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NON-NEIGHBOR TOPOLOGICAL INDICES OF HONEYCOMB NETWORKS

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Abstract Chemical graph theory is used as a tool to analyze chemical compounds using graph theory as a mathematical model. In this field, bioactivity of the chemical compounds can be predicted using topological index. Honeycomb network represents benzenoid hydrocarbons in chemistry. In this article, we study chemical graph of honeycomb networks and obtain an explicit formula for some non-neighbor topological indices of the line graphs of subdivision graphs of honeycomb networks which are helpful in studying the underlying topologies of these network. And also given the graphical representation to analyze the variation of non-neighbor indices for considered structures.

1 Introduction

In chemical graph theory, study of characteristics of the graph is important to understand the behaviour of the chemical combination, to understand the growth of the chemical combination and to make its comparison with other chemical combinations. In the analysis of structure-property relationships, especially in QSPR / QSAR studies, the application of molecular structure indices is now a standard procedure. Due to the chemical importance of these indices, the number of proposed molecular descriptors has increased rapidly in the last few years. The characteristics of the entire graph may be represented by a single value or a polynomial. This single value is called the topological index. It is possible to further categorize topological indices into various forms on the basis of their calculation criteria. Degree-based topological descriptors play a vital role in chemical graph theory. They involve calculations based on the degree of vertices of the graph.

Throughout the paper, $\mathcal{H}$ be a simple, connected and undirected graph. $V(\mathcal{H})$ and $E(\mathcal{H})$ be the vertex set and the edge set of $\mathcal{H}$, respectively and the degree of a vertex $a \in V(\mathcal{H})$ be represented as d_a.

The first and most investigated topological index in chemical graph theory is the Wiener index. In 1947, Wiener [13] introduced the topological index (Wiener index), while studying the boiling point of paraffin. This Wiener index has many applications in chemical graph theory [4, 5]. Randic introduced the Randic index, defined as $R(\mathcal{H}) = \sum_{ab\in E(\mathcal{H})} \frac{1}{\sqrt{d_a\ d_b}}$. The Randic index was generalized and is called as the general Randic index which is defined as $R_\alpha(\mathcal{H}) = \sum_{ab\in E(\mathcal{H})}(d_a\ d_b)^\alpha$, where α is a real number. Zhou proposed the general sum-connectivity index and defined as $\chi_\alpha(\mathcal{H}) = \sum_{ab\in E(\mathcal{H})}(d_a + d_b)^\alpha$, where α is a real number. The first general Zagreb index was introduced by Li and Zhao [10], defined as $M_\alpha(\mathcal{H}) = \sum_{a\in V(\mathcal{H})}(d_a)^\alpha$, where α is a real number. Estrada et al. introduced the atom-bond Connectivity (ABC) index which is given as $ABC(\mathcal{H}) = \sum_{ab\in E(\mathcal{H})} \sqrt{\frac{d_a+d_b-2}{d_a\ d_b}}$. The geometric-arithmetic (GA) index was introduced by Vukicevic and defined as $GA(\mathcal{H}) = \sum_{ab\in E(\mathcal{H})} \frac{2\sqrt{d_a\ d_b}}{d_a+d_b}$. A brief survey and a comparative study of these degree based indices is done in [6].

Let s_a be the sum of the degree of neighbour vertices in $\mathcal{H}$: $s_a = \sum_{b\in N_a} d_b$, where $N_a = \{b \in V(\mathcal{H}) | ab \in E(\mathcal{H})\}$, is known as the set of neighbour vertices of a. Ghorbani and Hosseinzadeh [7] in 2010 have introduced the fourth member of the class of ABC index which is given as $ABC_4(\mathcal{H}) = \sum_{ab\in E(\mathcal{H})} \sqrt{\frac{s_a+s_b-2}{s_a\ s_b}}$. In 2011, fifth version of GA index was proposed by Graovac

[8] and defined as $GA_5(\mathcal{H}) = \sum_{ab\in E(\mathcal{H})} \frac{2\sqrt{s_a\ s_b}}{s_a+s_b}$.

Motivated by these works, we define the non-neighbor indices. We define a set $\overline{N_{\mathcal{H}}(a)}$ of non-neighbors of a vertex a as $\overline{N_{\mathcal{H}}(a)} = \{b \in V(\mathcal{H}) : d(a,b) \neq 1\}$ and a non-neighbor degree $\overline{d_a}$ of a as $\overline{d_a} = p - 1 - d_a$, where p is the order of the graph $\mathcal{H}$. Throughout this paper we use the notation NN for non-neighbor. Some of the study on non-neighbor topological indices can be referred in [2, 3, 11].

Let $\overline{s_a}$ be the sum of the non-neighbor degree of the neighbour vertices of $a \in V(\mathcal{H})$: $\overline{s_a} = \sum_{b\in N_a} \overline{d_b}$, where $N_a = \{b \in V(\mathcal{H}) | ab \in E(\mathcal{H})\}$, is known as the set of neighbour vertices of $a \in V(\mathcal{H})$ and α be a real number. Following definitions are introduced and studied in this paper.

Definition 1.1. NN first general Zagreb index: $\overline{M_\alpha(\mathcal{H})} = \sum_{a\in V(\mathcal{H})} \left(\overline{d_a}\right)^\alpha$

Definition 1.2. NN general Randic index: $\overline{R_\alpha(\mathcal{H})} = \sum_{ab\in E(\mathcal{H})} \left(\overline{d_a}\ \overline{d_b}\right)^\alpha$

Definition 1.3. NN general sum-connectivity index: $\overline{\chi_\alpha(\mathcal{H})} = \sum_{ab\in E(\mathcal{H})} \left(\overline{d_a} + \overline{d_b}\right)^\alpha$

Definition 1.4. NN ABC index: $\overline{ABC(\mathcal{H})} = \sum_{ab\in E(\mathcal{H})} \sqrt{\frac{\overline{d_a}+\overline{d_b}-2}{\overline{d_a}\ \overline{d_b}}}$

Definition 1.5. NN GA index: $\overline{GA(\mathcal{H})} = \sum_{ab\in E(\mathcal{H})} \frac{2\sqrt{\overline{d_a}\ \overline{d_b}}}{\overline{d_a}+\overline{d_b}}$

Definition 1.6. NN ABC_4 index: $\overline{ABC_4(\mathcal{H})} = \sum_{ab\in E(\mathcal{H})} \sqrt{\frac{\overline{s_a}+\overline{s_b}-2}{\overline{s_a}\ \overline{s_b}}}$

Definition 1.7. NN GA_5 index: $\overline{GA_5(\mathcal{H})} = \sum_{ab\in E(\mathcal{H})} \frac{2\sqrt{\overline{s_a}\ \overline{s_b}}}{\overline{s_a}+\overline{s_b}}$

The study of topological for derived graphs such as line graph, subdivision graph, middle graph and total graph is an interesting area of research. The line graph of a graph $\mathcal{H}$ is represented as $L(\mathcal{H})$, whose vertices are the edges of $\mathcal{H}$, with $a, b \in E(L(\mathcal{H}))$ when a and b have a common endpoint in $\mathcal{H}$. The graph $S(\mathcal{H})$ depicts the subdivision graph of $\mathcal{H}$ which is obtained by inserting an additional vertex into each edge of $\mathcal{H}$. Related work can be referred in [9].

In this paper, we study the derived graph of honeycomb networks and obtain an explicit formula for above defined non-neighbor topological indices which are helpful in studying the underlying topologies of these network. And also given the graphical representation to analyze the variation of non-neighbor indices for considered structures.

2 Honeycomb networks

Honeycomb networks are widely used in computer graphics [12], cellular phone base stations, image processing, and in chemistry as the representation of benzenoid hydrocarbons. Honeycomb networks are obtained by recursively using hexagonal tiling in a particular pattern. HC_p is a p-dimensional honeycomb network, where p is the number of hexagons between the central and boundary hexagon. Honeycomb network HC_p is constructed from HC_{p-1} by adding a layer of hexagons around boundary of HC_{p-1}. The number of vertices in HC_p are $6n^2$ and number of edges are $9n^2 - 3n$.

Figure 1 is a graph of honeycomb networks HC_3 and subdivision graph of HC_3. The line graph of subdivision graph of honeycomb networks HC_3 is shown in Figure 2. We denote, honeycomb networks HC_p as $\mathcal{H}$ and line graph of subdivision graph of honeycomb networks as $L(S(\mathcal{H}))$.

In this section, we compute the first general Zagreb index, general Randic index, general sum connectivity index, ABC index, GA index, ABC_4 index and GA_5 index of line graph of subdivision graph of HC_p.

Theorem 2.1. *Let $\mathcal{A} = L(S(\mathcal{H}))$, where $\mathcal{H}$ be the graph of honeycomb networks HC_p $(p \geq 1)$. Then,*

(i) $\overline{M_\alpha(\mathcal{A})} = 18p(p-1)(k-4)^\alpha + 12p(k-3)^\alpha$

(ii) $\overline{R_\alpha(\mathcal{A})} = 12(p-1)(k-3)^\alpha(k-4)^\alpha + 6(p+1)(k-3)^{2\alpha} + 3(9p^2 - 11p + 2)(k-4)^{2\alpha}$

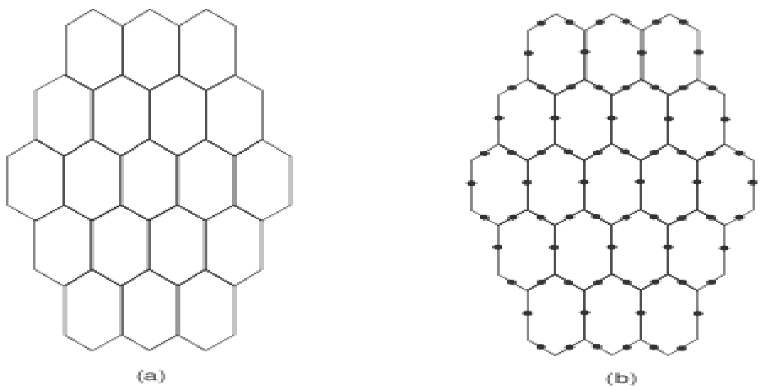

Figure 1. (a) Honeycomb networks HC_3, (b) subdivision of honeycomb networks HC_3.

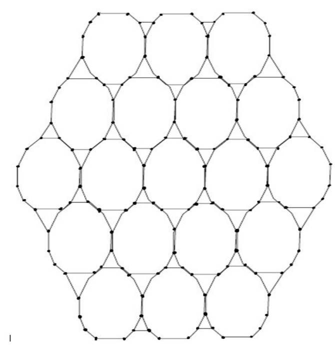

Figure 2. $L(S(HC_3))$.

(iii) $\overline{\chi_\alpha(\mathcal{A})} = 12(p-1)(2k-7)^\alpha + 6(p+1)2^\alpha(k-3)^\alpha + 3(9p^2-11p+2)2^\alpha(k-4)^\alpha$

(iv) $\overline{ABC(\mathcal{A})} = 12(p-1)\sqrt{\frac{2k-9}{(k-3)(k-4)}} + 6\sqrt{2}(p+1)\frac{\sqrt{k-4}}{k-3} + 3\sqrt{2}(9p^2-11p+2)\frac{\sqrt{k-5}}{k-4}$

(v) $\overline{GA(\mathcal{A})} = 24(p-1)\frac{\sqrt{(k-3)(k-4)}}{2k-7} + 27p(p-1) + 12$

where $k = 6p(3p-1)$ *and* α *is a real number.*

Proof. The graph $\mathcal{A}$ has total $6p(3p-1)$ vertices. Let $k = |V(\mathcal{A})| = 6p(3p-1)$. Here the vertex set V can be partitioned into V_1 and V_2 based on the degree of the vertices. Let V_1 and V_2 contains all the vertices of degree 3 and of degree 2, respectively. Thus, we have $|V_1| = 18(p-1)$ and $|V_2| = 12p$. We can note that, if $d_a = 2$ then $\overline{d_a} = k-3$ and if $d_a = 3$ then $\overline{d_a} = k-4$.

The graph $\mathcal{A}$ has total $3p(9p-5)$ edges. Based on the end degree of the edges, the edge set E of $\mathcal{A}$ is partitioned as E_1, E_2 and E_3 with $(2,3), (2,2)$ and $(3,3)$ as their end degree vertices, respectively. Thus, $|E_1| = 6(p+1)$, $|E_2| = 12(p-1)$ and $|E_3| = 3(9p^2-11p+2)$.

(i) $\overline{M_\alpha(\mathcal{A})} = \sum_{a\in V(\mathcal{A})}(\overline{d_a})^\alpha = \sum_{a\in V_1(\mathcal{A})}(\overline{d_a})^\alpha + \sum_{a\in V_2(\mathcal{A})}(\overline{d_a})^\alpha$

$\overline{M_\alpha(\mathcal{A})} = 18p(p-1)(k-4)^\alpha + 12p(k-3)^\alpha$

(ii) $\overline{R_\alpha(\mathcal{A})} = \sum_{ab\in E(\mathcal{A})}(\overline{d_a}\,\overline{d_b})^\alpha$

$= \sum_{ab\in E_1(\mathcal{A})}(\overline{d_a}\,\overline{d_b})^\alpha + \sum_{ab\in E_2(\mathcal{A})}(\overline{d_a}\,\overline{d_b})^\alpha + \sum_{ab\in E_3(\mathcal{A})}(\overline{d_a}\,\overline{d_b})^\alpha$

$\overline{R_\alpha(\mathcal{A})} = 12(p-1)(k-3)^\alpha(k-4)^\alpha + 6(p+1)(k-3)^{2\alpha} + 3(9p^2-11p+2)(k-4)^{2\alpha}$

(iii) $\overline{\chi_\alpha(\mathcal{A})} = \sum_{ab\in E(\mathcal{A})}(\overline{d_a}+\overline{d_b})^\alpha$

$= \sum_{ab\in E_1(\mathcal{A})}(\overline{d_a}+\overline{d_b})^\alpha + \sum_{ab\in E_2(\mathcal{A})}(\overline{d_a}+\overline{d_b})^\alpha + \sum_{ab\in E_3(\mathcal{A})}(\overline{d_a}+\overline{d_b})^\alpha$

$\overline{\chi_\alpha(\mathcal{A})} = 12(p-1)(2k-7)^\alpha + 6(p+1)2^\alpha(k-3)^\alpha + 3(9p^2-11p+2)2^\alpha(k-4)^\alpha$

(iv) $\overline{ABC(\mathcal{A})} = \sum_{ab\in E(\mathcal{A})} \sqrt{\frac{\overline{d_a}+\overline{d_b}-2}{\overline{d_a}\ \overline{d_b}}}$. Similar to the above, considering the edge partition of $\mathcal{A}$ we get the required result.

(v) $\overline{GA(\mathcal{A})} = \sum_{ab\in E(\mathcal{A})} \frac{2\sqrt{\overline{d_a}\ \overline{d_b}}}{\overline{d_a}+\overline{d_b}}$. Similar to the above, considering the edge partition of $\mathcal{A}$ we get the required result.

□

Corollary 2.2. *Let $\mathcal{A} = L(S(\mathcal{H}))$, where $\mathcal{H}$ be the graph of honeycomb networks HC_p $(p \geq 1)$. Then,*

(i) $\overline{M_1(\mathcal{A})} = 36p(9p^3 - 6p^2 - p + 1)$

(ii) $\overline{R(\mathcal{A})} = \frac{12(p-1)}{\sqrt{(k-3)(k-4)}} + \frac{6(p+1)}{k-3} + \frac{3(9p^2-11p+2)}{k-4}$

(iii) $\overline{\chi(\mathcal{A})} = \frac{12(p-1)}{\sqrt{2k-7}} + \frac{3(p+1)}{\sqrt{2(k-3)}} + \frac{3(9p^2-11p+2)}{\sqrt{2(k-4)}}$

where $k = 6p(3p-1)$.

$(s_a, s_b)\,; ab \in E(\mathcal{A})$	$(\overline{s_a}, \overline{s_b})\,; ab \in E(\mathcal{A})$	$\lvert E\rvert$
$(4,4)$	$(2k-6, 2k-6)$	6
$(5,5)$	$(2k-7, 2k-7)$	$6(p-2)$
$(8,8)$	$(3k-11, 3k-11)$	$6(p-1)$
$(9,9)$	$(3k-12, 3k-12)$	$3(9p^2-17p+8)$
$(4,5)$	$(2k-6, 2k-7)$	12
$(5,8)$	$(2k-7, 3k-11)$	$12(p-1)$
$(8,9)$	$(3k-11, 3k-12)$	$12(p-1)$

Table 1. Edge set partition based on the non-neighbor degree of end vertices

Theorem 2.3. *Let $\mathcal{A} = L(S(\mathcal{H}))$, where $\mathcal{H}$ be the graph of honeycomb networks HC_p $(p \geq 1)$. Then,*

(i)
$$\overline{ABC_4(\mathcal{A})} = \begin{cases} 3\sqrt{2}\frac{\sqrt{2k-7}}{k-3} + 12(p-2)\frac{\sqrt{k-4}}{2k-7} + 6\sqrt{6}(p-1)\frac{\sqrt{k-4}}{3k-11} \\ +\sqrt{2}(9p^2-17p+8)\frac{\sqrt{3k-13}}{k-4} + 12\sqrt{\frac{4k-15}{(2k-6)(2k-7)}} \\ +12\sqrt{5}(p-1)\sqrt{\frac{k-4}{(2k-7)(3k-11)}} + 12(p-1)\sqrt{\frac{6k-25}{(3k-11)(3k-12)}}, & n > 1 \\ 6\sqrt{2}\frac{\sqrt{2k-7}}{k-3}, & n = 1 \end{cases}$$

(ii)
$$\overline{GA_5(\mathcal{A})} = \begin{cases} 3(9p^2-13p+4) + 24(p-1)\left(\frac{\sqrt{(2k-7)(3k-11)}}{5k-18} + \frac{\sqrt{(3k-11)(3k-12)}}{6k-23}\right) \\ +24\frac{\sqrt{(2k-6)(2k-7)}}{4k-13}, & n > 1 \\ 12, & n = 1 \end{cases}$$

where $k = 6p(3p-1)$.

Proof. There are seven types of edges in the graph $\mathcal{A} = L(S(\mathcal{H}))$ based on the degree sum of neighbour vertices of end vertices of each edge, which are given in the Table 1. $ABC_4(\mathcal{A})$ and $GA_5(\mathcal{A})$ is computed using the definition of ABC_4 and GA_5 of a graph and the values from the Table 1. □

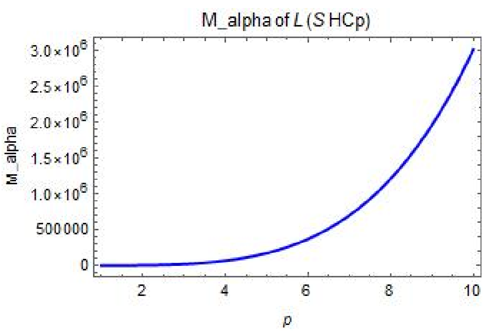

Figure 3. $\overline{M_1(\mathcal{A})}$

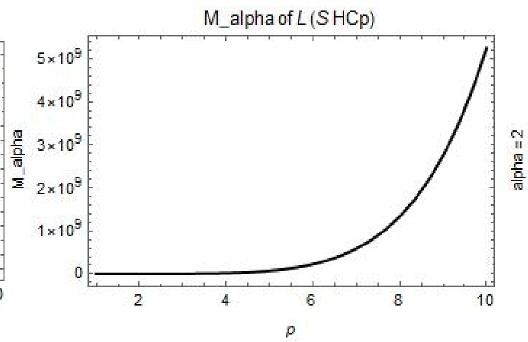

Figure 4. $\overline{M_2(\mathcal{A})}$

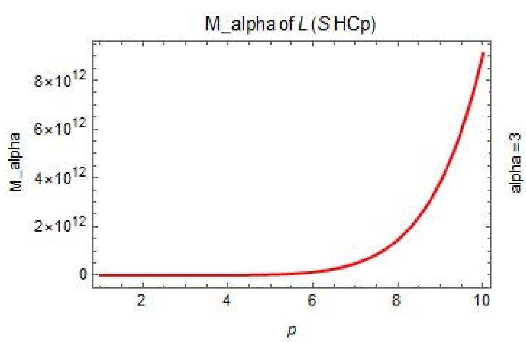

Figure 5. $\overline{M_3(\mathcal{A})}$

3 Analysis of line graph of subdivision of honeycomb networks HC_p

3.1 General non-neighbor Zagreb index $\overline{M_\alpha(\mathcal{A})}$

Figure 3, Figure 4 and Figure 5 represents the graphs of $\overline{M_\alpha(\mathcal{A})}$ when $\alpha = 1, 2, 3$, respectively for $1 \leq p \leq 10$. We can observe that the graphs are exponential in nature. $\overline{M_\alpha(\mathcal{A})}$ increases as increase in p. Also, we can note that the range of $\overline{M_\alpha(\mathcal{A})}$ increases as α increases. In particular when $\alpha = 1$, $\overline{M_1(\mathcal{A})}$ is called the non-neighbor first Zagreb index and it takes the least value compared to $\alpha \geq 2$ for a given p.

3.2 General non-neighbor Randic index $\overline{R_\alpha(\mathcal{A})}$

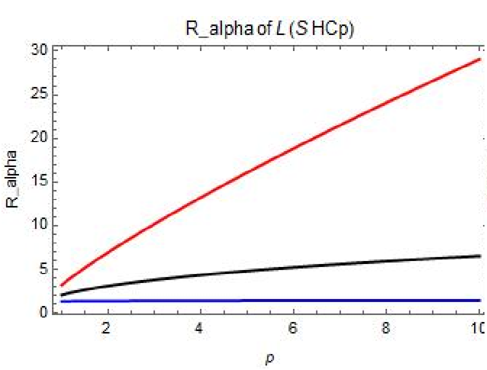

Figure 6. $R_\alpha(\mathcal{A})$: (a)

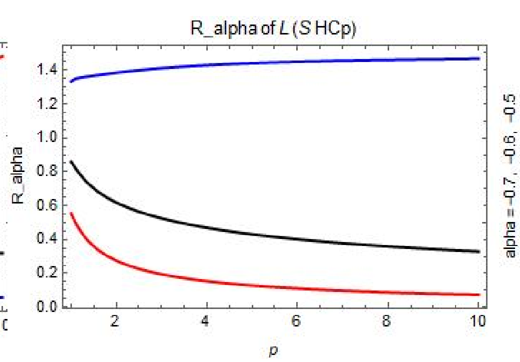

Figure 7. $R_\alpha(\mathcal{A})$: (b)

Figure 6 depicts the graph of $\overline{R_\alpha(\mathcal{A})}$ when $\alpha = -0.5, -0.4, -0.3$ for $1 \leq p \leq 10$. The range of $\overline{R_\alpha(\mathcal{A})}$ varies from 0 to 30. When $\alpha > -0.5$, the curves of $\overline{R_\alpha(\mathcal{A})}$ are above the curve of $\overline{R_{-0.5}(\mathcal{A})}$.

Figure 7 represents the graph of $\overline{R_\alpha(\mathcal{A})}$ when $\alpha = -0.5, -0.6, -0.7$ for $1 \leq p \leq 10$. $\overline{R_\alpha(\mathcal{A})}$ takes the values between 0 and 1.5 and when $\alpha < -0.5$, curve of $\overline{R_\alpha(\mathcal{A})}$ are below the curve of $\overline{R_{-0.5}(\mathcal{A})}$.

In particular, $\overline{R_{-0.5}(\mathcal{A})}$ is called the non-neighbor Randic index. We can mainly observe that, in Figure 6, $\overline{R_\alpha(\mathcal{A})}$ increases as p increases but in Figure 7, $\overline{R_\alpha(\mathcal{A})}$ decreases as p increases for $\alpha < -0.5$.

3.3 General non-neighbor sum-connectivity index $\overline{\chi_\alpha(\mathcal{A})}$

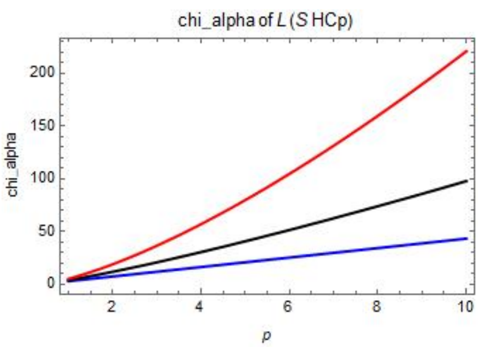

Figure 8. $\overline{\chi_\alpha(\mathcal{A})}$: (a)

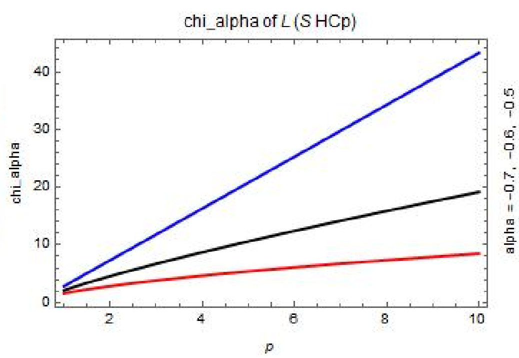

Figure 9. $\overline{\chi_\alpha(\mathcal{A})}$: (b)

Figure 8 represents the graph of $\overline{\chi_\alpha(\mathcal{A})}$ when $\alpha = -0.5, -0.4, -0.3$ for $1 \leq p \leq 10$. The range of $\overline{\chi_\alpha(\mathcal{A})}$ varies from 0 to 250. When $\alpha > -0.5$, the curves of $\overline{\chi_\alpha(\mathcal{A})}$ are above the curve of $\overline{\chi_{-0.5}(\mathcal{A})}$.

Figure 9 depicts the graph of $\overline{\chi_\alpha(\mathcal{A})}$ when $\alpha = -0.5, -0.6, -0.7$ for $1 \leq p \leq 10$. $\overline{\chi_\alpha(\mathcal{A})}$ takes the values between 0 and 45 and when $\alpha < -0.5$, curve of $\overline{\chi_\alpha(\mathcal{A})}$ are below the curve of $\overline{\chi_{-0.5}(\mathcal{A})}$.

In particular, $\overline{\chi_{-0.5}(\mathcal{A})}$ is called the non-neighbor sum-connectivity index. From both the figures we can observe that as p increases, $\overline{\chi_\alpha(\mathcal{A})}$ also increases.

4 Conclusion

We have studied the chemical graph of honeycomb networks and obtain an explicit formula for some non-neighbor topological indices of the line graphs of subdivision graphs of honeycomb and graphene networks. We have discussed the behaviour of some non-neighbor topological indices which are helpful in studying the underlying topologies of these network. Analyzing these indices for different chemical compounds, nanostructures to study their physical and chemical properties is an interesting topic in the field of chemical graph theory.

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