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Comparing the expected values of atom-bond connectivity and geometric–arithmetic indices in random spiro chains

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Abstract

The atom-bond connectivity (*ABC*) index and geometric–arithmetic (*GA*) index are two well-studied topological indices, which are useful tools in QSPR and QSAR investigations. In this paper, we first obtain explicit formulae for the expected values of *ABC* and *GA* indices in random spiro chains, which are graphs of a class of unbranched polycyclic aromatic hydrocarbons. Based on these formulae, we then present the average values of *ABC* and *GA* indices with respect to the set of all spiro chains with *n* hexagons and make a comparison between the expected values of *ABC* and *GA* indices in random spiro chains.

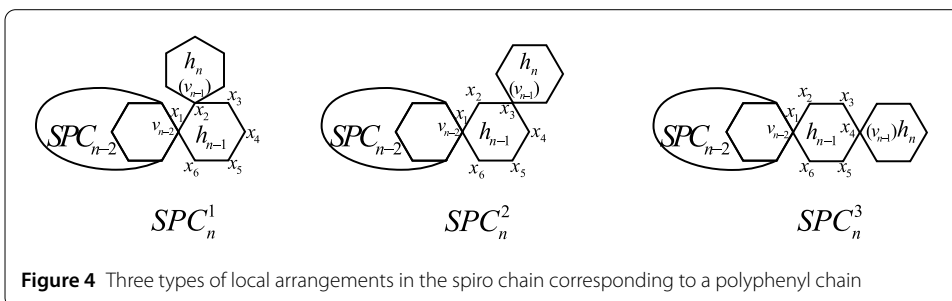
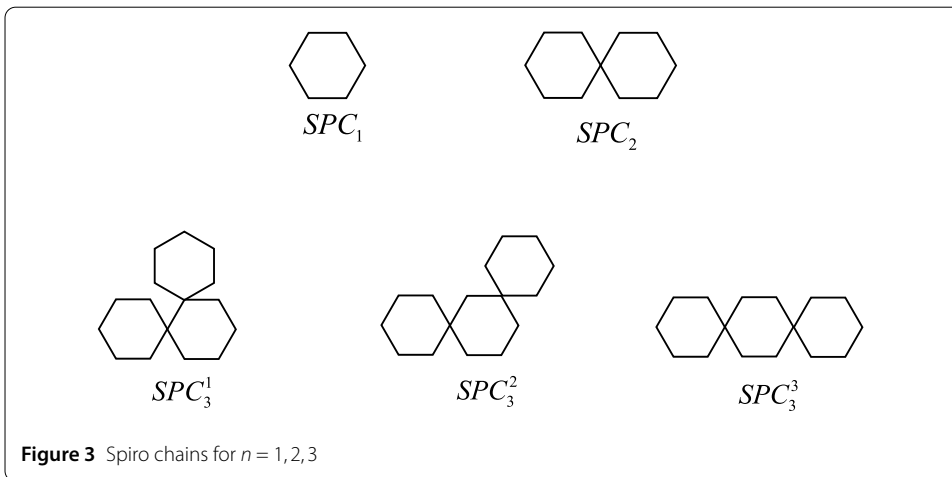
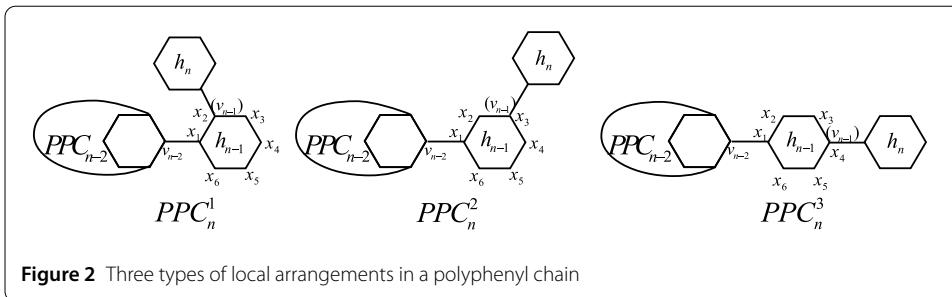
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1 Introduction

A connected graph with maximum vertex degree at most 4 is said to be a *molecular graph*. Its graphical representation may resemble a structural formula of some (usually organic) molecule. That was a primary reason for employing graph theory in chemistry. Nowadays this area of mathematical chemistry is called *chemical graph theory* [1]. Molecular descriptors play a significant role and have found wide applications in chemical graph theory especially in investigations of the quantitative structure–property relations (QSPR) and quantitative structure–activity relations (QSAR). Among them, topological indices have a prominent place [2]. There exists a legion of topological indices that have some applications in chemistry [2, 3]. One of the best known and widely used topological indices is the connectivity index (Randić index) introduced in 1975 by Randić [4], who has shown that this index can reflect molecular branching. Some results on molecular branching can be found in [5–9] and the references therein. However, many physico-chemical properties depend on factors rather different from branching.

All graphs considered in this paper are simple, undirected, and connected. The notation not defined in this paper can be found in the book [10]. Let *G* be a graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. Denote by d_i the degree of the vertex v_i in *G*. If an



A spiro chain of length n , denoted SPC_n , can be obtained from a polyphenyl chain PPC_n by contracting each cut edge between each pair of consecutive hexagons in PPC_n . Figure 3 shows the unique spiro chains for $n = 1, 2$ and all spiro chains for $n = 3$, and Figure 1(b) shows a general case, where v_{n-1} is a vertex of h_{n-1} in SPC_{n-1} . Similarly to the construction of a polyphenyl chain PPC_n , it is clear that SPC_n is also not unique when $n \geq 3$ and has three types of local arrangements, which are denoted by $SPC_n^1, SPC_n^2,$ and SPC_n^3 (Figure 4). We may assume that getting an SPC_n from a fixed SPC_{n-1} is a random process. Namely, the probabilities of getting $SPC_n^1, SPC_n^2,$ and SPC_n^3 from a fixed SPC_{n-1} are $p_1, p_2,$ and $1 - p_1 - p_2$, respectively. We also assume that the probabilities p_1 and p_2 are constants and independent of n , that is, the process described is a zeroth-order Markov process. After associating probabilities, such a spiro chain is called a *random spiro chain* and denoted by $SPC(n; p_1, p_2)$. For some contributions on spiro chains, the readers are referred to [27, 28, 33–35]. In 2015, Huang et al. [30] considered the expected value of the Kirchhoff index

in a random spiro chain. For more results concerning other random chains, we refer to [36–42] and the references therein.

The rest of this paper is organized as follows. In Section 2, we present explicit formulae for the expected values of the *ABC* and *GA* indices of random spiro chains. Based on these formulae, we then give the average values of the *ABC* and *GA* indices with respect to the set of all spiro chains with n hexagons in Section 3 and make a comparison between the expected values of the *ABC* and *GA* indices in random spiro chains in Section 4.

2 The *ABC* and *GA* indices in random spiro chains

In this section, we consider the *ABC* and *GA* indices in a random spiro chain. We keep the notation defined in Section 1. Let SPC_n be the spiro chain obtained by attaching a new hexagon h_n to SPC_{n-1} as described in Figure 1(b). Assume that $h_n = x_1x_2x_3x_4x_5x_6$ as shown in Figure 2. Clearly, there are only (2, 2)-, (2, 4)-, and (4, 4)-edges in a spiro chain SPC_n . By the definitions of the *ABC* and *GA* indices we can directly check that

$$ABC(SPC_n) = \frac{\sqrt{2}}{2}m_{22}(SPC_n) + \frac{\sqrt{2}}{2}m_{24}(SPC_n) + \frac{\sqrt{6}}{4}m_{44}(SPC_n) \tag{3}$$

and

$$GA(SPC_n) = m_{22}(SPC_n) + \frac{2\sqrt{2}}{3}m_{24}(SPC_n) + m_{44}(SPC_n). \tag{4}$$

Thus, to compute the *ABC* and *GA* indices of SPC_n , we just need to determine $m_{22}(SPC_n)$, $m_{24}(SPC_n)$, and $m_{44}(SPC_n)$.

Recall that $SPC(n; p_1, p_2)$ is a random spiro chain of length n . Clearly, both $ABC(SPC(n; p_1, p_2))$ and $GA(SPC(n; p_1, p_2))$ are random variables. For convenience, denote their expected values by $E_n^a = E[ABC(SPC(n; p_1, p_2))]$ and $E_n^g = E[GA(SPC(n; p_1, p_2))]$, respectively.

We first give a formula for the expected value of the *ABC* index of a random spiro chain.

Theorem 2.1 *Let $SPC(n; p_1, p_2)$ be a random spiro chain of length $n \geq 1$. Then*

$$E[ABC(SPC(n; p_1, p_2))] = \left[\left(\frac{\sqrt{6}}{4} - \frac{\sqrt{2}}{2} \right) p_1 + 3\sqrt{2} \right] n + \left(\frac{\sqrt{2}}{2} - \frac{\sqrt{6}}{4} \right) p_1.$$

Proof When $n = 1$, there is only one hexagon. So $E_1^a = 6 \times \frac{\sqrt{2}}{2} = 3\sqrt{2}$.

When $n \geq 2$, it is obvious that $m_{22}(SPC_n)$, $m_{24}(SPC_n)$, and $m_{44}(SPC_n)$ depend on the three possible constructions as shown in Figure 3.

(i) If $SPC_{n-1} \rightarrow SPC_n^1$ with probability p_1 , then we have

$$m_{22}(SPC_n^1) = m_{22}(SPC_{n-1}) + 3, m_{24}(SPC_n^1) = m_{24}(SPC_{n-1}) + 2$$

and

$$m_{44}(SPC_n^1) = m_{44}(SPC_{n-1}) + 1.$$

Therefore by (3) we have

$$ABC(SPC_n^1) = ABC(SPC_{n-1}) + \frac{5\sqrt{2}}{2} + \frac{\sqrt{6}}{4}.$$

(ii) If $SPC_{n-1} \rightarrow SPC_n^2$ with probability p_2 , then we have

$$m_{22}(SPC_n^2) = m_{22}(SPC_{n-1}) + 2, m_{24}(SPC_n^2) = m_{24}(SPC_{n-1}) + 4$$

and

$$m_{44}(SPC_n^2) = m_{44}(SPC_{n-1}).$$

Therefore by (3) we have

$$ABC(SPC_n^2) = ABC(SPC_{n-1}) + 3\sqrt{2}.$$

(iii) If $SPC_{n-1} \rightarrow SPC_n^3$ with probability $1 - p_1 - p_2$, then we have

$$m_{22}(SPC_n^3) = m_{22}(SPC_{n-1}) + 2, m_{24}(SPC_n^3) = m_{24}(SPC_{n-1}) + 4$$

and

$$m_{44}(SPC_n^3) = m_{44}(SPC_{n-1}).$$

Therefore by (3) we have

$$ABC(SPC_n^3) = ABC(SPC_{n-1}) + 3\sqrt{2}.$$

Thus we obtain

$$\begin{aligned} E_n^a &= E[ABC(SPC(n, p_1, p_2))] \\ &= p_1 ABC(SPC_n^1) + p_2 ABC(SPC_n^2) + (1 - p_1 - p_2) ABC(SPC_n^3) \\ &= ABC(SPC_{n-1}) + \left(\frac{\sqrt{6}}{4} - \frac{\sqrt{2}}{2}\right) p_1 + 3\sqrt{2}. \end{aligned}$$

Note that $E[E_n^a] = E_n^a$. Applying the expectation operator to the last equation, we get

$$E_n^a = E_{n-1}^a + \left(\frac{\sqrt{6}}{4} - \frac{\sqrt{2}}{2}\right) p_1 + 3\sqrt{2} \quad \text{for } n \geq 2. \tag{5}$$

Since equation (5) is a first-order nonhomogeneous linear difference equation with constant coefficients. It is clear that the general solution of the homogeneous part of equation (5) is $E^a = c$, a constant.

Let $E^{a*} = an$ be a particular solution of equation (5). Substituting E^{a*} into equation (5) and comparing the constant term, we have

$$a = \left(\frac{\sqrt{6}}{4} - \frac{\sqrt{2}}{2}\right) p_1 + 3\sqrt{2}.$$

Consequently, the general solution of equation (5) is

$$E_n^a = E^{a*} + E^a = E[ABC(SPC(n; p_1, p_2))] = \left[\left(\frac{\sqrt{6}}{4} - \frac{\sqrt{2}}{2}\right) p_1 + 3\sqrt{2}\right] n + C \quad \text{for } n \geq 1.$$

Substituting the initial condition, we obtain

$$C = \left(\frac{\sqrt{2}}{2} - \frac{\sqrt{6}}{4} \right) p_1.$$

Therefore we have

$$E_n^a = \left[\left(\frac{\sqrt{6}}{4} - \frac{\sqrt{2}}{2} \right) p_1 + 3\sqrt{2} \right] n + \left(\frac{\sqrt{2}}{2} - \frac{\sqrt{6}}{4} \right) p_1.$$

This completes the proof. □

We now give the formula for the expected value of the GA index of a random spiro chain.

Theorem 2.2 *Let $SPC(n; p_1, p_2)$ be a random spiro chain of length $n \geq 1$. Then*

$$E[GA(SPC(n; p_1, p_2))] = \left[\left(2 - \frac{4\sqrt{2}}{3} \right) p_1 + 2 + \frac{8\sqrt{2}}{3} \right] n + \left(\frac{4\sqrt{2}}{3} - 2 \right) p_1 + \left(4 - \frac{8\sqrt{2}}{3} \right).$$

Proof When $n = 1$, there is only one hexagon. So $E_1^g = E[GA(SPC(1; p_1, p_2))] = 6$.

When $n \geq 2$, it is obvious that $m_{22}(SPC_n)$, $m_{24}(SPC_n)$, and $m_{44}(SPC_n)$ depend on the three possible constructions as shown in Figure 3.

(i) If $SPC_{n-1} \rightarrow SPC_n^1$ with probability p_1 , then we get

$$m_{22}(SPC_n^1) = m_{22}(SPC_{n-1}) + 3, m_{24}(SPC_n^1) = m_{24}(SPC_{n-1}) + 2$$

and

$$m_{44}(SPC_n^1) = m_{44}(SPC_{n-1}) + 1.$$

Therefore by (4) we have

$$GA(SPC_n^1) = GA(SPC_{n-1}) + 4 + \frac{4\sqrt{2}}{3}.$$

(ii) If $SPC_{n-1} \rightarrow SPC_n^2$ with probability p_2 , then we get

$$m_{22}(SPC_n^2) = m_{22}(SPC_{n-1}) + 2, m_{24}(SPC_n^2) = m_{24}(SPC_{n-1}) + 4$$

and

$$m_{44}(SPC_n^2) = m_{44}(SPC_{n-1}).$$

Therefore by (4) we have

$$GA(SPC_n^2) = GA(SPC_{n-1}) + 2 + \frac{8\sqrt{2}}{3}.$$

(iii) If $SPC_{n-1} \rightarrow SPC_n^3$ with probability $1 - p_1 - p_2$, then we have

$$m_{22}(SPC_n^3) = m_{22}(SPC_{n-1}) + 2, m_{24}(SPC_n^3) = m_{24}(SPC_{n-1}) + 4$$

and

$$m_{44}(SPC_n^3) = m_{44}(SPC_{n-1}).$$

Therefore by (4) we have

$$GA(SPC_n^3) = GA(SPC_{n-1}) + 2 + \frac{8\sqrt{2}}{3}.$$

Thus we obtain

$$\begin{aligned} E_n^g &= E[GA(SPC(n, p_1, p_2))] \\ &= p_1 GA(SPC_n^1) + p_2 GA(SPC_n^2) + (1 - p_1 - p_2) GA(SPC_n^3) \\ &= GA(SPC_{n-1}) + \left(2 - \frac{4\sqrt{2}}{3}\right)p_1 + \left(2 + \frac{8\sqrt{2}}{3}\right). \end{aligned}$$

Note that $E[E_n^g] = E_n^g$. Applying the expectation operator to the last equation, we get

$$E_n^g = E_{n-1}^g + \left(2 - \frac{4\sqrt{2}}{3}\right)p_1 + \left(2 + \frac{8\sqrt{2}}{3}\right), \quad \text{for } n \geq 2. \tag{6}$$

Since equation (6) is a first-order nonhomogeneous linear difference equation with constant coefficients, it is clear that the general solution of the homogeneous part of equation (6) is $E^g = c$, a constant.

Let $E^{g*} = an$ be a particular solution of equation (6). Substituting E^{g*} into equation (6) and comparing the constant term, we have

$$a = \left(2 - \frac{4\sqrt{2}}{3}\right)p_1 + \left(2 + \frac{8\sqrt{2}}{3}\right).$$

Consequently, the general solution of equation (6) is

$$\begin{aligned} E_n^g &= E^{g*} + E^g = E[GA(SPC(n; p_1, p_2))] \\ &= \left[\left(2 - \frac{4\sqrt{2}}{3}\right)p_1 + \left(2 + \frac{8\sqrt{2}}{3}\right)\right]n + C \quad \text{for } n \geq 1. \end{aligned}$$

Substituting the initial condition, we obtain

$$C = \left(\frac{4\sqrt{2}}{3} - 2\right)p_1 + \left(4 - \frac{8\sqrt{2}}{3}\right).$$

Therefore we have

$$E_n^g = \left[\left(2 - \frac{4\sqrt{2}}{3}\right)p_1 + \left(2 + \frac{8\sqrt{2}}{3}\right)\right]n + \left(\frac{4\sqrt{2}}{3} - 2\right)p_1 + \left(4 - \frac{8\sqrt{2}}{3}\right),$$

and the proof is completed. □

In Theorems 2.1 and 2.2, we observe that both $E[ABC(SPC(n; p_1, p_2))]$ and $E[GA(SPC(n; p_1, p_2))]$ are asymptotic to n and linear in p_1 . Therefore, by Theorems 2.1 and 2.2 we can easily obtain the ABC and GA indices of spiro meta-chain O_n , spiro orth-chain M_n , and spiro para-chain P_n (defined in [30]).

Corollary 2.3 *The ABC indices of the spiro meta-chain O_n , the spiro orth-chain M_n , and the spiro para-chain P_n are*

$$ABC(O_n) = \left(\frac{\sqrt{6}}{4} + \frac{5\sqrt{2}}{2}\right)n + \frac{\sqrt{2}}{2} - \frac{\sqrt{6}}{4}$$

and

$$ABC(M_n) = ABC(P_n) = 3\sqrt{2}n.$$

Corollary 2.4 *The GA indices of the spiro meta-chain O_n , the spiro orth-chain M_n , and the spiro para-chain P_n are*

$$GA(O_n) = \left(4 + \frac{4\sqrt{2}}{3}\right)n + 2 - \frac{4\sqrt{2}}{3}$$

and

$$GA(M_n) = GA(P_n) = \left(2 + \frac{8\sqrt{2}}{3}\right)n + 4 - \frac{8\sqrt{2}}{3}.$$

3 The average values of ABC and GA indices

In this section, we present the average values of the ABC and GA indices with respect to the set of all spiro chains with n hexagons.

Let \mathcal{SP}_n be the set of all spiro chains with n hexagons. The average values of the ABC and GA indices of \mathcal{SP}_n are defined by

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

and

$$GA_{\text{avr}}(\mathcal{SP}_n) = \frac{1}{|\mathcal{SP}_n|} \sum_{G \in \mathcal{SP}_n} GA(G),$$

respectively. In fact, this is the population mean of the ABC and GA indices of all elements in \mathcal{SP}_n . Since every element occurring in \mathcal{SP}_n has the same probability, we have $p_1 = p_2 = 1 - p_1 - p_2$. Thus we can apply Theorems 2.1 and 2.2 by putting $p_1 = p_2 = 1 - p_1 - p_2 = \frac{1}{3}$ and obtain the following result.

Theorem 3.1 *The average values of the ABC and GA indices with respect to \mathcal{SP}_n are*

$$ABC_{\text{avr}}(\mathcal{SP}_n) = \left(\frac{\sqrt{6}}{12} + \frac{17\sqrt{2}}{6}\right)n + \frac{\sqrt{2}}{6} - \frac{\sqrt{6}}{12}$$

and

$$GA_{avr}(\mathcal{S}\mathcal{P}_n) = \left(\frac{8}{3} + \frac{20\sqrt{2}}{9}\right)n + \frac{10}{3} - \frac{20\sqrt{2}}{9}.$$

From Theorem 3.1, as well as from Corollaries 2.3 and 2.4, it is no difficult to see that the average values of the *ABC* and *GA* indices with respect to $\{O_n, M_n, P_n\}$ are

$$\frac{ABC(O_n) + ABC(M_n) + ABC(P_n)}{3} = \left(\frac{\sqrt{6}}{12} + \frac{17\sqrt{2}}{6}\right)n + \frac{\sqrt{2}}{6} - \frac{\sqrt{6}}{12}$$

and

$$\frac{GA(O_n) + GA(M_n) + GA(P_n)}{3} = \left(\frac{8}{3} + \frac{20\sqrt{2}}{9}\right)n + \frac{10}{3} - \frac{20\sqrt{2}}{9},$$

which indicate that the average values of the *ABC* and *GA* indices with respect to $\mathcal{S}\mathcal{P}_n$ are exactly equal to the average values of the *ABC* and *GA* indices with respect to $\{O_n, M_n, P_n\}$, respectively.

4 A comparison between the expected values of *ABC* and *GA* indices

Das and Trinajstić [15] compared the first *GA* index and *ABC* index for chemical trees, molecular graphs, and simple graphs with some restricted conditions. Recently, Ke [40] also compared the expected values of the *GA* index and *ABC* index for a random polyphenyl chain. Using Theorems 2.1 and 2.2, we now make a comparison between the expected values for the *ABC* and *GA* indices of a random spiro chain with the same probability p_i ($i = 1, 2$).

Theorem 4.1 *Let $SPC(n; p_1, p_2)$ be a random spiro chain with n hexagons. Then*

$$E[GA(SPC(n; p_1, p_2))] > E[ABC(SPC(n; p_1, p_2))].$$

Proof When $n = 1$, it is clear that

$$E[GA(SPC(1; p_1, p_2))] = 6 > 3\sqrt{2} = E[ABC(SPC(1; p_1, p_2))].$$

When $n \geq 2$, by Theorems 2.1 and 2.2 we have

$$\begin{aligned} & E[GA(SPC(n; p_1, p_2))] - E[ABC(SPC(n; p_1, p_2))] \\ &= \left[\left(2 - \frac{\sqrt{6}}{4} - \frac{4\sqrt{2}}{3} + \frac{\sqrt{2}}{2} \right) p_1 + 2 + \frac{8\sqrt{2}}{3} - 3\sqrt{2} \right] n \\ & \quad + \left(\frac{4\sqrt{2}}{3} - 2 - \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} \right) p_1 + 4 - \frac{8\sqrt{2}}{3}. \end{aligned}$$

Noting that $2 - \frac{\sqrt{6}}{4} - \frac{4\sqrt{2}}{3} + \frac{\sqrt{2}}{2} > 0$ and $0 \leq p_1 \leq 1$, we get

$$\begin{aligned} & E[GA(SPC(n; p_1, p_2))] - E[ABC(SPC(n; p_1, p_2))] \\ & \geq \left(2 + \frac{8\sqrt{2}}{3} - 3\sqrt{2}\right)n + \left(\frac{4\sqrt{2}}{3} - 2 - \frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4}\right) \times 1 + 4 - \frac{8\sqrt{2}}{3} \\ & = \left(2 - \frac{\sqrt{2}}{3}\right)n + 2 + \frac{\sqrt{6}}{4} - \frac{11\sqrt{2}}{6} \\ & \geq \left(2 - \frac{\sqrt{2}}{3}\right) \times 2 + 2 + \frac{\sqrt{6}}{4} - \frac{11\sqrt{2}}{6} \\ & > 0, \end{aligned}$$

as desired. This completes the proof. \square

Theorem 4.1 states that the expected value of the *ABC* index is less than the expected value of the *GA* index for a random spiro chain, which is similar to the result for a random polyphenyl chain [40].

5 Conclusions

In this paper, we mainly study the *ABC* and *GA* indices in random spiro chains. Firstly, we study explicit formulae for the expected values of the *ABC* and *GA* indices in random spiro chains, similar to the results obtained in [30, 33]. Secondly, we present the average values of the *ABC* and *GA* indices with respect to the set of all spiro chains with n hexagons. Finally, we compare the expected values of the *ABC* and *GA* indices in random spiro chains and show that the expected value of the *ABC* index is less than the expected value of the *GA* index.

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Competing interests

The authors declare that they have no competing interests.

Authors' contributions

SW carried out the proofs of the main results in the manuscript. XK and GH participated in the design of the study and drafted the manuscript. All the authors read and approved the final manuscript.

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References

1. Trinajstić, N.: *Chemical Graph Theory*. CRC Press, Boca Raton (1983)
2. Todeschini, R., Consonni, V.: *Handbook of Molecular Descriptors*. Wiley-VCH, Weinheim (2000)
3. Todeschini, R., Consonni, V.: *Molecular Descriptors for Chemoinformatics*. Wiley-VCH, Weinheim (2009)
4. Randić, M.: On characterization of molecular branching. *J. Am. Chem. Soc.* **97**, 6609–6615 (1975)

5. Gutman, I., Vukičević, D., Žerovnik, J.: A class of modified Wiener indices. *Croat. Chem. Acta* **77**, 103–109 (2004)
6. Vukičević, D.: Distinction between modifications of Wiener indices. *MATCH Commun. Math. Comput. Chem.* **47**, 87–105 (2003)
7. Vukičević, D., Gutman, I.: Note on a class of modified Wiener indices. *MATCH Commun. Math. Comput. Chem.* **47**, 107–117 (2003)
8. Vukičević, D., Žerovnik, J.: Variable Wiener indices. *MATCH Commun. Math. Comput. Chem.* **53**, 385–402 (2005)
9. Vukičević, D., Žerovnik, J.: New indices based on the modified Wiener indices. *MATCH Commun. Math. Comput. Chem.* **60**, 119–132 (2008)
10. Bondy, J.A., Murty, U.S.R.: *Graph Theory with Applications*. MacMillan, New York (1976)
11. Estrada, E., Torres, L., Rodríguez, L., Gutman, I.: An atom-bond connectivity index: modelling the enthalpy of formation of alkanes. *Indian J. Chem.* **37A**, 849–855 (1998)
12. Estrada, E.: Atom-bond connectivity and the energetic of branched alkanes. *Chem. Phys. Lett.* **463**, 422–425 (2008)
13. Chen, J., Guo, X.: Extreme atom-bond connectivity index of graphs. *MATCH Commun. Math. Comput. Chem.* **65**, 713–722 (2011)
14. Das, K.C.: Atom-bond connectivity index of graphs. *Discrete Appl. Math.* **158**, 1181–1188 (2010)
15. Das, K.C., Trinajstić, N.: Comparison between first geometric–arithmetic index and atom-bond connectivity index. *Chem. Phys. Lett.* **497**, 149–151 (2010)
16. Ke, X.: Atom-bond connectivity index of benzenoid systems and fluoranthene congeners. *Polycycl. Aromat. Compd.* **32**, 27–35 (2012)
17. Furtula, B., Graovac, A., Vukičević, D.: Atom-bond connectivity index of trees. *Discrete Appl. Math.* **157**, 2828–2835 (2009)
18. Vukičević, D., Furtula, B.: Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. *J. Math. Chem.* **46**, 1369–1376 (2009)
19. Das, K.C.: On geometric–arithmetic index of graphs. *MATCH Commun. Math. Comput. Chem.* **64**(3), 619–630 (2010)
20. Divnić, T., Milivojević, M., Pavlović, L.: Extremal graphs for the geometric–arithmetic index with given minimum degree. *Discrete Appl. Math.* **162**, 386–390 (2014)
21. Rodríguez, J.M., Sigarreta, J.M.: Spectral properties of geometric–arithmetic index. *Appl. Math. Comput.* **277**, 142–153 (2016)
22. Yuan, Y., Zhou, B., Trinajstić, N.: On geometric–arithmetic index. *J. Math. Chem.* **47**, 833–841 (2010)
23. Zhou, B., Gutman, I., Furtula, B., Du, Z.: On two types of geometric–arithmetic index. *Chem. Phys. Lett.* **482**, 153–155 (2009)
24. Flower, D.R.: On the properties of bit string-based measures of chemical similarity. *J. Chem. Inf. Comput. Sci.* **38**, 379–386 (1998)
25. Li, Q.R., Yang, Q., Yin, H., Yang, S.: Analysis of by-products from improved Ullmann reaction using TOFMS and GC/TOFMS. *J. Univ. Sci. Technol. China* **34**, 335–341 (2004)
26. Tepavčević, S., Wroble, A.T., Bissen, M., Wallace, D.J., Choi, Y., Hanley, L.: Photoemission studies of polythiophene and polyphenyl films produced via surface polymerization by ion-assisted deposition. *J. Phys. Chem. B* **109**, 7134–7140 (2005)
27. Deng, H.: Wiener indices of spiro and polyphenyl hexagonal chains. *Math. Comput. Model.* **55**, 634–644 (2012)
28. Deng, H., Tang, Z.: Kirchhoff indices of spiro and polyphenyl hexagonal chains. *Util. Math.* **95**, 113–128 (2014)
29. Došlić, T., Litz, M.S.: Matchings and independent sets in polyphenylene chains. *MATCH Commun. Math. Comput. Chem.* **67**, 313–330 (2012)
30. Huang, G., Kuang, M., Deng, H.: The expected values of Kirchhoff indices in the random polyphenyl and spiro chains. *Ars Math. Contemp.* **9**, 197–207 (2015)
31. Huang, G., Kuang, M., Deng, H.: The expected values of Hosoya index and Merrifield–Simmons index in a random polyphenylene chain. *J. Comb. Optim.* **32**, 550–562 (2016)
32. Yang, W., Zhang, F.: Wiener index in random polyphenyl chains. *MATCH Commun. Math. Comput. Chem.* **68**, 371–376 (2012)
33. Chen, X., Zhao, B., Zhao, P.: Six-membered ring spiro chains with extremal Merrifield–Simmons index and Hosoya index. *MATCH Commun. Math. Comput. Chem.* **62**, 657–665 (2009)
34. Yang, Y., Liu, H., Wang, H., Fu, H.: Subtrees of spiro and polyphenyl hexagonal chains. *Appl. Math. Comput.* **268**, 547–560 (2015)
35. Yang, Y., Liu, H., Wang, H., Sun, S.: On spiro and polyphenyl hexagonal chains with respect to the number of BC-subtrees. *Int. J. Comput. Math.* **94**(4), 774–799 (2017)
36. Chen, A., Zhang, F.: Wiener index and perfect matchings in random phenylene chains. *MATCH Commun. Math. Comput. Chem.* **61**, 623–630 (2009)
37. Gutman, I., Kennedy, J.W., Quintas, L.V.: Wiener numbers of random benzenoid chains. *Chem. Phys. Lett.* **173**, 403–408 (1990)
38. Gutman, I.: The number of perfect matchings in a random hexagonal chain. *Graph Theory Notes N. Y.* **16**, 26–28 (1989)
39. Gutman, I., Kennedy, J.W., Quintas, L.V.: Perfect matchings in random hexagonal chain graphs. *J. Math. Chem.* **6**, 377–383 (1991)
40. Ke, X.: Atom-bond connectivity and geometric–arithmetic indices in random polyphenyl chains. Submitted
41. Wei, S., Ke, X., Lin, F.: Perfect matchings in random polyomino chain graphs. *J. Math. Chem.* **54**, 690–697 (2016)
42. Wei, S., Ke, X.: Wiener and Kirchhoff indices in random generalized polyomino chains. *Ars Comb.* (in press)