-\rho_1-\rho_2)GA\prod(\mathbb{S}_{n-1})(\frac{2\sqrt{2}}{3})^4 \\
&= GA\prod(\mathbb{S}_{n-1})[\frac{8}{9}\rho_1 - \rho_1(\frac{8}{9})^2 + (\frac{8}{9})^2] \\
&= GA\prod(\mathbb{S}_{n-1})[\rho_1(1-\frac{8}{9})\frac{8}{9} + (\frac{8}{9})^2] \\
&= GA\prod(\mathbb{S}_{n-1})[\frac{8\rho_1+64}{81}] \qquad (2.4)
\end{aligned}
$$

As $E[E_n] = E$, so apply E on Eqs (2.3) and (2.4), which gives the following:

$$E_n^{ABC} = E_{n-1}^{ABC}[\rho_1\frac{\sqrt{3}-2}{16} + \frac{1}{8}]. \qquad (2.5)$$

$$E_n^{GA} = E_{n-1}^{GA}[\frac{8\rho_1+64}{81}]. \qquad (2.6)$$

Solving the linear recurrence relation of Eqs (2.5) and (2.6) with the initial condition, we get

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

$$E_n^{GA} = \frac{64}{81}(\frac{8\rho_1+64}{81})^{n-2}.$$

□

From Theorem 1, we noted that E_n^{ABC} and E_n^{GA} are polynomial in rho_1 and asymptotic to n. It is easy to note that these indices can be computed for three special chains: meta $PM_n = \mathbb{S}(n; 0, 1)$, para $PP_n = \mathbb{S}(n; 0, 0)$, and ortho $PO_n = \mathbb{S}(n; 1, 0)$ chains as shown in Figure 3.

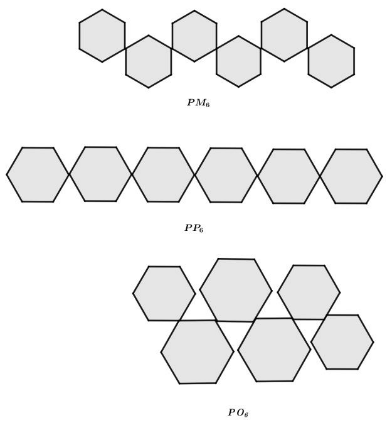

Figure 3. Special Polyphenyl ortho ($\overline{PO}_6$, meta $\overline{PM}_6$ and para $\overline{PP}_6$ chains).

Corollary. *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. • $GA\prod(P_n) = GA\prod(M_n) = (\frac{64}{81})^{n-1}$.

   • $GA\prod(O_n) = (\frac{8}{9})^{n}$.

If $\mathbb{P}_n$ is the polyphenyl chain as shown in Figure 1. There are only $(2,2),(2,3)$ and $(3,3)$ edges in $\mathbb{P}_n$ and from Eqs (1.1) and (1.2) one can get the following:

$$ABC\prod(\mathbb{P}_n) = (\frac{\sqrt{2}}{2})^{x_{22}(\mathbb{P}_n)+x_{24}(\mathbb{P}_n)} * (\frac{\sqrt{6}}{4})^{x_{44}(\mathbb{P}_n)} \tag{2.7}$$

$$GA\prod(\mathbb{P}_n) = (1)^{x_{22}(\mathbb{P}_n)+x_{44}(\mathbb{P}_n)} * (\frac{2\sqrt{2}}{3})^{x_{24}(\mathbb{P}_n)} \tag{2.8}$$

As we know that the multiplicative GA and ABC indices are random variables in random polyphenyl chain and their expected values are denoted by $E_n^ABC = E[ABC\prod(\mathbb{P}(n;\rho_1,\rho_2))]$ and $E_n^{GA} = E[GA\prod(\mathbb{P}(n;\rho_1,\rho_2))]$ respectively.

Theorem 2. *For $n > 1$, and a random polyphenyl chains $\mathbb{P}(n;\rho_1,\rho_2)$, we have*
1) $E_n^{ABC} = ABC\prod(\mathbb{P}_n) = \frac{[3+\rho_1(2\sqrt{2}-3)]^{n-2}}{2^{2n+1}*3^{2n-3}}$.
2) $E_n^{GA} = (\frac{2\sqrt{6}}{5})^4\Big[(\frac{2\sqrt{6}}{5})^4 + \rho_1\{(\frac{2\sqrt{6}}{5})^2 - (\frac{2\sqrt{6}}{5})^4\}\Big]^{n-2}$.

Proof. For $n = 2$, we have $E_2^{ABC} = 1/96$ and $E_2^{GA} = 576/625$. If $n > 2$, then we have to consider three local arrangements (see Figure 1).

1). If $\mathbb{P}_{n-1} \rightarrow \mathbb{P}_n^1$ with probability ρ_1, then
$x_{22}(\mathbb{P}_n^1) = x_{22}(\mathbb{P}_{n-1}) + 3$, $x_{23}(\mathbb{P}_n^1) = x_{23}(\mathbb{P}_{n-1}) + 2$ and $x_{33}(\mathbb{P}_n^1) = x_{33}(\mathbb{P}_{n-1}) + 2$. Then from (2.7) and (2.8), we have
$ABC\prod(\mathbb{P}_n^1) = \frac{\sqrt{2}}{18}ABC\prod(\mathbb{P}_{n-1})$
$GA\prod(\mathbb{P}_n^1) = (\frac{2\sqrt{6}}{5})^2 GA\prod(\mathbb{P}_{n-1})$

2). If $\mathbb{P}_{n-1} \rightarrow \mathbb{P}_n^2$ with probability ρ_2, then
$x_{22}(\mathbb{P}_n^2) = x_{22}(\mathbb{P}_{n-1}) + 2$, $x_{23}(\mathbb{P}_n^2) = x_{23}(\mathbb{P}_{n-1}) + 4$ and $x_{33}(\mathbb{P}_n^2) = x_{33}(\mathbb{P}_{n-1}) + 1$. Then from (2.7) and (2.8), we have
$ABC\prod(\mathbb{P}_n^2) = (\frac{\sqrt{2}}{2})^6(\frac{2}{3})ABC\prod(\mathbb{P}_{n-1}) = (\frac{1}{12})ABC\prod(\mathbb{P}_{n-1})$
$GA\prod(\mathbb{P}_n^2) = (\frac{2\sqrt{6}}{5})^4 GA\prod(\mathbb{P}_{n-1})$

3). If $\mathbb{RPC}_{n-1} \rightarrow \mathbb{RPC}_n^3$ with probability $1-\rho_1-\rho_2$, then
$x_{22}(\mathbb{P}_n^3) = x_{22}(\mathbb{P}_{n-1}) + 2$, $x_{23}(\mathbb{P}_n^3) = x_{23}(\mathbb{P}_{n-1}) + 4$ and $x_{33}(\mathbb{P}_n^3) = x_{33}(\mathbb{P}_{n-1}) + 1$. Then from (2.7) and (2.8), we have
$ABC\prod(\mathbb{P}_n^3) = (\frac{\sqrt{2}}{2})^6(\frac{2}{3})ABC\prod(\mathbb{P}_{n-1}) = (\frac{1}{12})ABC\prod(\mathbb{P}_{n-1})$
$GA\prod(\mathbb{P}_n^3) = (\frac{2\sqrt{6}}{5})^4 GA\prod(\mathbb{P}_{n-1})$

By the above three types of local arrangements, we have

$$\begin{aligned}
E_n^{ABC} &= \rho_1 ABC\prod(\mathbb{P}_n^1) + \rho_2 ABC\prod(\mathbb{P}_n^2) + (1-\rho_1-\rho_2)ABC\prod(\mathbb{P}_n^3)\\
&= \rho_1[ABC\prod(\mathbb{P}_{n-1})\frac{\sqrt{2}}{18}] + \rho_2[ABC\prod(\mathbb{P}_{n-1})\frac{1}{12}]\\
&+ (1-\rho_1-\rho_2)ABC\prod(\mathbb{P}_{n-1})\frac{1}{12}\\
&= ABC\prod(\mathbb{P}_{n-1})[\rho_1\frac{\sqrt{2}}{18} + \rho_2\frac{1}{12} + \frac{1}{12} - \rho_1\frac{1}{12} - \rho_2\frac{1}{12}]\\
&= ABC\prod(\mathbb{P}_{n-1})[\frac{3+\rho_1(2\sqrt{2}-3)}{36}] \qquad (2.9)
\end{aligned}$$

and also, we have

$$\begin{aligned}
E_n^{GA} &= \rho_1 GA\prod(\mathbb{P}_n^1) + \rho_2 GA\prod(\mathbb{P}_n^2) + (1-\rho_1-\rho_2)GA\prod(\mathbb{P}_n^3)\\
&= \rho_1(\frac{2\sqrt{6}}{5})^2 GA\prod(\mathbb{P}_{n-1}) + \rho_2(\frac{2\sqrt{6}}{5})^4 GA\prod(\mathbb{P}_{n-1})\\
&+ (1-\rho_1-\rho_2)(\frac{2\sqrt{6}}{5})^4 GA\prod(\mathbb{P}_{n-1})\\
&= GA\prod(\mathbb{P}_{n-1})\Big[(\frac{2\sqrt{6}}{5})^4 + \rho_1\{(\frac{2\sqrt{6}}{5})^2 - (\frac{2\sqrt{6}}{5})^4\}\Big] \qquad (2.10)
\end{aligned}$$

As $E[E_n] = E$, so apply E on Eqs (2.9) and (2.10), which gives the following:

$$E_n^{ABC} = E_{n-1}^{ABC}[\frac{3+\rho_1(2\sqrt{2}-3)}{36}]. \qquad (2.11)$$

$$E_n^{GA} = E_{n-1}^{GA}\Big[(\frac{2\sqrt{6}}{5})^4 + \rho_1\{(\frac{2\sqrt{6}}{5})^2 - (\frac{2\sqrt{6}}{5})^4\}\Big]. \qquad (2.12)$$

Solving the linear recurrence relation of Eqs (2.11) and (2.12) with the initial condition, we get our results and finish the proof. □

From Theorem 2, we noted that E_n^{ABC} and E_n^{GA} are polynomial in ρ_1 and asymptotic to n. It is easy to note that these indices can be computed for three special chains: meta $\overline{PM}_n = \mathbb{P}(n;0,1)$, para $\overline{PP}_n = \mathbb{P}(n;0,0)$, and ortho $\overline{PO}_n = \mathbb{P}(n;1,0)$ chains as shown in Figure 4.

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

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

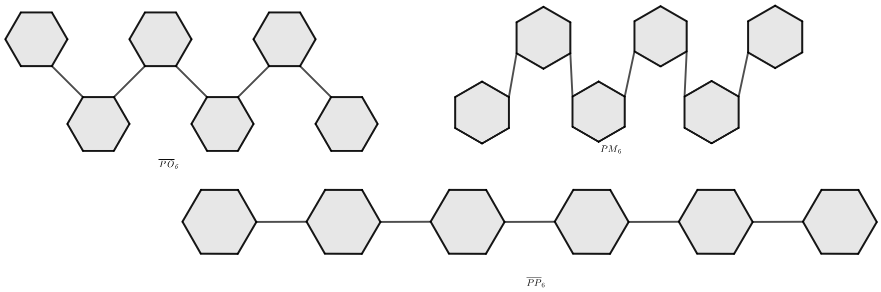

Figure 4. Special Polyphenyl ortho ($\overline{PO}_6$, meta $\overline{PM}_6$ and para $\overline{PP}_6$ chains).

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

A comparison between the expected values of multiplicative ABC and GA indices for these two types of random chains has been considered in this part. As an application of Theorems 1 and 2, an analytical and numerical comparison (see Tables 1–8) between the expected values for these indices of a random spiro and random polyphenyl chains has been outlined. Moreover, Figures 5 and 6 gives the comparison of both indices. The following lemma is easy to prove by induction, we omit its proof.

Lemma 1. *For all $n \geq 2$, we have*

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

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

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

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

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

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

□

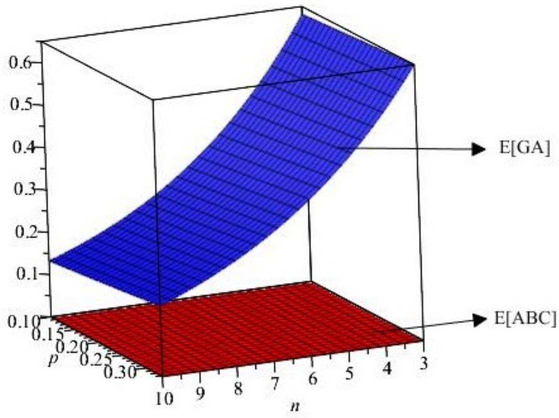

Figure 5. Comparison between E[ABC] and E[GA] in random polyphenyl chain.

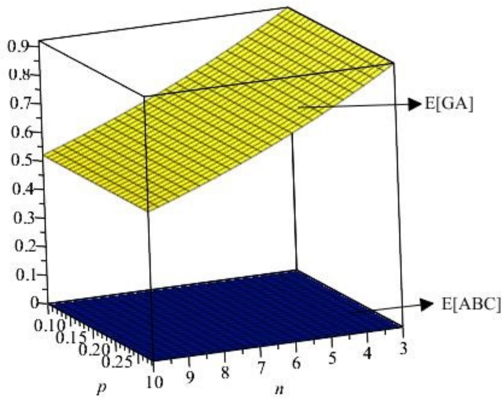

Figure 6. Comparison between E[ABC] and E[GA] in random spiro chain.

Table 1. For probability $\rho_1 = 0$.

n	$E_n^{ABC}(\mathbb{S}_n)$	$E_n^{GA}(\mathbb{S}_n)$
2	0.015625	0.790123457
3	0.001953125	0.624295077
4	0.000244141	0.493270184
5	3.05176×10^{-5}	0.389744343
6	3.8147×10^{-6}	0.307946148
7	4.76837×10^{-7}	0.243315475
8	5.96046×10^{-8}	0.192249264
9	7.45058×10^{-9}	0.151900653
10	9.31323×10^{-10}	0.120020269

Theorem 4. *For $n \geq 2$, we have*

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

Proof. When $n > 2$, by Theorem 2, we have

$$\begin{aligned} & E[GA\prod(\mathbb{P}(n;\rho_1,\rho_2))] - E[ABC\prod(\mathbb{P}(n;\rho_1,\rho_2))] \\ = & (\frac{24}{25})^2\Big[\frac{24}{25^2}(24+\rho_1)\Big]^{n-2} - \frac{[3+\rho_1(2\sqrt{2}-3)]^{n-2}}{2^{2n+1}3^{2n-3}} \\ = & (\frac{24}{25})^n - \frac{(\sqrt{2})^{n-2}}{2^{n+3}3^{2n-3}} \quad \because 0 \leq \rho_1 \leq 1 \\ = & (\sqrt{2})^{n-2}\Big[\frac{4^n(\sqrt{2})^{n+2}3^n}{5^{2n}} - \frac{1}{2^{n+3}3^{2n-3}}\Big] \\ = & (\sqrt{2})^{n-2}\Big[2(\frac{12\sqrt{2}}{25})^n - \frac{1}{2^{n+3}3^{2n-3}}\Big] > 0 \end{aligned}$$

□

Table 2. For probability $\rho_1 = 1/2$.

n	$E_n^{ABC}(\mathbb{S}_n)$	$E_n^{GA}(\mathbb{S}_n)$
2	0.015625	0.790123457
3	0.00182229	3.784788904
4	0.000212528	18.12960611
5	2.47864×10^{-5}	86.84305148
6	2.89075×10^{-6}	415.988938
7	3.37138×10^{-7}	1992.63837
8	3.93193×10^{-8}	9544.983795
9	4.58567×10^{-9}	45721.65077
10	5.34811×10^{-10}	219012.3518

Table 3. For probability $\rho_1 = 1/3$.

n	$E_n^{ABC}(\mathbb{S}_n)$	$E_n^{GA}(\mathbb{S}_n)$
2	0.015625	0.790123457
3	0.001865902	2.731290962
4	0.000222822	9.441499621
5	2.66089×10^{-5}	32.63728264
6	3.17757×10^{-6}	112.8202363
7	3.79458×10^{-7}	389.9958785
8	4.5314×10^{-8}	1348.133901
9	5.4113×10^{-9}	4660.215954
10	6.46205×10^{-10}	16109.38848

Table 4. For probability $\rho_1 = 1$.

n	$E_n^{ABC}(\mathbb{S}_n)$	$E_n^{GA}(\mathbb{S}_n)$
2	0.015625	0.790123457
3	0.001691456	6.945282731
4	0.000183105	61.04989265
5	1.98217×10^{-5}	536.6360934
6	2.14577×10^{-6}	4717.097513
7	2.32286×10^{-7}	41463.86949
8	2.51457×10^{-8}	364472.5318
9	2.7221×10^{-9}	3203758.551
10	2.94676×10^{-10}	28161433.19

From Tables 1–4, we can note that the expected value of the GA index is greater than ABC index for spiro chain.

Table 5. For probability $\rho_1 = 0$.

n	$E_n^{ABC}(\mathbb{P}_n)$	$E_n^{GA}(\mathbb{P}_n)$
2	0.010416667	0.9216
3	0.000868056	0.84934656
4	7.2338×10^{-5}	0.78275779
5	6.02816×10^{-6}	0.721389579
6	5.02347×10^{-7}	0.664832636
7	4.18622×10^{-8}	0.612709757
8	3.48852×10^{-9}	0.564673312
9	2.9071×10^{-10}	0.520402925
10	2.42258×10^{-11}	0.479603335

Table 6. For probability $\rho_1 = 1/2$.

n	$E_n^{ABC}(\mathbb{P}_n)$	$E_n^{GA}(\mathbb{P}_n)$
2	0.010416667	0.9216
3	0.000843233	0.86704128
4	6.826×10^{-5}	0.815712436
5	5.52568×10^{-6}	0.76742226
6	4.47306×10^{-7}	0.721990862
7	3.62096×10^{-8}	0.679249003
8	2.93118×10^{-9}	0.639037462
9	2.3728×10^{-10}	0.601206444
10	1.92079×10^{-11}	0.565615023

Table 7. For probability $\rho_1 = 1/3$.

n	$E_n^{ABC}(\mathbb{P}_n)$	$E_n^{GA}(\mathbb{P}_n)$
2	0.010416667	0.9216
3	0.000851507	0.86114304
4	6.96062×10^{-5}	0.804652057
5	5.68994×10^{-6}	0.751866882
6	4.65122×10^{-7}	0.702544414
7	3.80213×10^{-8}	0.656457501
8	3.10804×10^{-9}	0.613393889
9	2.54066×10^{-10}	0.57315525
10	2.07685×10^{-11}	0.535556265

Table 8. For probability $\rho_1 = 1$.

n	$E_n^{ABC}(\mathbb{P}_n)$	$E_n^{GA}(\mathbb{P}_n)$
2	0.010416667	0.9216
3	0.000818411	0.884736
4	6.43004×10^{-5}	0.84934656
5	5.05192×10^{-6}	0.815372698
6	3.96916×10^{-7}	0.78275779
7	3.11847×10^{-8}	0.751447478
8	2.4501×10^{-9}	0.721389579
9	1.92498×10^{-10}	0.692533996
10	1.51241×10^{-11}	0.664832636

From Tables 5–8, we can note that the expected value of the GA index is greater than ABC index for polyphenyl chain $\mathbb{P}_n$.

3.1. The average value of multiplicative ABC and GA for a random and spiro chains

In order to compute the average values of aforementioned indices over the set of all spiro chains $\mathbb{S}(n, \rho_1, \rho_2)$ of order n, which will be denoted by $\mathbb{SS}_n$. The average values over the set $\mathbb{SS}_n$ are defined by

$$ABC_{ave}\prod(\mathbb{SS}_n) = \frac{1}{|\mathbb{SS}_n|}\sum_{\Gamma\in\mathbb{SS}_n} ABC\prod(\Gamma)$$

and

$$GA_{ave}\prod(\mathbb{SS}_n) = \frac{1}{|\mathbb{SS}_n|}\sum_{\Gamma\in\mathbb{SS}_n} GA\prod(\Gamma)$$

respectively. It is easy to see that these are the population means of these indices over all elements in $\mathbb{SS}_n$ that is $\rho_1 = \rho_2 = 1 - \rho_1 - \rho_2$¿ Hence by putting $\rho_1 = \rho_2 = 1 - \rho_1 - \rho_2 = \frac{1}{3}$ in Theorem 1 we, will get the following result.

Theorem 5. *If $\mathbb{SS}_n$ is the set of spiro chains, then*

$$ABC_{ave}\prod(\mathbb{SS}_n) = \frac{(\frac{\sqrt{3}+4}{3})^{n-2}}{2^{4n-2}}.$$

$$GA_{ave}\prod(\mathbb{SS}_n) = 5^{2n-4} * \frac{2^{3n}}{3^{5n-1}}.$$

It is easy to see from Corollary 2, we have

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

and

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

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 these aforementioned indices is always greater or equal to their average value over the set $\{PO_n, PP_n, PM_n\}$ of three special chains.

4. Conclusions

The multiplicative ABC and GA indices have been considered in the following article. We also determine the expected values, and give a comparison of the expected values of both indices in random polyphenyl and spiro chains. The results of these calculations have potential opportunities in many engineering states. Particularly, the related theories gives the mathematical features in reverse engineering and explicit values of compounds with extraordinary compound attributes. Therefore far the values are concerned, the basic features of the compound are concluded from the topological index that provides a theoretical point for the synthesis of drug investigation, great materials, and extraordinary chemical substances. In addition, we make it clear that the estimation model described in the current article takes many limitations in the chemical field. For instance, hexagonal and spiro structures typically appear in different polybenzene arrangements. Although the stability of polybenzene arrangements has been dictated through its absolute arrangement. Furthermore, steric impact, e.g., steric hindrance, assumes a vital part in computing the overall steadiness of orth, meta, and para isomers. Subsequently, the final structural arrangement of such a hexagonal chain is not random in general. Steric limitations prevent the final arrangement of cycloalkane chains. Thus, more research is required on how to describe the chemical structure of odors and oppressive barriers.

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Conflict of interest

The authors declare there is no conflict of interest.

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