



Expected Values of Molecular Descriptors in Random Polyphenyl Chains

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Abstract

A chemical graph is a model used to indicate a chemical combination. In a molecular graph, vertices define atoms, and edges are represented as chemical bonds. A topological index is a single number to characterize the graph of a molecule. In this article, we study the topological properties of some special chains. The polyphenyl chains with hexagons are graphs of aromatic organic compounds. The key purpose of this article is to explore the expected value of Sombor, reduced Sombor, and average Sombor index for this category of organic compounds. It was investigated that the Sombor, reduced Sombor and average Sombor index revealed adequate discriminative potential of alkanes. It has been tested that these indicators can be used effectively in modeling chemical thermodynamic structures. The average value of the Sombor, reduced Sombor, and average Sombor index for the set of all spiro and random polyphenyl chains has been determined. Finally, the ratio between the expected values of these mentioned indices for both random chains has been resolved.

Keywords:

Sombor Index;
Reduced Sombor Index;
Average Sombor Index;
Spiro Chain; Polyphenyl Chains.

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1- Introduction

Aromatic organic compounds are main building blocks for many natural and synthetic chemical compounds as well as constituents of petrochemicals. Topological index was first created in 1971 by Hosoya. The simplest topological index does not acknowledge double bonds in hydrocarbons. Polycyclic aromatic hydrocarbons are well studied and much explored chemicals in food. Polyphenols are plant defense system (secondary metabolites) originate in vegetables, fruits and seeds. Polyphenols have diversity in their chemical structure along with a wide range in their properties and applications like as natural antioxidants, cardiovascular inflammatory, and neurodegenerative diseases, food supplements, pharmaceutical and cosmetic additive. These days, there are many topological indicators [1], some of which are incorporated into chemistry. They can be distinguished by the structure of the graphs used for their calculation. For example, there is a Hosoya index, which is calculated by counting non-incident edges on a graph. In addition, the Estrada index is based on graph width, the Randić link index, and the Zagreb group indicators are calculated using degrees of vertices, etc. Topological indices have many applications in QSPR/QSAR research. The degree based topological index play an important part in chemical graph theory. The Sombor index [2-4] family was introduced by Gutman with a view to a chemical graph. In this article we are concerned about Sombor's index of chemical graphs. Topological indices are related to vertex adjacency or the topological distances in a graph. Wiener index [5-7] is the first topological index, which is equal to the sum of all distances between the vertices. In this article, we will compute the topological index like SO , SO_{red} and SO_{avg} . The SO , SO_{red} and SO_{avg} [8] are defined as:

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$$SO(G) = \sum_{e_{ij} \in E(G)} \sqrt{\deg(v_i)^2 + \deg(v_j)^2} \tag{1}$$

$$SO_{red}(G) = \sum_{e_{ij} \in E(G)} \sqrt{\deg((v_i) - 1)^2 + \deg((v_j) - 1)^2} \tag{2}$$

$$SO_{avg}(G) = \sum_{e_{ij} \in E(G)} \sqrt{\left(\deg(v_i) - \frac{2m}{n}\right)^2 + \left(\deg(v_j) - \frac{2m}{n}\right)^2} \tag{3}$$

where m denotes the number of edges and n denotes the number of vertices. Let us consider hexagons $h_1, h_2, h_3, \dots, h_k$. We can get a Polyphenyl chains ($\acute{R}PC$) by adding an edge to each pair of successive hexagons [9]. Since two successive hexagons can be attached by three different schemes as shown in Figure 1. For $k > 2$, random Polyphenyl chains ($\acute{R}PC_k$) may not be unique. The three types of order denoted by $\acute{R}PC_k^1$, $\acute{R}PC_k^2$, and $\acute{R}PC_k^3$. Let us associate the probabilities ζ_1, ζ_2 and $1 - \zeta_1 - \zeta_2$ for acquiring $\acute{R}PC_k^1$, $\acute{R}PC_k^2$, and $\acute{R}PC_k^3$.

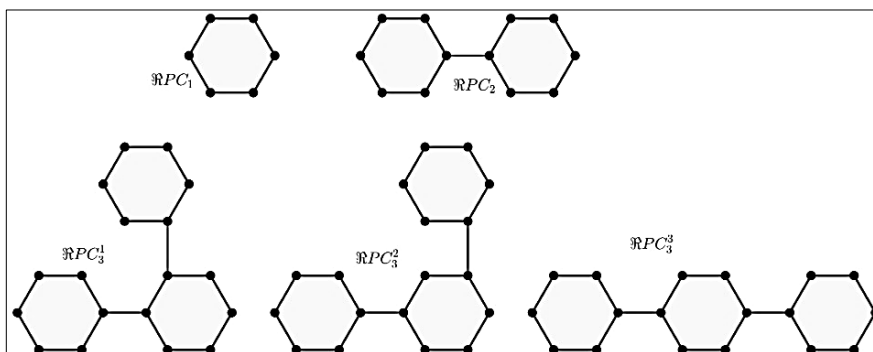


Figure 1. Polyphenyl Chains

If we squeeze each bridge between successive hexagons in ($\acute{R}PC_k$), after that we will get a spiro-chain which is symbolized by ($\acute{R}SC_k$). For $k > 2$, spiro chain [6, 10, 11] is not unique and has following three arrangements as shown in Figure 2, denoted by $\acute{R}SC_k^1$, $\acute{R}SC_k^2$, and $\acute{R}SC_k^3$. Let us link the probabilities ζ_1, ζ_2 and $1 - \zeta_1 - \zeta_2$ for acquiring $\acute{R}SC_k^1$, $\acute{R}SC_k^2$, and $\acute{R}SC_k^3$.

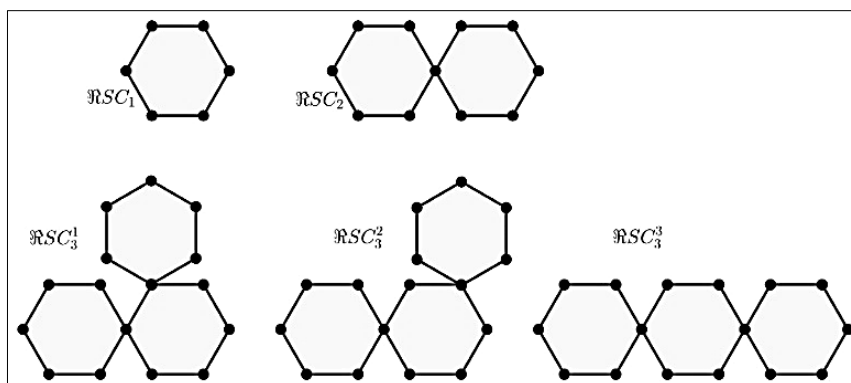


Figure 2. Spiro Chain

2- Sombor, Reduced Sombor and Average Sombor in Random Polyphenyl Chains

In this part, we examine the SO , SO_{red} and SO_{avg} in the random Polyphenyl chains $\acute{R}PC_k$. Let $\acute{R}PC_k$ be the polyphenyl chain [12] obtained by $\acute{R}PC_{k-1}$. Clearly, there are only (2,2), (2,3) and (3,3) – edges in $\acute{R}PC_k$. By using the Equations 1 and 2 and Equation 3 in random Polyphenyl chains [13] we have the following equations:

$$SO(\acute{R}PC_k) = 2\sqrt{2}\omega_{22}(\acute{R}PC_k) + \sqrt{13}\omega_{23}(\acute{R}PC_k) + 3\sqrt{2}\omega_{33}(\acute{R}PC_k) \tag{4}$$

$$SO_{red}(\acute{R}PC_k) = \sqrt{2}\omega_{22}(\acute{R}PC_k) + \sqrt{5}\omega_{23}(\acute{R}PC_k) + 2\sqrt{2}\omega_{33}(\acute{R}PC_k) \tag{5}$$

$$SO_{avg}(\acute{R}PC_k) = \sqrt{2} \left(\frac{k-1}{3k}\right) \omega_{22}(\acute{R}PC_k) + \frac{\sqrt{5k^2+2k+2}}{3k} \omega_{23}(\acute{R}PC_k) + \sqrt{2} \left(\frac{2k+1}{3k}\right) \omega_{33}(\acute{R}PC_k) \tag{6}$$

Thus, to find the SO , SO_{red} and SO_{avg} of $\acute{R}PC_k$, we just need to evaluate the $\omega_{22}(\acute{R}PC_k)$, $\omega_{23}(\acute{R}PC_k)$ and $\omega_{33}(\acute{R}PC_k)$. Since $\acute{R}PC_k(k, \zeta_1, \zeta_2)$ is a random Polyphenyl chains. So, $SO(\acute{R}PC_k(k, \zeta_1, \zeta_2))$, $SO_{red}(\acute{R}PC_k(k, \zeta_1, \zeta_2))$ and $SO_{avg}(\acute{R}PC_k(k, \zeta_1, \zeta_2))$ are also arbitrary variables. We symbolize the anticipated values of given indices by $E_k^{SO} = E^{SO} [SO(\acute{R}PC_k(k, \zeta_1, \zeta_2))]$, $E_k^{red} = E^{red} [SO(\acute{R}PC_k(k, \zeta_1, \zeta_2))]$ and $E_k^{avg} = E^{avg} [SO(\acute{R}PC_k(k, \zeta_1, \zeta_2))]$ respectively.

2-1-Theorem

Let $\acute{R}PC_k(k, \zeta_1, \zeta_2)$ be an arbitrary Polyphenyl chains of length k , where $k \geq 2$. Then:

$$E_k^{SO} = [(5\sqrt{2} - 2\sqrt{13})\zeta_1 + (7\sqrt{2} + 4\sqrt{13})]k - (10\sqrt{2} - 4\sqrt{13})\zeta_1 + (5\sqrt{2} - 4\sqrt{13})$$

Proof: For $k = 2$, we have $E_2^{SO} = 19\sqrt{2} + 4\sqrt{13}$. Now, when $k \geq 2$, it is obvious that ω_{22} , ω_{23} and ω_{33} depend on the following three cases:

1. If $\acute{R}PC_{k-1} \rightarrow \acute{R}PC_k^1$ with probability ζ_1

$$\omega_{22}(\acute{R}PC_k^1) = \omega_{22}(\acute{R}PC_{k-1}) + 3$$

$$\omega_{23}(\acute{R}PC_k^1) = \omega_{23}(\acute{R}PC_{k-1}) + 2$$

$$\omega_{33}(\acute{R}PC_k^1) = \omega_{33}(\acute{R}PC_{k-1}) + 2$$

by using Equation 4, we have:

$$SO(\acute{R}PC_k^1) = SO(\acute{R}PC_{k-1}) + 12\sqrt{2} + 2\sqrt{13}$$

2. If $\acute{R}PC_{k-1} \rightarrow \acute{R}PC_k^2$ with probability ζ_2

$$\omega_{22}(\acute{R}PC_k^2) = \omega_{22}(\acute{R}PC_{k-1}) + 2$$

$$\omega_{23}(\acute{R}PC_k^2) = \omega_{23}(\acute{R}PC_{k-1}) + 4$$

$$\omega_{33}(\acute{R}PC_k^2) = \omega_{33}(\acute{R}PC_{k-1}) + 1$$

by using Equation 4, we have:

$$SO(\acute{R}PC_k^2) = SO(\acute{R}PC_{k-1}) + 7\sqrt{2} + 4\sqrt{13}$$

3. If $\acute{R}PC_{k-1} \rightarrow \acute{R}PC_k^3$ with probability $1 - \zeta_1 - \zeta_2$

$$\omega_{22}(\acute{R}PC_k^3) = \omega_{22}(\acute{R}PC_{k-1}) + 2$$

$$\omega_{23}(\acute{R}PC_k^3) = \omega_{23}(\acute{R}PC_{k-1}) + 4$$

$$\omega_{33}(\acute{R}PC_k^3) = \omega_{33}(\acute{R}PC_{k-1}) + 1$$

by using Equation 4, we have:

$$SO(\acute{R}PC_k^3) = SO(\acute{R}PC_{k-1}) + 7\sqrt{2} + 4\sqrt{13}$$

Thus:

$$E_k^{SO} = \zeta_1 SO(\acute{R}PC_k^1) + \zeta_2 SO(\acute{R}PC_k^2) + (1 - \zeta_1 - \zeta_2) SO(\acute{R}PC_k^3)$$

$$E_k^{SO} = \zeta_1 SO(\acute{R}PC_{k-1}) + (12\sqrt{2} + 2\sqrt{13})\zeta_1 + \zeta_2 SO(\acute{R}PC_{k-1}) + (7\sqrt{2} + 4\sqrt{13})\zeta_2 + (1 - \zeta_1 - \zeta_2) SO(\acute{R}PC_{k-1}) + (1 - \zeta_1 - \zeta_2)(12\sqrt{2} + 2\sqrt{13})$$

$$E_k^{SO} = SO(\acute{R}PC_{k-1}) + (5\sqrt{2} - 2\sqrt{13})\zeta_1 + (7\sqrt{2} + 4\sqrt{13}) \tag{7}$$

Since $E[E_k]^{SO} = E_k^{SO}$ so apply the operator E on Equation 7, we get:

$$E_k^{SO} = E_{k-1}^{SO} + (5\sqrt{2} - 2\sqrt{13})\zeta_1 + (7\sqrt{2} + 4\sqrt{13}), \quad k > 2 \tag{8}$$

and after solving the recurrence relation in Equation 8 with $E_2^{SO} = 19\sqrt{2} + 4\sqrt{13}$, we get

$$E_k^{SO} = [(5\sqrt{2} - 2\sqrt{13})\zeta_1 + (7\sqrt{2} + 4\sqrt{13})]k - (10\sqrt{2} - 4\sqrt{13})\zeta_1 + (5\sqrt{2} - 4\sqrt{13}).$$

2-2-Theorem

Let $\acute{R}PC_k(k, \zeta_1, \zeta_2)$ be an arbitrary Polyphenyl chains of length k , where $k \geq 2$. Then

$$E_k^{red} = [(3\sqrt{2} - 2\sqrt{5})\zeta_1 + (4\sqrt{2} + 4\sqrt{5})]k - (6\sqrt{2} - 4\sqrt{5})\zeta_1 + (2\sqrt{2} - 4\sqrt{5}).$$

Proof: For $k = 2$, we have $E_2^{red} = 10\sqrt{2} + 4\sqrt{5}$. Now, when $k \geq 3$, it is obvious that ω_{22} , ω_{23} and ω_{33} depend on the following three cases:

If $\acute{R}PC_{k-1} \rightarrow \acute{R}PC_k^1$ with probability ζ_1

$$\omega_{22}(\acute{R}PC_k^1) = \omega_{22}(\acute{R}PC_{k-1}) + 3$$

$$\omega_{23}(\acute{R}PC_k^1) = \omega_{23}(\acute{R}PC_{k-1}) + 2$$

$$\omega_{33}(\acute{R}PC_k^1) = \omega_{33}(\acute{R}PC_{k-1}) + 2$$

by using Equation 5, we have:

$$SO_{red}(\acute{R}PC_k^1) = SO_{red}(\acute{R}PC_{k-1}) + 7\sqrt{2} + 2\sqrt{5}$$

1. If $\acute{R}PC_{k-1} \rightarrow \acute{R}PC_k^2$ with probability ζ_2

$$\omega_{22}(\acute{R}PC_k^2) = \omega_{22}(\acute{R}PC_{k-1}) + 2$$

$$\omega_{23}(\acute{R}PC_k^2) = \omega_{23}(\acute{R}PC_{k-1}) + 4$$

$$\omega_{33}(\acute{R}PC_k^2) = \omega_{33}(\acute{R}PC_{k-1}) + 1$$

by using Equation 5, we have:

$$SO_{red}(\acute{R}PC_k^2) = SO_{red}(\acute{R}PC_{k-1}) + 4\sqrt{2} + 4\sqrt{5}$$

1. If $\acute{R}PC_{k-1} \rightarrow \acute{R}PC_k^3$ with probability $1 - \zeta_1 - \zeta_2$

$$\omega_{22}(\acute{R}PC_k^3) = \omega_{22}(\acute{R}PC_{k-1}) + 2$$

$$\omega_{23}(\acute{R}PC_k^3) = \omega_{23}(\acute{R}PC_{k-1}) + 4$$

$$\omega_{33}(\acute{R}PC_k^3) = \omega_{33}(\acute{R}PC_{k-1}) + 1$$

by using Equation 5, we have:

$$SO_{red}(\acute{R}PC_k^3) = SO_{red}(\acute{R}PC_{k-1}) + 4\sqrt{2} + 4\sqrt{5}$$

Thus:

$$E_k^{red} = \zeta_1 SO_{red}(\acute{R}PC_k^1) + \zeta_2 SO_{red}(\acute{R}PC_k^2) + (1 - \zeta_1 - \zeta_2) SO_{red}(\acute{R}PC_k^3)$$

$$E_k^{red} = \zeta_1 SO_{red}(\acute{R}PC_{k-1}) + (7\sqrt{2} + 2\sqrt{5})\zeta_1 + \zeta_2 SO_{red}(\acute{R}PC_{k-1}) + (4\sqrt{2} + 4\sqrt{5})\zeta_2 + (1 - \zeta_1 - \zeta_2) SO_{red}(\acute{R}PC_{k-1}) + (1 - \zeta_1 - \zeta_2)(4\sqrt{2} + 2\sqrt{5})$$

$$E_k^{red} = SO_{red}(\acute{R}PC_{k-1}) + (3\sqrt{2} - 2\sqrt{13})\zeta_1 + (4\sqrt{2} + 4\sqrt{5}) \quad (9)$$

Since $E[E_k]^{red} = E_k^{red}$ so apply the operator E on Equation 9, we get:

$$E_k^{red} = E_{k-1}^{red} + (3\sqrt{2} - 2\sqrt{5})\zeta_1 + (4\sqrt{2} + 4\sqrt{5}), \quad k > 2 \quad (10)$$

And after solving the recurrence relation in Equation 10 with $E_2^{red} = 10\sqrt{2} + 4\sqrt{5}$, we get:

$$E_k^{red} = [(3\sqrt{2} - 2\sqrt{5})\zeta_1 + (4\sqrt{2} + 4\sqrt{5})]k - (6\sqrt{2} - 4\sqrt{5})\zeta_1 + (2\sqrt{2} - 4\sqrt{5}).$$

2-3-Theorem

Let $\acute{R}PC_k(k, \zeta_1, \zeta_2)$ be an arbitrary Polyphenyl chains of length k , where $k \geq 2$. Then

$$E_k^{avg} = \left[\left(\sqrt{2} - \frac{2\sqrt{5k^2+2k+2}}{3k} \right) \zeta_1 + \left(\frac{4\sqrt{2k-\sqrt{2}}}{3k} + \frac{4\sqrt{5k^2+2k+2}}{3k} \right) \right] k - \left(2\sqrt{2} - \frac{4\sqrt{5k^2+2k+2}}{3k} \right) \zeta_1 - \left(\frac{8\sqrt{2k-2\sqrt{2}}}{3k} + \frac{8\sqrt{5k^2+2k+2}}{3k} \right) + \frac{13\sqrt{2}}{6} + \frac{2\sqrt{26}}{3}.$$

Proof: For $k = 2$, we have $E_2^{avg} = \frac{13\sqrt{2}}{6} + \frac{2\sqrt{26}}{3}$. Now, when $k \geq 3$, it is obvious that ω_{22} , ω_{23} and ω_{33} depend on the following three cases:

1. If $\acute{R}PC_{k-1} \rightarrow \acute{R}PC_k^1$ with probability ζ_1

$$\omega_{22}(\acute{R}PC_k^1) = \omega_{22}(\acute{R}PC_{k-1}) + 3$$

$$\omega_{23}(\acute{R}PC_k^1) = \omega_{23}(\acute{R}PC_{k-1}) + 2$$

$$\omega_{33}(\acute{R}PC_k^1) = \omega_{33}(\acute{R}PC_{k-1}) + 2$$

by using Equation 5, we have:

$$SO_{\text{avg}}(\acute{R}PC_k^1) = SO_{\text{avg}}(\acute{R}PC_{k-1}) + \left(\frac{7\sqrt{2}k-\sqrt{2}}{3k}\right) + \left(\frac{2\sqrt{5k^2+2k+2}}{3k}\right)$$

2. If $\acute{R}PC_{k-1} \rightarrow \acute{R}PC_k^2$ with probability ζ_2

$$\omega_{22}(\acute{R}PC_k^2) = \omega_{22}(\acute{R}PC_{k-1}) + 2$$

$$(\acute{R}PC_k^2) = \omega_{23}(\acute{R}PC_{k-1}) + 4$$

$$\omega_{33}(\acute{R}PC_k^2) = \omega_{33}(\acute{R}PC_{k-1}) + 1$$

by using Equation 5, we have:

$$SO_{\text{avg}}(\acute{R}PC_k^2) = SO_{\text{avg}}(\acute{R}PC_{k-1}) + \left(\frac{4\sqrt{2}k-\sqrt{2}}{3k}\right) + \left(\frac{4\sqrt{5k^2+2k+2}}{3k}\right)$$

3. If $\acute{R}PC_{k-1} \rightarrow \acute{R}PC_k^3$ with probability $1 - \zeta_1 - \zeta_2$

$$\omega_{22}(\acute{R}PC_k^3) = \omega_{22}(\acute{R}PC_{k-1}) + 2$$

$$\omega_{23}(\acute{R}PC_k^3) = \omega_{23}(\acute{R}PC_{k-1}) + 4$$

$$\omega_{33}(\acute{R}PC_k^3) = \omega_{33}(\acute{R}PC_{k-1}) + 1$$

by using Equation 5, we have:

$$SO_{\text{avg}}(\acute{R}PC_k^3) = SO_{\text{avg}}(\acute{R}PC_{k-1}) + \left(\frac{4\sqrt{2}k-\sqrt{2}}{3k}\right) + \left(\frac{4\sqrt{5k^2+2k+2}}{3k}\right)$$

Thus:

$$E_k^{\text{avg}} = \zeta_1 SO_{\text{avg}}(\acute{R}PC_k^1) + \zeta_2 SO_{\text{avg}}(\acute{R}PC_k^2) + (1 - \zeta_1 - \zeta_2) SO_{\text{avg}}(\acute{R}PC_k^3)$$

$$E_k^{\text{avg}} = \zeta_1 SO_{\text{avg}}(\acute{R}PC_{k-1}) + \left[\left(\frac{7\sqrt{2}k-\sqrt{2}}{3k}\right) + \left(\frac{2\sqrt{5k^2+2k+2}}{3k}\right)\right] \zeta_1 + \zeta_2 SO_{\text{avg}}(\acute{R}PC_{k-1}) + \left[\left(\frac{4\sqrt{2}k-\sqrt{2}}{3k}\right) + \left(\frac{4\sqrt{5k^2+2k+2}}{3k}\right)\right] \zeta_2 + (1 - \zeta_1 - \zeta_2) SO_{\text{avg}}(\acute{R}PC_k^3) + (1 - \zeta_1 - \zeta_2) \left[\left(\frac{4\sqrt{2}k-\sqrt{2}}{3k}\right) + \left(\frac{4\sqrt{5k^2+2k+2}}{3k}\right)\right]$$

$$E_k^{\text{avg}} = SO_{\text{avg}}(\acute{R}PC_{k-1}) + \left(\sqrt{2} - \frac{2\sqrt{5k^2+2k+2}}{3k}\right) \zeta_1 + \left[\frac{4\sqrt{2}k-\sqrt{2}}{3k} + \frac{4\sqrt{5k^2+2k+2}}{3k}\right] \zeta_2 \quad (11)$$

Since $E[E_k]^{\text{avg}} = E_k^{\text{avg}}$ so apply the operator E on Equation 11, we get:

$$E_k^{\text{avg}} = E_{k-1}^{\text{avg}} + \left[\sqrt{2} - \frac{2\sqrt{5k^2+2k+2}}{3k}\right] \zeta_1 + \left[\frac{4\sqrt{2}k-\sqrt{2}}{3k} + \frac{4\sqrt{5k^2+2k+2}}{3k}\right] \zeta_2, \quad k > 2 \quad (12)$$

and after solving the recurrence relation in Equation 12 with $E_2^{\text{avg}} = \frac{13\sqrt{2}}{6} + \frac{2\sqrt{26}}{3}$, we get:

$$E_k^{\text{avg}} = \left[\left[\sqrt{2} - \frac{2\sqrt{5k^2+2k+2}}{3k}\right] \zeta_1 + \left[\frac{4\sqrt{2}k-\sqrt{2}}{3k} + \frac{4\sqrt{5k^2+2k+2}}{3k}\right] \zeta_2\right] k - \left(2\sqrt{2} - \frac{4\sqrt{5k^2+2k+2}}{3k}\right) \zeta_1 - \left(\frac{8\sqrt{2}k-2\sqrt{2}}{3k} + \frac{8\sqrt{5k^2+2k+2}}{3k}\right) + \frac{13\sqrt{2}}{6} + \frac{2\sqrt{26}}{3}.$$

These indices can be computed for three chains meta $M_k = \acute{R}PC(k; 0, 1)$ para $P_k = \acute{R}PC(k; 0, 0)$ and ortho $O_k = \acute{R}PC(k; 1, 0)$.

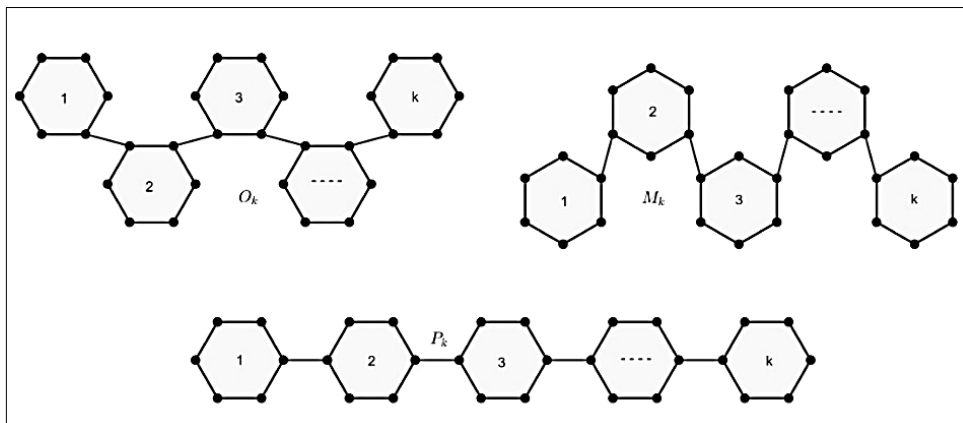


Figure 1. Polyphenyl ortho, meta and para Chains

2-4-Corollary

For $k \geq 2$, we have:

$$\bullet SO(O_k) = (12\sqrt{2} + 2\sqrt{13})k - 5\sqrt{2}$$

$$\bullet SO(P_k) = SO(M_k) = (7\sqrt{2} + 4\sqrt{13})k + (5\sqrt{2} - 4\sqrt{13})$$

$$\bullet SO_{red}(O_k) = (7\sqrt{2} + 2\sqrt{5})k - 4\sqrt{2}$$

$$\bullet SO_{red}(P_k) = SO_{red}(M_k) = (4\sqrt{2} + 4\sqrt{5})k + (2\sqrt{2} - 4\sqrt{5})$$

$$\bullet SO_{avg}(O_k) = \left(\frac{7\sqrt{2}-\sqrt{2}}{3k} + \frac{2\sqrt{5k^2+2k+2}}{3k} \right) k - \frac{5\sqrt{2}}{2} + \frac{2\sqrt{2}}{3k} - \frac{4\sqrt{5k^2+2k+2}}{3k} + \frac{2\sqrt{26}}{3}$$

$$\bullet SO_{avg}(P_k) = SO_{avg}(M_k) = \left(\frac{4\sqrt{2}-\sqrt{2}}{3k} + \frac{4\sqrt{5k^2+2k+2}}{3k} \right) k - \left[\frac{8\sqrt{2}k}{3k} - \frac{2\sqrt{2}}{3k} + \frac{8\sqrt{5k^2+2k+2}}{3k} \right] + \frac{13\sqrt{2}}{6} + \frac{2\sqrt{26}}{3}$$

3- Average Value of Indices in Polyphenyl chains

In this part, the average values of SO , SO_{red} and SO_{avg} have been resolved for the set of random Polyphenyl chains [14]. The average values over the set $\hat{R}P_k$ are:

$$SO_{avg}(\hat{R}P_k) = \frac{1}{|\hat{R}P_k|} \sum_{G \in \hat{R}P_k} SO(G)$$

$$(SO_{red})_{avg}(\hat{R}P_k) = \frac{1}{|\hat{R}P_k|} \sum_{G \in \hat{R}P_k} SO_{red}(G)$$

$$(SO_{avg})_{avg}(\hat{R}P_k) = \frac{1}{|\hat{R}P_k|} \sum_{G \in \hat{R}P_k} SO_{avg}(G)$$

As a result $\zeta_1 = \zeta_2 = 1 - \zeta_1 - \zeta_2$, we can use theorem (2-1, 2-2, 2-3) by setting $\zeta_1 = \zeta_2 = 1 - \zeta_1 - \zeta_2 = \frac{1}{3}$ and the results will be in the form of following expression.

3-1-Theorem

Let $\hat{R}P_k$ be the set of arbitrary Polyphenyl chains, then:

$$SO(\hat{R}P_k) = \left[\frac{26\sqrt{2}}{3} + \frac{10\sqrt{13}}{3} \right] k + \frac{5\sqrt{2}}{3} - \frac{8\sqrt{13}}{3}$$

$$SO_{red}(\hat{R}P_k) = \left[5\sqrt{2} + \frac{10\sqrt{5}}{3} \right] k - \frac{8\sqrt{5}}{3}$$

$$SO_{avg}(\hat{R}P_k) = \left[\frac{5\sqrt{2}}{3} + \frac{\sqrt{2}}{3k} + \frac{10\sqrt{5k^2+2k+2}}{9k} \right] k - \frac{20\sqrt{5k^2+2k+2}}{9k} - \frac{7\sqrt{2}}{6} + \frac{2\sqrt{2}}{3k} + \frac{2\sqrt{26}}{3}$$

from corollary (2-4);

$$\frac{1}{3} [SO(O_k) + SO(P_k) + SO(M_k)] = \left[\frac{26\sqrt{2}}{3} + \frac{10\sqrt{13}}{3} \right] k + \frac{5\sqrt{2}}{3} - \frac{8\sqrt{13}}{3}$$

$$\frac{1}{3} [SO(O_k) + SO(P_k) + SO(M_k)] = \left[5\sqrt{2} + \frac{10\sqrt{5}}{3} \right] k - \frac{8\sqrt{5}}{3}$$

$$\frac{1}{3} [SO(O_k) + SO(P_k) + SO(M_k)] = \left[\frac{5\sqrt{2}}{3} + \frac{\sqrt{2}}{3k} + \frac{10\sqrt{5k^2+2k+2}}{9k} \right] k - \frac{20\sqrt{5k^2+2k+2}}{9k} - \frac{7\sqrt{2}}{6} + \frac{2\sqrt{2}}{3k} + \frac{2\sqrt{26}}{3}$$

Thus the average value of these indices $SO(\hat{R}PC(k, \zeta_1, \zeta_2))$, $SO_{red}(\hat{R}PC(k, \zeta_1, \zeta_2))$ or $SO_{avg}(\hat{R}PC(k, \zeta_1, \zeta_2))$ is always equal over the set $\{O_k, P_k, M_k\}$.

4- Ratio between Sombor, Reduced Sombor and Average Sombor Index for Polyphenyl Chains

Now, by getting results from theorem (2-1, 2-2) and (2-3) we will assemble the ratio between the anticipated values for the SO , SO_{red} and SO_{avg} of an arbitrary Polyphenyl chains [15] with probability ζ_1 and ζ_2 .

4-1-Theorem

If $k \geq 2$, then:

$$E^{SO} [SO(\hat{R}PC(k, \zeta_1, \zeta_2))] > E^{red} [redSO(\hat{R}PC(k, \zeta_1, \zeta_2))].$$

Proof: The statement is true for $k = 2$. Thus for $k > 2$, by applying theorem (2-1) and (2-2) we get;

$$\begin{aligned}
E^{SO}[SO(\acute{R}PC(k, \zeta_1, \zeta_2))] - E^{red}[redSO(\acute{R}PC(k, \zeta_1, \zeta_2))] \\
&= \{[(5\sqrt{2} - 2\sqrt{13})\zeta_1 + (7\sqrt{2} + 4\sqrt{13})](k-2) + (19\sqrt{2} + 4\sqrt{13})\} \\
&\quad - \{[(3\sqrt{2} - 2\sqrt{5})\zeta_1 + (4\sqrt{2} + 4\sqrt{5})](k-2) + (10\sqrt{2} + 4\sqrt{5})\} \\
&= [(2\sqrt{2} - 2\sqrt{13} + 2\sqrt{5})\zeta_1 + (3\sqrt{2} + 4\sqrt{13} - 4\sqrt{5})](k-2) + (9\sqrt{2} + 4\sqrt{13} - 4\sqrt{5})
\end{aligned}$$

Since:

$$(2\sqrt{2} - 2\sqrt{13} + 2\sqrt{5}) > 0, (3\sqrt{2} + 4\sqrt{13} - 4\sqrt{5}) > 0, (9\sqrt{2} + 4\sqrt{13} - 4\sqrt{5}) > 0$$

So

$$= [(2\sqrt{2} - 2\sqrt{13} + 2\sqrt{5})\zeta_1 + (3\sqrt{2} + 4\sqrt{13} - 4\sqrt{5})](k-2) + (9\sqrt{2} + 4\sqrt{13} - 4\sqrt{5}) > 0,$$

$$\therefore k \geq 2, 0 < \zeta_1 < 1$$

4-2-Theorem

If $k \geq 2$, then:

$$E^{red}[redSO(\acute{R}PC(k, \zeta_1, \zeta_2))] > E^{avg}[avgSO(\acute{R}PC(k, \zeta_1, \zeta_2))].$$

Proof: The statement is true for $k = 2$. Thus for $k > 2$, by applying theorem (2-2) and (2-3), we get;

$$\begin{aligned}
E^{red}[redSO(\acute{R}PC(k, \zeta_1, \zeta_2))] - E^{avg}[avgSO(\acute{R}PC(k, \zeta_1, \zeta_2))] &= \{[(3\sqrt{2} - 2\sqrt{5})\zeta_1 + (4\sqrt{2} + 4\sqrt{5})](k-2) + \\
(10\sqrt{2} + 4\sqrt{5})\} - \left\{ \left[\left(\sqrt{2} - \frac{2\sqrt{5k^2+2k+2}}{3k} \right) \zeta_1 + \left(\frac{4\sqrt{2k-\sqrt{2}}}{3k} + \frac{4\sqrt{5k^2+2k+2}}{3k} \right) \right] (k-2) + \left(\frac{13\sqrt{2}}{6} + \frac{2\sqrt{26}}{3} \right) \right\} \\
&= \left[\left(2\sqrt{2} - 2\sqrt{5} + \frac{2\sqrt{5k^2+2k+2}}{3k} \right) \zeta_1 + \left(\frac{8\sqrt{2}}{3} + 4\sqrt{5} - \frac{\sqrt{2}}{3k} - \frac{4\sqrt{5k^2+2k+2}}{3k} \right) \right] (k-2) + \left(\frac{47\sqrt{2}}{6} + 4\sqrt{5} - \frac{2\sqrt{26}}{3} \right) \\
&= \left[\left(2\sqrt{5} - \frac{2\sqrt{5k^2+2k+2}}{3k} \right) (2 - \zeta_1) + \left(\frac{8\sqrt{2}}{3} - \frac{\sqrt{2}}{3k} - 2\sqrt{2}\zeta_1 \right) \right] (k-2) + \left(\frac{47\sqrt{2}}{6} + 4\sqrt{5} - \frac{2\sqrt{26}}{3} \right)
\end{aligned}$$

Since:

$$\left(2\sqrt{5} - \frac{2\sqrt{5\frac{2}{k} + \frac{2}{k^2}}}{3} \right) > 0, \left(\frac{\sqrt{2}}{3} \left(\frac{8k-1}{k} \right) + 2\sqrt{2}\zeta_1 \right) > 0, \left(\frac{47\sqrt{2}}{6} + 4\sqrt{5} - \frac{2\sqrt{26}}{3} \right) > 0, k \geq 2$$

So

$$= \left[\left(2\sqrt{5} - \frac{2\sqrt{5k^2+2k+2}}{3k} \right) (2 - \zeta_1) + \left(\frac{8\sqrt{2}}{3} - \frac{\sqrt{2}}{3k} - 2\sqrt{2}\zeta_1 \right) \right] (k-2) + \left(\frac{47\sqrt{2}}{6} + 4\sqrt{5} - \frac{2\sqrt{26}}{3} \right) > 0,$$

$$\therefore k \geq 2, 0 < \zeta_1 < 1$$

4-3-Theorem

If $k \geq 2$, then:

$$E^{SO}[SO(\acute{R}PC(k, \zeta_1, \zeta_2))] > E^{avg}[avgSO(\acute{R}PC(k, \zeta_1, \zeta_2))].$$

Proof: The statement is true for $k = 2$. Thus for $k > 2$, by applying theorem (2-1) and (2-3) we get;

$$\begin{aligned}
E^{SO}[SO(\acute{R}PC(k, \zeta_1, \zeta_2))] - E^{avg}[avgSO(\acute{R}PC(k, \zeta_1, \zeta_2))] &= \{[(5\sqrt{2} - 2\sqrt{13})\zeta_1 + (7\sqrt{2} + 4\sqrt{13})](k-2) + \\
(19\sqrt{2} + 4\sqrt{13})\} - \left\{ \left[\left(\sqrt{2} - \frac{2\sqrt{5k^2+2k+2}}{3k} \right) \zeta_1 + \left(\frac{4\sqrt{2k-\sqrt{2}}}{3k} + \frac{4\sqrt{5k^2+2k+2}}{3k} \right) \right] (k-2) + \left(\frac{13\sqrt{2}}{6} + \frac{2\sqrt{26}}{3} \right) \right\} \\
&= \left[\left(4\sqrt{2} - 2\sqrt{13} + \frac{2\sqrt{5k^2+2k+2}}{3k} \right) \zeta_1 + \left(\frac{17\sqrt{2}}{3} + 4\sqrt{13} - \frac{\sqrt{2}}{3k} - \frac{4\sqrt{5k^2+2k+2}}{3k} \right) \right] (k-2) + \left(\frac{101\sqrt{2}}{6} + 4\sqrt{13} - \frac{2\sqrt{26}}{3} \right) \\
&= \left[\left(2\sqrt{13} - \frac{2\sqrt{5k^2+2k+2}}{3k} \right) (2 - \zeta_1) + \left(\frac{17\sqrt{2}}{3} - \frac{\sqrt{2}}{3k} - 4\sqrt{2}\zeta_1 \right) \right] (k-2) + \left(\frac{101\sqrt{2}}{6} + 4\sqrt{13} - \frac{2\sqrt{26}}{3} \right)
\end{aligned}$$

Since

$$\left(2\sqrt{13} - \frac{2\sqrt{5\frac{2}{k} + \frac{2}{k^2}}}{3} \right) > 0, \left(\frac{101\sqrt{2}}{6} + 4\sqrt{13} - \frac{2\sqrt{26}}{3} \right) > 0, \left(\frac{8\sqrt{2}}{3} - \frac{\sqrt{2}}{3k} + 2\sqrt{2}\zeta_1 \right) > 0, k \geq 2.$$

So

$$= \left[\left(2\sqrt{13} - \frac{2\sqrt{5k^2+2k+2}}{3k} \right) (2 - \zeta_1) + \left(\frac{17\sqrt{2}}{3} - \frac{\sqrt{2}}{3k} - 4\sqrt{2}\zeta_1 \right) (k - 2) + \left(\frac{101\sqrt{2}}{6} + 4\sqrt{13} - \frac{2\sqrt{26}}{3} \right) \right] > 0,$$

$$\because k \geq 2, 0 < \zeta_1 < 1.$$

4-4-Corollary

For $k \geq 2$, $E^{SO}[SO(\acute{R}PC(k, \zeta_1, \zeta_2))] > E^{red}[redSO(\acute{R}PC(k, \zeta_1, \zeta_2))] > E^{avg}[avgSO(\acute{R}PC(k, \zeta_1, \zeta_2))]$ as shown in Figure 4.

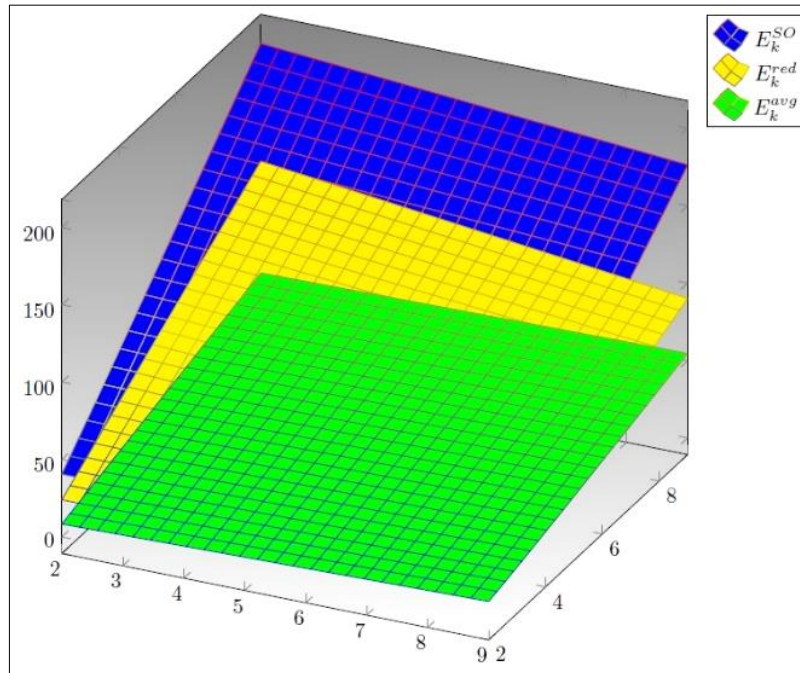


Figure 2. Comparison between the expected values of Sombor E_k^{SO} (blue), reduced Sombor E_k^{red} (yellow) and average Sombor E_k^{avg} (green) index in random Polyphenyl chains

5- Sombor, Reduced Sombor and Average Sombor Index in Random Spiro Chain

In the following part, we consider the SO , SO_{red} and SO_{avg} in the arbitrary spiro-chain $\acute{R}SC_k$. Let $\acute{R}SC_k$ be the spiro chain [16-20] acquired by $\acute{R}SC_{k-1}$. Clearly, there are only (2,2), (2,4) and (4,4) – edges in $\acute{R}SC_k$. By using the definition of SO , SO_{red} and SO_{avg} , we have the following equation:

$$SO(\acute{R}SC_k) = 2\sqrt{2}\omega_{22}(\acute{R}SC_k) + 2\sqrt{5}\omega_{24}(\acute{R}SC_k) + 4\sqrt{2}\omega_{44}(\acute{R}SC_k) \quad (13)$$

$$SO_{red}(\acute{R}SC_k) = \sqrt{2}\omega_{22}(\acute{R}SC_k) + \sqrt{10}\omega_{24}(\acute{R}SC_k) + 3\sqrt{2}\omega_{44}(\acute{R}SC_k) \quad (14)$$

$$SO_{avg}(\acute{R}SC_k) = 2\sqrt{2} \left(\frac{k-1}{5k+1} \right) \omega_{22}(\acute{R}SC_k) + \frac{2\sqrt{17k^2+14k+5}}{5k+1} \omega_{24}(\acute{R}SC_k) + 4\sqrt{2} \left(\frac{2k+1}{5k+1} \right) \omega_{44}(\acute{R}SC_k) \quad (15)$$

Thus, to find the SO , SO_{red} and SO_{avg} of $\acute{R}SC_k$, we just need to evaluate the $\omega_{22}(\acute{R}SC_k)$, $\omega_{24}(\acute{R}SC_k)$ and $\omega_{44}(\acute{R}SC_k)$. Since $\acute{R}SC(k; \zeta_1, \zeta_2)$ is an arbitrary spiro-chain. So, $SO(\acute{R}SC(k; \zeta_1, \zeta_2))$, $SO_{red}(\acute{R}SC(k; \zeta_1, \zeta_2))$ and $SO_{avg}(\acute{R}SC(k; \zeta_1, \zeta_2))$ are also arbitrary variables. We symbolize the anticipated values of these indices by $E_k^{SO} = E^{SO}[SO(\acute{R}SC(k; \zeta_1, \zeta_2))]$, $E_k^{red} = E^{red}[SO_{red}(\acute{R}SC(k; \zeta_1, \zeta_2))]$ and $E_k^{avg} = E^{avg}[SO_{avg}(\acute{R}SC(k; \zeta_1, \zeta_2))]$ respectively.

5-1-Theorem

Let $\acute{R}SC(k; \zeta_1, \zeta_2)$ be an arbitrary spiro-chain of length k , where $k \geq 2$. Then:

$$E_k^{SO} = [(6\sqrt{2} - 4\sqrt{5})\zeta_1 + (4\sqrt{2} + 8\sqrt{5})]k - (12\sqrt{2} - 8\sqrt{5})\zeta_1 + (8\sqrt{2} - 8\sqrt{5}).$$

Proof: For $k = 2$, we have $E_2^{SO} = 16\sqrt{2} + 8\sqrt{5}$. Now, when $k \geq 3$, it is obvious that ω_{22} , ω_{24} and ω_{44} depend on the following three cases:

1. If $\acute{R}SC_{k-1} \rightarrow \acute{R}SC_k^1$ with probability ζ_1

$$\omega_{22}(\acute{R}SC_k^1) = \omega_{22}(\acute{R}SC_{k-1}) + 3$$

$$\omega_{24}(\acute{R}SC_k^1) = \omega_{24}(\acute{R}SC_{k-1}) + 2$$

$$\omega_{44}(\acute{R}SC_k^1) = \omega_{44}(\acute{R}SC_{k-1}) + 1$$

by using Equation 13:

$$SO(\acute{R}SC_k^1) = SO(\acute{R}SC_{k-1}) + 10\sqrt{2} + 4\sqrt{5}$$

2. If $\acute{R}SC_{k-1} \rightarrow \acute{R}SC_k^2$ with probability ζ_2

$$\omega_{22}(\acute{R}SC_k^2) = \omega_{22}(\acute{R}SC_{k-1}) + 2$$

$$\omega_{24}(\acute{R}SC_k^2) = \omega_{24}(\acute{R}SC_{k-1}) + 4$$

$$\omega_{44}(\acute{R}SC_k^2) = \omega_{44}(\acute{R}SC_{k-1})$$

by using Equation 13:

$$SO(\acute{R}SC_k^2) = SO(\acute{R}SC_{k-1}) + 4\sqrt{2} + 8\sqrt{5}$$

3. If $\acute{R}SC_{k-1} \rightarrow \acute{R}SC_k^3$ with probability $1 - \zeta_1 - \zeta_2$

$$\omega_{22}(\acute{R}SC_k^3) = \omega_{22}(\acute{R}SC_{k-1}) + 2$$

$$\omega_{24}(\acute{R}SC_k^3) = \omega_{24}(\acute{R}SC_{k-1}) + 4$$

$$\omega_{44}(\acute{R}SC_k^3) = \omega_{44}(\acute{R}SC_{k-1})$$

by using Equation 13:

$$SO(\acute{R}SC_k^3) = SO(\acute{R}SC_{k-1}) + 4\sqrt{2} + 8\sqrt{5}$$

Thus:

$$E_k^{SO} = \zeta_1 SO(\acute{R}SC_k^1) + \zeta_2 SO(\acute{R}SC_k^2) + (1 - \zeta_1 - \zeta_2) SO(\acute{R}SC_k^3)$$

$$E_k^{SO} = \zeta_1 SO(\acute{R}SC_{k-1}) + (10\sqrt{2} + 4\sqrt{5})\zeta_1 + \zeta_2 SO(\acute{R}SC_{k-1}) + (4\sqrt{2} + 8\sqrt{5})\zeta_2 + (1 - \zeta_1 - \zeta_2) SO(\acute{R}SC_k^3) + (1 - \zeta_1 - \zeta_2)(4\sqrt{2} + 8\sqrt{5})$$

$$E_k^{SO} = SO(\acute{R}SC_{k-1}) + (6\sqrt{2} - 4\sqrt{5})\zeta_1 + (4\sqrt{2} + 8\sqrt{5}) \tag{16}$$

Since $E[E_k]^{SO} = E_k^{SO}$ so apply the operator E on Equation 16, we get:

$$E_k^{SO} = E_{k-1}^{SO} + (6\sqrt{2} - 4\sqrt{5})\zeta_1 + (4\sqrt{2} + 8\sqrt{5}), \quad k > 2 \tag{17}$$

and after solving the recurrence relation in Equation 17 with $E_2^{SO} = 16\sqrt{2} + 8\sqrt{5}$, we get:

$$E_k^{SO} = [(6\sqrt{2} - 4\sqrt{5})\zeta_1 + (4\sqrt{2} + 8\sqrt{5})]k - (12\sqrt{2} - 8\sqrt{5})\zeta_1 + (8\sqrt{2} - 8\sqrt{5})$$

5-2-Theorem

Let $\acute{R}SC(k; \zeta_1, \zeta_2)$ be an arbitrary spiro chain of length k , where $k \geq 2$. Then;

$$E_k^{red} = [(4\sqrt{2} - 2\sqrt{10})\zeta_1 + (2\sqrt{2} + 4\sqrt{10})]k - (8\sqrt{2} - 4\sqrt{10})\zeta_1 + (4\sqrt{2} - 4\sqrt{10}).$$

Proof: For $k = 2$, we have $E_2^{red} = 8\sqrt{2} + 4\sqrt{10}$. Now, when $k \geq 3$, it is obvious that ω_{22}, ω_{24} and ω_{44} depend on the following three cases:

1. If $\acute{R}SC_{k-1} \rightarrow \acute{R}SC_k^1$ with probability ζ_1

$$\omega_{22}(\acute{R}SC_k^1) = \omega_{22}(\acute{R}SC_{k-1}) + 3$$

$$\omega_{24}(\acute{R}SC_k^1) = \omega_{24}(\acute{R}SC_{k-1}) + 2$$

$$\omega_{44}(\acute{R}SC_k^1) = \omega_{44}(\acute{R}SC_{k-1}) + 1$$

by using Equation 14:

$$SO_{red}(\acute{R}SC_k^1) = SO_{red}(\acute{R}SC_{k-1}) + 6\sqrt{2} + 2\sqrt{10}$$

2. If $\acute{R}SC_{k-1} \rightarrow \acute{R}SC_k^2$ with probability ζ_2

$$\omega_{22}(\acute{R}SC_k^2) = \omega_{22}(\acute{R}SC_{k-1}) + 2$$

$$\omega_{24}(\acute{R}SC_k^2) = \omega_{24}(\acute{R}SC_{k-1}) + 4$$

$$\omega_{44}(\acute{R}SC_k^2) = \omega_{44}(\acute{R}SC_{k-1})$$

by using Equation 14:

$$SO_{red}(\acute{R}SC_k^2) = SO_{red}(\acute{R}SC_{k-1}) + 2\sqrt{2} + 4\sqrt{10}$$

3. If $\acute{R}SC_{k-1} \rightarrow \acute{R}SC_k^3$ with probability $1 - \zeta_1 - \zeta_2$

$$\omega_{22}(\acute{R}SC_k^3) = \omega_{22}(\acute{R}SC_{k-1}) + 2$$

$$\omega_{24}(\acute{R}SC_k^3) = \omega_{24}(\acute{R}SC_{k-1}) + 4$$

$$\omega_{44}(\acute{R}SC_k^3) = \omega_{44}(\acute{R}SC_{k-1})$$

by using Equation 14:

$$SO_{red}(\acute{R}SC_k^3) = SO_{red}(\acute{R}SC_{k-1}) + 2\sqrt{2} + 4\sqrt{10}$$

Thus:

$$E_k^{red} = \zeta_1 SO_{red}(\acute{R}SC_k^1) + \zeta_2 SO_{red}(\acute{R}SC_k^2) + (1 - \zeta_1 - \zeta_2) SO_{red}(\acute{R}SC_k^3)$$

$$E_k^{red} = \zeta_1 SO_{red}(\acute{R}SC_{k-1}) + (6\sqrt{2} + 2\sqrt{10})\zeta_1 + \zeta_2 SO_{red}(\acute{R}SC_{k-1}) + (2\sqrt{2} + 4\sqrt{10})\zeta_2 + (1 - \zeta_1 - \zeta_2) SO_{red}(\acute{R}SC_{k-1}) + (1 - \zeta_1 - \zeta_2)(2\sqrt{2} + 4\sqrt{10})$$

$$E_k^{red} = SO_{red}(\acute{R}SC_{k-1}) + (4\sqrt{2} - 2\sqrt{10})\zeta_1 + (2\sqrt{2} + 4\sqrt{10}) \tag{18}$$

Since $E[E_k]^{red} = E_k^{red}$ so apply the operator E on Equation 18, we get;

$$E_k^{red} = E_{k-1}^{red} + (4\sqrt{2} - 2\sqrt{10})\zeta_1 + (2\sqrt{2} + 4\sqrt{10}), \quad k > 2 \tag{19}$$

and after solving the recurrence relation in Equation 19 with initial condition, we get:

$$E_k^{red} = [(4\sqrt{2} - 2\sqrt{10})\zeta_1 + (2\sqrt{2} + 4\sqrt{10})]k - (8\sqrt{2} - 4\sqrt{10})\zeta_1 + (4\sqrt{2} - 4\sqrt{10})$$

5-3-Theorem

Let $\acute{R}SC(k; \zeta_1, \zeta_2)$ be an arbitrary spiro chain of length k , where $k \geq 2$. Then;

$$E_k^{avg} = \left[\left(\frac{10\sqrt{2}k+2\sqrt{2}}{5k+1} - \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) \zeta_1 + \left(\frac{4\sqrt{2}k-4\sqrt{2}}{5k+1} + \frac{8\sqrt{17k^2+14k+5}}{5k+1} \right) \right] k - \left(\frac{20\sqrt{2}k+4\sqrt{2}}{5k+1} - \frac{8\sqrt{17k^2+14k+5}}{5k+1} \right) \zeta_1 + \left(\frac{8\sqrt{2}k-4\sqrt{2}}{5k+1} + \frac{16\sqrt{17k^2+14k+5}}{5k+1} \right) + \frac{16\sqrt{2}}{11} + \frac{8\sqrt{101}}{11}$$

Proof: For $k = 2$, we have $E_2^{avg} = \frac{16\sqrt{2}}{11} + \frac{8\sqrt{101}}{11}$. Now, when $k \geq 3$, it is obvious that ω_{22}, ω_{24} and ω_{44} depend on the following three cases:

1. If $\acute{R}SC_{k-1} \rightarrow \acute{R}SC_k^1$ with probability ζ_1

$$\omega_{22}(\acute{R}SC_k^1) = \omega_{22}(\acute{R}SC_{k-1}) + 3$$

$$\omega_{24}(\acute{R}SC_k^1) = \omega_{24}(\acute{R}SC_{k-1}) + 2$$

$$\omega_{44}(\acute{R}SC_k^1) = \omega_{44}(\acute{R}SC_{k-1}) + 1$$

by using Equation 15:

$$SO_{avg}(\acute{R}SC_k^1) = SO_{avg}(\acute{R}SC_{k-1}) + \left(\frac{14\sqrt{2}k-2\sqrt{2}}{5k+1} \right) + \left(\frac{4\sqrt{17k^2+14k+5}}{5k+1} \right)$$

2. If $\acute{R}SC_{k-1} \rightarrow \acute{R}SC_k^2$ with probability ζ_2

$$\omega_{22}(\dot{R}SC_k^2) = \omega_{22}(\dot{R}SC_{k-1}) + 2$$

$$\omega_{24}(\dot{R}SC_k^2) = \omega_{24}(\dot{R}SC_{k-1}) + 4$$

$$\omega_{44}(\dot{R}SC_k^2) = \omega_{44}(\dot{R}SC_{k-1})$$

by using Equation 15:

$$SO_{avg}(\dot{R}SC_k^2) = SO_{avg}(\dot{R}SC_{k-1}) + 4\sqrt{2} \left(\frac{k-1}{5k+1} \right) + \left(\frac{8\sqrt{17k^2+14k+5}}{5k+1} \right)$$

3. If $\dot{R}SC_{k-1} \rightarrow \dot{R}SC_k^3$ with probability $1 - \zeta_1 - \zeta_2$

$$\omega_{22}(\dot{R}SC_k^3) = \omega_{22}(\dot{R}SC_{k-1}) + 2$$

$$\omega_{24}(\dot{R}SC_k^3) = \omega_{24}(\dot{R}SC_{k-1}) + 4$$

$$\omega_{44}(\dot{R}SC_k^3) = \omega_{44}(\dot{R}SC_{k-1})$$

by using Equation 15:

$$SO_{avg}(\dot{R}SC_k^3) = SO_{avg}(\dot{R}SC_{k-1}) + 4\sqrt{2} \left(\frac{k-1}{5k+1} \right) + \left(\frac{8\sqrt{17k^2+14k+5}}{5k+1} \right)$$

Thus:

$$E_k^{avg} = \zeta_1 SO_{avg}(\dot{R}SC_k^1) + \zeta_2 SO_{avg}(\dot{R}SC_k^2) + (1 - \zeta_1 - \zeta_2) SO_{avg}(\dot{R}SC_k^3)$$

$$E_k^{avg} = \zeta_1 SO_{avg}(\dot{R}SC_{k-1}) + \left[\left(\frac{14\sqrt{2}k-2\sqrt{2}}{5k+1} \right) + \left(\frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) \right] \zeta_1 + \zeta_2 SO_{avg}(\dot{R}SC_{k-1}) + \left[\left(\frac{4\sqrt{2}k-4\sqrt{2}}{5k+1} \right) + \left(\frac{8\sqrt{17k^2+14k+5}}{5k+1} \right) \right] \zeta_2 + (1 - \zeta_1 - \zeta_2) SO_{avg}(\dot{R}SC_k^3) + (1 - \zeta_1 - \zeta_2) \left[\left(\frac{4\sqrt{2}k-4\sqrt{2}}{5k+1} \right) + \left(\frac{8\sqrt{17k^2+14k+5}}{5k+1} \right) \right]$$

$$E_k^{avg} = SO_{avg}(\dot{R}SC_{k-1}) + \left[\frac{10\sqrt{2}k+2\sqrt{2}}{5k+1} - \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right] \zeta_1 + \left[\frac{4\sqrt{2}k-4\sqrt{2}}{5k+1} + \frac{8\sqrt{17k^2+14k+5}}{5k+1} \right] \zeta_2 \quad (20)$$

Since $E[E_k]^{avg} = E_k^{avg}$ so apply the operator E on Equation 20, we get:

$$E_k^{avg} = E_{k-1}^{avg} + \left[\frac{10\sqrt{2}k+2\sqrt{2}}{5k+1} - \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right] \zeta_1 + \left[\frac{4\sqrt{2}k-4\sqrt{2}}{5k+1} + \frac{8\sqrt{17k^2+14k+5}}{5k+1} \right] \zeta_2, \quad k > 2 \quad (21)$$

And after solving the recurrence relation in Equation 21 with initial condition, we get:

$$E_k^{avg} = \left[\left(\frac{10\sqrt{2}k+2\sqrt{2}}{5k+1} - \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) \zeta_1 + \left(\frac{10\sqrt{2}k+2\sqrt{2}}{5k+1} - \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) \right] k - \left(\frac{20\sqrt{2}k+4\sqrt{2}}{5k+1} - \frac{8\sqrt{17k^2+14k+5}}{5k+1} \right) \zeta_1 - \left(\frac{8\sqrt{2}k-8\sqrt{2}}{5k+1} + \frac{16\sqrt{17k^2+14k+5}}{5k+1} \right) \zeta_2 + \frac{16\sqrt{2}}{11} + \frac{8\sqrt{101}}{11}.$$

These indices can be computed for three chains meta $\overline{M}_k = \dot{R}SC(k; 0,1)$, para $\overline{P}_k = \dot{R}SC(k; 0,0)$ and ortho $\overline{O}_k = \dot{R}SC(k; 1,0)$ as shown in Figure 5.

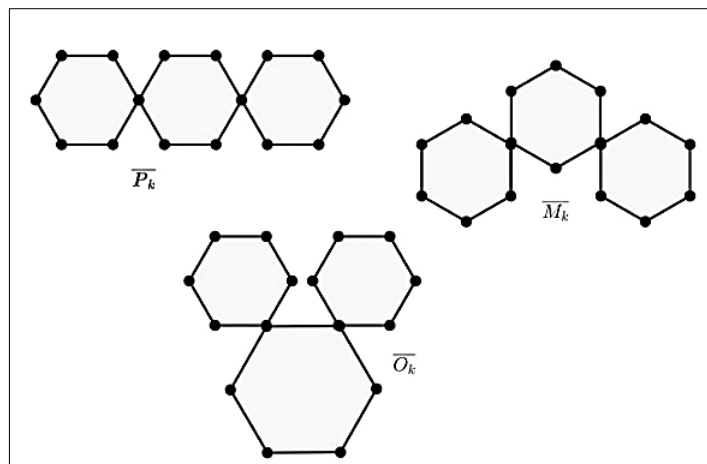


Figure 5. Special spiro ortho, meta and para chains

5-4-Corollary

For $k \geq 2$, we have:

$$\bullet SO(\overline{O}_k) = (10\sqrt{2} + 4\sqrt{5})k - 4\sqrt{2}$$

$$\bullet SO(\overline{P}_k) = SO(\overline{M}_k) = (4\sqrt{2} + 8\sqrt{5})k + (8\sqrt{2} - 8\sqrt{5})$$

$$\bullet SO_{red}(\overline{O}_k) = (6\sqrt{2} + 2\sqrt{10})k - 4\sqrt{2}$$

$$\bullet SO_{red}(\overline{P}_k) = SO_{red}(\overline{M}_k) = (2\sqrt{2} + 4\sqrt{10})k + (4\sqrt{2} - 4\sqrt{10})$$

$$\bullet SO_{avg}(\overline{O}_k) = \left(\frac{14\sqrt{2}k + 4\sqrt{2}}{5k+1} + \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) k + \frac{28\sqrt{2}k}{5k+1} + \frac{4\sqrt{2}}{5k+1} - \frac{8\sqrt{17k^2+14k+5}}{5k+1} + \frac{16\sqrt{2}}{11} + \frac{8\sqrt{101}}{11}$$

$$\bullet SO_{avg}(\overline{P}_k) = SO_{avg}(\overline{M}_k) = \left(\frac{4\sqrt{2}k - 4\sqrt{2}}{5k+1} + \frac{8\sqrt{17k^2+14k+5}}{5k+1} \right) k + \frac{28\sqrt{2}k}{5k+1} + \frac{4\sqrt{2}}{5k+1} - \frac{8\sqrt{17k^2+14k+5}}{5k+1} + \frac{16\sqrt{2}}{11} + \frac{8\sqrt{101}}{11}$$

6- Average Value of Indices for Spiro Chain

In this part, the average value of SO , SO_{red} and SO_{avg} have been resolved for the set of arbitrary spiro chain. The average values over the set SP_k are:

$$SO_{avg}(SP_k) = \frac{1}{|SP_k|} \sum_{G \in SP_k} SO(G)$$

$$(SO_{red})_{avg}(SP_k) = \frac{1}{|SP_k|} \sum_{G \in SP_k} SO_{red}(G)$$

$$(SO_{avg})_{avg}(SP_k) = \frac{1}{|SP_k|} \sum_{G \in SP_k} SO_{avg}(G)$$

As a result $\zeta_1 = \zeta_2 = 1 - \zeta_1 - \zeta_2$, we can use theorems (5-1, 5-2, 5-3) by setting $\zeta_1 = \zeta_2 = 1 - \zeta_1 - \zeta_2 = \frac{1}{3}$ and the results will be in the form of following expression:

6-1-Theorem

Let SP_k be the set of spiro chain, then;

$$SO(\overline{RP}_k) = \left[16\sqrt{2} + \frac{20\sqrt{5}}{3} \right] k + 4\sqrt{2} - \frac{16\sqrt{5}}{3}$$

$$SO_{red}(\overline{RP}_k) = \left[\frac{10\sqrt{2}}{3} + \frac{10\sqrt{10}}{3} \right] k + \frac{4\sqrt{2}}{3} - \frac{8\sqrt{10}}{3}$$

$$SO_{avg}(\overline{RP}_k) = \left[\frac{22\sqrt{2}k}{3(5k+1)} - \frac{10\sqrt{2}}{3(5k+1)} + \frac{20\sqrt{17k^2+14k+5}}{3(5k+1)} \right] k - \frac{44\sqrt{2}}{3(5k+1)} + \frac{20\sqrt{2}}{3(5k+1)} - \frac{40\sqrt{17k^2+14k+5}}{3(5k+1)} + \frac{16\sqrt{2}}{11} + \frac{8\sqrt{101}}{11}$$

from corollary (5-4);

$$\frac{1}{3} [SO(\overline{O}_k) + SO(\overline{P}_k) + SO(\overline{M}_k)] = \left[16\sqrt{2} + \frac{20\sqrt{5}}{3} \right] k + 4\sqrt{2} - \frac{16\sqrt{5}}{3}$$

$$\frac{1}{3} [SO_{red}(\overline{O}_k) + SO_{red}(\overline{P}_k) + SO_{red}(\overline{M}_k)] = \left[\frac{10\sqrt{2}}{3} + \frac{10\sqrt{10}}{3} \right] k + \frac{4\sqrt{2}}{3} - \frac{8\sqrt{10}}{3}$$

$$\frac{1}{3} [SO_{avg}(\overline{O}_k) + SO_{avg}(\overline{P}_k) + SO_{avg}(\overline{M}_k)] = \left[\frac{22\sqrt{2}k}{3(5k+1)} - \frac{10\sqrt{2}}{3(5k+1)} + \frac{20\sqrt{17k^2+14k+5}}{3(5k+1)} \right] k - \frac{44\sqrt{2}}{3(5k+1)} + \frac{20\sqrt{2}}{3(5k+1)} - \frac{40\sqrt{17k^2+14k+5}}{3(5k+1)} + \frac{16\sqrt{2}}{11} + \frac{8\sqrt{101}}{11}$$

Thus, the average value of these indices $SO(\overline{RSC}(k, \zeta_1, \zeta_2))$, $SO_{red}(\overline{RSC}(k, \zeta_1, \zeta_2))$ or $SO_{avg}(\overline{RSC}(k, \zeta_1, \zeta_2))$ is equal to the average value of the special chains in the set $\{\overline{O}_k, \overline{P}_k, \overline{M}_k\}$.

7- Ratio between Sombor, Reduced Sombor and Average Sombor Index for Spiro Chain

By getting results from theorem (5-1, 5-2) and (5-3), we will make the ratio between the expected values for the SO , SO_{red} and SO_{avg} with the same probabilities ζ_1 and ζ_2 of a random spiro-chain.

7-1-Theorem

If $k \geq 2$, then:

$$E^{SO}[\text{SO}(\acute{R}SC(k, \zeta_1, \zeta_2))] > E^{\text{red}}[\text{redSO}(\acute{R}SC(k, \zeta_1, \zeta_2))].$$

Proof: The statement is true for $k = 2$. Thus for $k > 2$, by applying theorem (5-1) and (5-2), we get;

$$\begin{aligned} E^{SO}[\text{SO}(\acute{R}SC(k, \zeta_1, \zeta_2))] - E^{\text{red}}[\text{redSO}(\acute{R}SC(k, \zeta_1, \zeta_2))] &= \{[(6\sqrt{2} - 4\sqrt{5})\zeta_1 + (4\sqrt{2} + 8\sqrt{5})](k-2) + \\ & (16\sqrt{2} + 8\sqrt{5})\} - \{[(4\sqrt{2} - 2\sqrt{10})\zeta_1 + (2\sqrt{2} + 4\sqrt{10})](k-2) + (8\sqrt{2} + 4\sqrt{10})\} \\ &= [(2\sqrt{2} - 4\sqrt{5} + 2\sqrt{10})\zeta_1 + (2\sqrt{2} + 8\sqrt{5} - 4\sqrt{10})](k-2) + (8\sqrt{2} + 8\sqrt{5} - 4\sqrt{5}) \end{aligned}$$

Since;

$$(2\sqrt{2} - 4\sqrt{5} + 2\sqrt{10}) > 0, (2\sqrt{2} + 8\sqrt{5} - 4\sqrt{10}) > 0, (8\sqrt{2} + 8\sqrt{5} - 4\sqrt{5}) > 0$$

So;

$$= [(2\sqrt{2} - 4\sqrt{5} + 2\sqrt{10})\zeta_1 + (2\sqrt{2} + 8\sqrt{5} - 4\sqrt{10})](k-2) + (8\sqrt{2} + 8\sqrt{5} - 4\sqrt{5}) > 0,$$

$$\because k \geq 2, 0 < \zeta_1 < 1$$

7-2-Theorem

If $k \geq 2$, then;

$$E^{\text{red}}[\text{redSO}(\acute{R}SC(k, \zeta_1, \zeta_2))] > E^{\text{avg}}[\text{avgSO}(\acute{R}SC(k, \zeta_1, \zeta_2))].$$

Proof: The statement is true for $k = 2$. Thus for $k > 2$, by applying theorem (5-2) and (5-3), we get:

$$\begin{aligned} E^{\text{red}}[\text{redSO}(\acute{R}SC(k, \zeta_1, \zeta_2))] - E^{\text{avg}}[\text{avgSO}(\acute{R}SC(k, \zeta_1, \zeta_2))] &= \{[(4\sqrt{2} - 2\sqrt{10})\zeta_1 + (2\sqrt{2} + 4\sqrt{10})](k-2) + \\ & (8\sqrt{2} + 4\sqrt{10})\} - \left\{ \left[\left(\frac{10\sqrt{2}k+2\sqrt{2}}{5k+1} - \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) \zeta_1 + \left(\frac{4\sqrt{2}k-4\sqrt{2}}{5k+1} + \frac{8\sqrt{17k^2+14k+5}}{5k+1} \right) \right] (k-2) + \left(\frac{16\sqrt{2}}{11} + \frac{8\sqrt{101}}{11} \right) \right\} \\ &= \left[\left(2\sqrt{2} - 2\sqrt{10} + \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) \zeta_1 + \left(\frac{16\sqrt{2}(k+1)}{5k+1} + 4\sqrt{10} - \frac{8\sqrt{17k^2+14k+5}}{5k+1} \right) \right] (k-2) + \left(\frac{72\sqrt{2}}{11} + 4\sqrt{10} - \frac{8\sqrt{101}}{11} \right) \\ &= \left[\left(2\sqrt{10} - \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) (2 - \zeta_1) + \left(2\sqrt{10} + \frac{16\sqrt{2}(k+1)}{5k+1} \right) \right] (k-2) + \left(\frac{72\sqrt{2}}{11} + 4\sqrt{10} - \frac{8\sqrt{101}}{11} \right) \end{aligned}$$

Since;

$$\left(2\sqrt{10} - \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) > 0, \left(2\sqrt{10} + \frac{16\sqrt{2}(k+1)}{5k+1} \right) > 0, \left(\frac{72\sqrt{2}}{11} + 4\sqrt{10} - \frac{8\sqrt{101}}{11} \right) > 0, k \geq 2$$

So;

$$= \left[\left(2\sqrt{10} - \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) (2 - \zeta_1) + \left(2\sqrt{10} + \frac{16\sqrt{2}(k+1)}{5k+1} \right) \right] (k-2) + \left(\frac{72\sqrt{2}}{11} + 4\sqrt{10} - \frac{8\sqrt{101}}{11} \right) > 0, \because k \geq 2, 0 < \zeta_1 < 1$$

7-3-Theorem

If $k \geq 2$, then;

$$E^{SO}[\text{SO}(\acute{R}SC(k, \zeta_1, \zeta_2))] > E^{\text{avg}}[\text{avgSO}(\acute{R}SC(k, \zeta_1, \zeta_2))].$$

Proof: The statement is true for $k = 2$. Thus for $k > 2$, by applying theorem (5-1) and (5-3) we get;

$$\begin{aligned} E^{SO}[\text{SO}(\acute{R}SC(k, \zeta_1, \zeta_2))] - E^{\text{avg}}[\text{avgSO}(\acute{R}SC(k, \zeta_1, \zeta_2))] &= \{[(6\sqrt{2} - 4\sqrt{5})\zeta_1 + (4\sqrt{2} + 8\sqrt{5})](k-2) + \\ & (16\sqrt{2} + 8\sqrt{5})\} - \left\{ \left[\left(\frac{10\sqrt{2}k+2\sqrt{2}}{5k+1} - \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) \zeta_1 + \left(\frac{4\sqrt{2}k-4\sqrt{2}}{5k+1} + \frac{8\sqrt{17k^2+14k+5}}{5k+1} \right) \right] (k-2) + \left(\frac{16\sqrt{2}}{11} + \frac{8\sqrt{101}}{11} \right) \right\} \\ &= \left[\left(4\sqrt{2} - 4\sqrt{5} + \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) \zeta_1 + \left(14\sqrt{2} \left(\frac{19k+5}{5k+1} \right) + 8\sqrt{5} - \frac{8\sqrt{17k^2+14k+5}}{5k+1} \right) \right] (k-2) + \left(\frac{160\sqrt{2}}{11} + 8\sqrt{5} - \frac{8\sqrt{101}}{11} \right) \\ &= \left[\left(4\sqrt{5} - \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) (2 - \zeta_1) + \left(4\sqrt{2} + 14\sqrt{2} \left(\frac{19k+5}{5k+1} \right) \right) \right] (k-2) + \left(\frac{160\sqrt{2}}{11} + 8\sqrt{5} - \frac{8\sqrt{101}}{11} \right) \end{aligned}$$

Since

$$\left(4\sqrt{5} - \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) > 0, \left(4\sqrt{2} + 14\sqrt{2} \left(\frac{19k+5}{5k+1} \right) \right) > 0, \left(\frac{160\sqrt{2}}{11} + 8\sqrt{5} - \frac{8\sqrt{101}}{11} \right) > 0, k \geq 2.$$

So;

$$= \left[\left(4\sqrt{5} - \frac{4\sqrt{17k^2+14k+5}}{5k+1} \right) (2 - \zeta_1) + \left(4\sqrt{2} + 14\sqrt{2} \left(\frac{19k+5}{5k+1} \right) \right) \right] (k - 2) + \left(\frac{160\sqrt{2}}{11} + 8\sqrt{5} - \frac{8\sqrt{101}}{11} \right) > 0, \because k \geq 2, 0 < \zeta_1 < 1.$$

7-4-Corollary

For $k \geq 2$, $E^{SO}[SO(\acute{R}SC(k, \zeta_1, \zeta_2))] > E^{red}[\text{red}SO(\acute{R}SC(k, \zeta_1, \zeta_2))] > E^{avg}[\text{avg}SO(\acute{R}SC(k, \zeta_1, \zeta_2))]$ as shown in Figure 6:

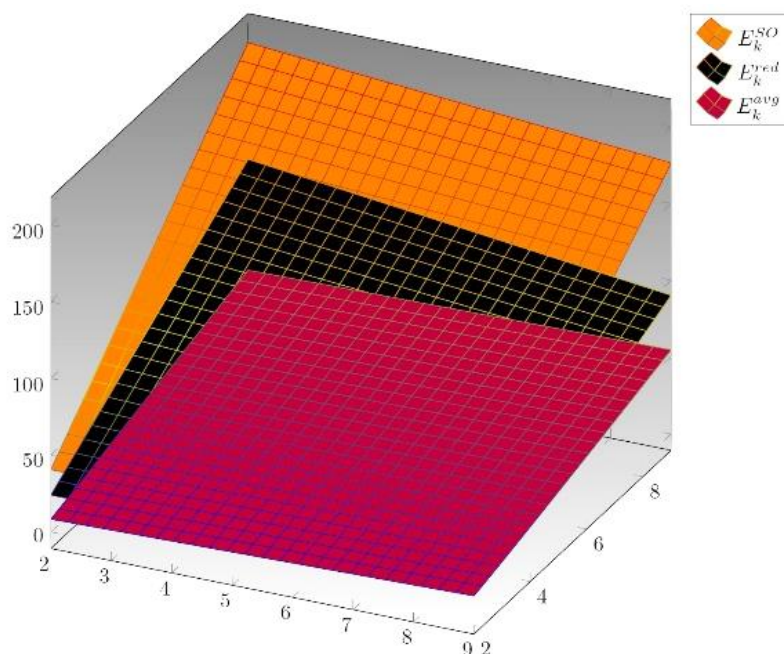


Figure 3. Comparison between the expected values of Sombor E_k^{SO} (blue), reduced Sombor E_k^{red} (red) and average Sombor E_k^{avg} (green) index in random spiro chains

8- Conclusion

The study of topological index is very helpful in discovering the basic topologies of different networks. Gutman introduced the SO index as a new indicator of mathematical formulation. Many topological indices are described in the literature, and many of them have been found to have applications such as physical modeling, chemical, pharmaceutical, and other molecular properties. We have discussed the SO , SO_{red} and SO_{avg} to find the expected value of random Polyphenyl chains and random spiro-chain. The average value of indices for both chains have been resolved. Finally, we have computed the comparison between the expected value of all Sombor indices. Figures 4 and 6 show that the expected value of the Sombor index is always greater than the other two mentioned indices. One can also deduce from it that the Sombor index is much better correlated, as compared to the other indices, with the physical properties of the compounds which are formed by these chains. Finding chemical applications for this Sombor index is an alluring task for the near future. We are also interested in building new networks and studying their geographical indications, which will greatly help to understand their priorities.

9- Declarations

9-1-Author Contributions

Conceptualization, Z.R.; methodology, Z.R.; software, K.N.; validation, Z.R., K.N. and S.A.; formal analysis, Z.R.; investigation, S.A.; resources, Z.R.; data curation, K.N.; writing—original draft preparation, Z.R.; writing—review and editing, K.N. and S.A.; visualization, K.N.; supervision, S.A.; project administration, Z.R.; funding acquisition, Z.R. All authors have read and agreed to the published version of the manuscript.

9-2-Data Availability Statement

The data presented in this study are available on request from the corresponding author.

9-3- Funding

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9-4- Conflicts of Interest

The authors declare that there is no conflict of interests regarding the publication of this manuscript. In addition, the ethical issues, including plagiarism, informed consent, misconduct, data fabrication and/or falsification, double publication and/or submission, and redundancies have been completely observed by the authors.

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