



Computation of Topological Indices for Inner Dual Graph of Honeycomb and Graphene Network

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Abstract

In QSPR/QSAR study, the molecular structure indices are now standard methods for studying structure-property relations. Due to the chemical significance of these indices, the number of proposed molecular descriptors is quickly rising in the last few years. A topological index is a transformation of a chemical structure into a real number. In mathematics, honeycomb networks are widely used because of their extreme importance in computer graphics, image processing, cellular phone base stations, and in chemistry to represent benzenoid hydrocarbons. They are formed by recursively using hexagonal tiling in a particular pattern. $HC(n)$ represents the honeycomb network of dimension n , where n is the number of hexagons between boundary and central hexagon. An atomic-scale honeycomb structure composed of carbon atoms is known as graphene. Professor Andre Geim and Professor Kostya Novoselov separated it from graphite in 2004. It is the first 2D material that is one million times thinner than human hair, two hundred times stronger than steel, and the world's most conductive material. The graph 2D graphene is expressed as $G(r, s)$ where “ r ” means the number of rows, and “ s ” is the number of hexagons in a row. This paper uses the inner dual graph of honeycomb networks and 2D graphene network, which are named as $HcID(n)$ and $GID(r, s)$ respectively. We derive some results related to topological indices for these graphs. We compute degree-based indices, first general Zagreb index, general Randić connectivity index, general sum-connectivity index, first Zagreb index, Second Zagreb index, Randić index, Atom-bond Connectivity (ABC) index, and Geometric-Arithmetic (GA) index of inner dual graphs of honeycomb networks and graphene network

Keywords: Honeycomb structure, Inner dual graph, Graphene network, Topological indices.

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1. Introduction

A numerical value mathematically derived from the graph structure is known as the topological index. It helps to establish correlations between a molecular compound's structure and its physicochemical properties

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or biological activity. Topological indices are also used to foretell physicochemical properties like boiling point, the heat of combustion, enthalpy of vaporization, stability, etc. In 1947, the first topological index was founded by Harold Wiener while he was working on the boiling point of paraffin. He defined this index as a path number, and later it was renamed as Wiener index [17]. There are several types of topological indices such as degree-based, distance-based, counting-related topological indices, etc. The most essential and crucial indices in degree-based topological indices are the Atom-bond connectivity, Geometric–arithmetic. The Atom-Bond Connectivity (ABC) index gives a great model for the stability of the linear and branched alkanes and cycloalkanes’ strain energy. Randić index is closely related to various chemical properties and is observed parallel to the boiling point and Kovats constants. In chemical graph theory, a graph is used to express a molecule by viewing the atoms as the vertices of the graph and the molecular bonds as the edges. Let G be a simple, undirected, and connected graph with $V(G)$ vertices and $E(G)$ edges throughout this paper. If edges share a typical end vertex, they are called adjacent edges, and if they share a common vertex, they are incident to each other.

Table 1: Some Degree-based Topological indices in which the degree of vertices p and q is denoted by d_p and d_q respectively and α is a real number.

Topological index	Formulation
First Zagreb index [11]	$M_1(G) = \sum_{pq \in E(G)} (d_p + d_q)$
Second Zagreb index [8]	$M_2(G) = \sum_{pq \in E(G)} (d_p * d_q)$
First general Zagreb index [18]	$M_\alpha(G) = \sum_{q \in V(G)} (d_q)^\alpha$
Randić index [15]	$R(G) = \sum_{pq \in E(G)} (d_p d_q)^{-1/2}$
General Randić index [6]	$R_\alpha(G) = \sum_{pq \in E(G)} (d_p d_q)^\alpha$
General Sum-connectivity index [4]	$\chi_\alpha(G) = \sum_{pq \in E(G)} (d_p + d_q)^\alpha$
Atom-Bond Connectivity index [10]	$ABC(G) = \sum_{pq \in E(G)} \sqrt{\frac{(d_p + d_q) - 2}{d_p d_q}}$
Geometric-Arithmetic (GA) index [9]	$GA(G) = \sum_{pq \in E(G)} \frac{2\sqrt{(d_p * d_q)}}{d_p + d_q}$

2. Honeycomb Networks

For the construction of the honeycomb network of dimension n expressed as $HC(n)$, we use $HC(n - 1)$ and add a layer of hexagons around the boundary of $HC(n - 1)$. The number of vertices in the honeycomb network $HC(n)$ is $6n^2$ and the total number of edges $9n^2 - 3n$ [1, 5]. Some other networks with interesting topological properties are studied in [13, 14]. The n -dimensional inner dual graph of the honeycomb network is expressed as $HcID(n)$, where n is the number of hexagons between the central and boundary hexagon. The Inner dual graph of honeycomb network $HcIN(n)$ is formed by using $HcID(n - 1)$, we add a layer of hexagons around the boundary of $HcID(n - 1)$, and its inner dual graph is made by putting a vertex in the center of all hexagons and connecting those vertices that are in adjacent hexagons. The number of vertices in the inner dual graph of honeycomb networks $HcID(n)$ is $3n^2 - 3n + 1$ and the number of edges $9n^2 - 15n + 6$. Honeycomb network of dimension 3 and its inner dual graph is shown in Figure 1.

(d_p, d_q) where $pq \in E(G)$	No. of Edges
(3,4)	12
(3,6)	6
(4,4)	$6(n - 3)$
(4,6)	$12(n - 2)$
(6,6)	$9n^2 - 33n + 30$

Table 2: Edge partition of $HcID(n)$, $n \geq 3$ based on end points vertices degree of all edges

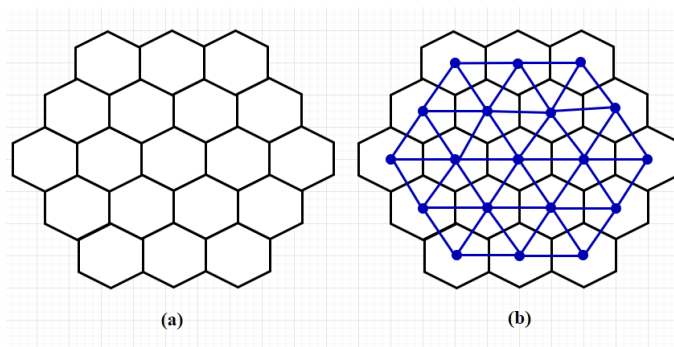


Figure 1: figure

(a) Honeycomb network of dimension 3 (b) Inner dual graph of 3-dimensional honeycomb network

3. Graphene Network

The graph 2D graphene is expressed as $G(r, s)$ where “ r ” means the number of rows, and “ s ” is the number of hexagons in a row. Some topological indices of graphene, subdivision graph of graphene, and its line graph are calculated in [1, 12]. The Inner dual graph of the 2D graphene is denoted as $GID(r, s)$ where “ r ” expresses the number of rows and “ s ” is the number of hexagons in a row. Its inner dual graph is made by putting a vertex in the center of all hexagons and connecting those vertices that are in adjacent hexagons. The number of vertices in the inner dual graph of graphene network $GID(r, s)$ is rs and number of edges $3rs - 2r - 2s + 1$. Graphene network with four rows and four hexagons in each row and its inner dual graph is shown in Figure 2. For inner dual graph of graphene network, we have eleven types of edges

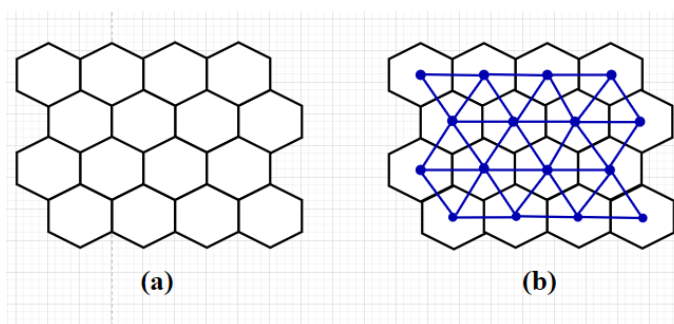


Figure 2: (a) Graphene network, $G(4, 4)$ (b) Inner dual graph of $G(4, 4)$

given in the Table 3.

4. Main results

We calculated the general Randić connectivity index, general sum connectivity index, first general Zagreb index, Atom-bond Connectivity (ABC) index, Geometric-arithmetic (GA) index, Randić index, first Zagreb index, and second Zagreb index of the inner dual graphs of honeycomb networks and 2D graphene network. In the following theorem, we calculate the Zagreb index for the inner dual graph of the n -dimensional honeycomb network.

Theorem 4.1. *Let $HcID(n)$ be the inner dual graph of honeycomb network of dimension $n \geq 3$, then*

a) *first Zagreb index is equal to*

$$M_1(HcID(n)) = 108n^2 - 288n + 144$$

(d_p, d_q) where $pq \in E(G)$	No. of Edges
(3,6)	r
(4,5)	2
(3,5)	$2r - 6$
(4,4)	$2s - 6$
(2,5)	2
(3,4)	2
(3,3)	2
(2,4)	2
(6,6)	$(3r - 8)s - (8r - 21)$
(5,6)	$3r - 8$
(4,6)	$4s - 10$

Table 3: Edge partition of $GID(r, s)$, $r \geq 3$ and $s \geq 3$ based on end points vertices degree of all edges

b) second Zagreb index is equal to

$$M_2(HcID(n)) = 324n^2 - 804n + 468$$

c) The first general Zagreb index is equal to

$$M_\alpha(HcID(n)) = 6 * 3^\alpha + (6n - 12)2^{2\alpha} + (3n^2 - 9n + 7)6^\alpha$$

where α is a real number.

Proof. (a) As we know that $M_1(G)$ is the first Zagreb index, from Table 1 for $HcID(n)$, we get

$$M_1(HcID(n)) = \sum_{pq \in E(HcID(n))} (d_p + d_q)$$

Using edge types and the total number of edges in each type from the Table 2, we get

$$M_1(HcID(n)) = 12(3 + 4) + 6(3 + 6) + 6(n - 3)(4 + 4) + 12(n - 2)(4 + 6) + (9n^2 - 33n + 30)(6 + 6)$$

So first Zagreb index for $n \geq 3$ is

$$M_1(HcID(n)) = 108n^2 - 288n + 144$$

(c) The graph $HcID(n)$ have total $3n^2 - 3n + 1$ vertices among which 6, $6n - 12$ and $3n^2 - 9n + 7$ number of vertices are of degree 3, 4 and 6, respectively. Using these values, we get

$$M_\alpha(HcID(n)) = 6 * 3^\alpha + (6n - 12)2^{2\alpha} + (3n^2 - 9n + 7)6^\alpha$$

□

From Table 1 and Table 2, the part b) can be proved easily. In the next theorem, we calculate the general Randić index for the inner dual graph of the n -dimensional honeycomb network.

Theorem 4.2. Let $HcID(n)$ be the inner dual graph of honeycomb network of dimension $n \geq 3$, then

a) Randić index is equal to

$$R_{-1/2}(HcID(n)) = \frac{3n^2}{2} + (\sqrt{6} - 4)n + (2\sqrt{3} + \sqrt{2} + \frac{1}{2} - 2\sqrt{6})$$

b) The general Randić index is equal to

$$R_\alpha(HcID(n)) = 12 * 12^\alpha + 6 * 18^\alpha + 6(n - 3) * 4^{2\alpha} + 12(n - 2) * 24^\alpha + (9n^2 - 33n + 30)6^{2\alpha}$$

where α is a real number.

Proof. b) As we know that $R_{-1/2}(G)$ is the Randić index, from Table 1 for $HcID(n)$, we get

$$R_{-1/2}(HcID(n)) = \sum_{pq \in E(HcID(n))} (d_p * d_q)^{-1/2}$$

Using edge types and the total number of edges in all types from the Table 2, we get

$$R_{-1/2}(HcID(n)) = 12(3 * 4)^{-1/2} + 6(3 * 6)^{-1/2} + 6(n - 3)(4 * 4)^{-1/2} + 12(n - 2)(4 * 6)^{-1/2} + (9n^2 - 33n + 30)(6 * 6)^{-1/2}$$

So Randić index for $n \geq 3$ is

$$R_{-1/2}(HcID(n)) = \frac{3n^2}{2} + (\sqrt{6} - 4)n + (2\sqrt{3} + \sqrt{2} + \frac{1}{2} - 2\sqrt{6})$$

□

Proof of a) can be done using similar method. Now we compute the general Sum-connectivity index of the inner dual graph of the n -dimensional honeycomb network.

Theorem 4.3. Let $HcID(n)$ be the inner dual graph of honeycomb network of dimension n , for $n \geq 3$ its general Sum-connectivity index is equal to

$$\chi_\alpha(HcID(n)) = 12 * 7^\alpha + 6 * 3^{2\alpha} + 6(n - 3)8^\alpha + 12(n - 2)10^\alpha + (9n^2 - 33n + 30)12^\alpha$$

where α is a real number.

Proof. As we know that $\chi_\alpha(G)$ is the general Sum-connectivity index, from Table 1 for $HcID(n)$, we get

$$\chi_\alpha(HcID(n)) = \sum_{pq \in E(HcID(n))} (d_p + d_q)^\alpha$$

Putting edge types and total number of edges in each type from the Table 2 and on simplifying the above equation, we get

$$\chi_\alpha(HcID(n)) = 12 * 7^\alpha + 6 * 3^{2\alpha} + 6(n - 3)8^\alpha + 12(n - 2)10^\alpha + (9n^2 - 33n + 30)12^\alpha$$

□

In the following theorem, we calculate Atom-bond Connectivity (ABC) index of $HcID(n)$.

Theorem 4.4. Let $HcID(n)$ be the inner dual graph of honeycomb network of dimension n , for $n \geq 3$ its Atom-bond Connectivity (ABC) index is equal to

$$ABC(HcID(n)) = \frac{3\sqrt{10}}{2}n^2 + (\frac{3\sqrt{6}}{2} + 4\sqrt{3} - \frac{11\sqrt{10}}{2})n + (2\sqrt{15} + \sqrt{14} - \frac{9\sqrt{6}}{2} - 8\sqrt{3} + 5\sqrt{10})$$

Proof. As we know that $ABC(G)$ is the Atom-bond Connectivity index, from Table 1 for $HcID(n)$, we get

$$ABC(HcID(n)) = \sum_{pq \in E(HcID(n))} \sqrt{\frac{(d_p + d_q) - 2}{d_p d_q}}$$

Using edge types and the total number of edges in all types from the Table 2, we get

$$ABC(HcID(n)) = 12\sqrt{\frac{(3+4)-2}{3*4}} + 6\sqrt{\frac{(3+6)-2}{3*6}} + 6(n-3)\sqrt{\frac{(4+4)-2}{4*4}} \\ + 12(n-2)\sqrt{\frac{(4+6)-2}{4*6}} + (9n^2 - 33n + 30)\sqrt{\frac{(6+6)-2}{6*6}}$$

So ABC index for $n \geq 3$ is

$$ABC(HcID(n)) = \frac{3\sqrt{10}}{2}n^2 + (\frac{3\sqrt{6}}{2} + 4\sqrt{3} - \frac{11\sqrt{10}}{2})n + (2\sqrt{15} + \sqrt{14} - \frac{9\sqrt{6}}{2} - 8\sqrt{3} + 5\sqrt{10})$$

□

In the next theorem, the Geometric-arithmetic (GA) index of the inner dual graph of $HcID(n)$ is computed.

Theorem 4.5. *Let $HcID(n)$ be the inner dual graph of honeycomb network of dimension n , for $n \geq 3$ its Geometric-arithmetic (GA) index is equal to*

$$GA(HcID(n)) = 9n^2 + (\frac{24\sqrt{6}}{5} - 27)n + (\frac{48\sqrt{3}}{7} + 4\sqrt{2} - \frac{48\sqrt{6}}{5} + 12)$$

Proof. As we know that $GA(G)$ is the Geometric-arithmetic index, from Table 1 for $HcID(n)$, we get

$$GA(HcID(n)) = \sum_{pq \in E(HcID(n))} \frac{2\sqrt{(d_p * d_q)}}{d_p + d_q}$$

Using edge types and the total number of edges in each type from the Table 2, we get

$$GA(HcID(n)) = 12(\frac{2\sqrt{3*4}}{3+4}) + 6(\frac{2\sqrt{3*6}}{3+6}) + 6(n-3)(\frac{2\sqrt{4*4}}{4+4}) + 12(n-2)(\frac{2\sqrt{4*6}}{4+6}) \\ + (9n^2 - 33n + 30)(\frac{2\sqrt{6*6}}{6+6})$$

So GA index for $n \geq 3$ is

$$GA(HcID(n)) = 9n^2 + (\frac{24\sqrt{6}}{5} - 27)n + (\frac{48\sqrt{3}}{7} + 4\sqrt{2} - \frac{48\sqrt{6}}{5} + 12)$$

□

In the following theorem, we calculate the first general Zagreb index for the inner dual graph of the 2D graphene network.

Theorem 4.6. *Let $GID(r,s)$ be the inner dual graph of 2D graphene network with r rows of hexagons and s hexagons in each row, for $r \geq 3$ & $s \geq 2$ its first general Zagreb index is equal to*

$$M_\alpha(GID(r,s)) = 2 * 2^\alpha + r * 3^\alpha + (2s - 4)4^\alpha + (r - 2)5^\alpha + [(r - 2)s - (2r - 4)]6^\alpha$$

where α is a real number.

Proof. As we know that $M_\alpha(G)$ is the first general Zagreb index, by from Table 1 for $GID(r, s)$, we have

$$M_\alpha(GID(r, s)) = \sum_{q \in V(GID(r, s))} (d_q)^\alpha$$

For $r \geq 3$ & $s \geq 2$, the graph $GID(r, s)$ have total rs vertices among which 2, r , $(2s - 4)$, $(r - 2)$ and $(r - 2)s - (2r - 4)$ number of vertices are of degree 2, 3, 4, 5, and 6 respectively. Using these values in above equation, we get

$$M_\alpha(GID(r, s)) = 2 * 2^\alpha + r * 3^\alpha + (2s - 4)4^\alpha + (r - 2)5^\alpha + [(r - 2)s - (2r - 4)]6^\alpha$$

□

In the next theorem, the general sum-connectivity index of the inner dual graph of the 2D graphene network is computed.

Theorem 4.7. *Let $GID(r, s)$ be the inner dual graph of 2D graphene network with r rows of hexagons and s hexagons in each row, for $r, s \geq 3$ its general sum-connectivity index is equal to*

$$\begin{aligned} \chi_\alpha(GID(r, s)) = & (r + 2)3^{2\alpha} + (2r + 2s - 12)8^\alpha + 4 * 7^\alpha + 4 * 6^\alpha + [(3r - 8)s - (8r - 21)]12^\alpha \\ & + (3r - 8)11^\alpha + (4s - 10)10^\alpha \end{aligned}$$

where α is a real number.

Proof. As we know that $\chi_\alpha(G)$ is the general sum-connectivity index, from Table 1 for $GID(r, s)$, we have

$$\chi_\alpha(GID(r, s)) = \sum_{pq \in E(GID(r, s))} (d_p + d_q)^\alpha$$

For $r, s \geq 3$, using edge types and the total number of edges from the Table 3, we get

$$\begin{aligned} \chi_\alpha(GID(r, s)) = & r(3 + 6)^\alpha + 2(4 + 5)^\alpha + (2r - 6)(3 + 5)^\alpha + (2s - 6)(4 + 4)^\alpha + 2(2 + 5)^\alpha \\ & + 2(3 + 4)^\alpha + 2(3 + 3)^\alpha + 2(2 + 4)^\alpha + [(3r - 8)s - (8r - 21)](6 + 6)^\alpha + (3r - 8)(5 + 6)^\alpha + (4s - 10)(4 + 6)^\alpha \end{aligned}$$

By simplifying the above equation, we get

$$\begin{aligned} \chi_\alpha(GID(r, s)) = & (r + 2)3^{2\alpha} + (2r + 2s - 12)8^\alpha + 4 * 7^\alpha + 4 * 6^\alpha + [(3r - 8)s - (8r - 21)]12^\alpha \\ & + (3r - 8)11^\alpha + (4s - 10)10^\alpha \end{aligned}$$

□

In the following theorem, we calculate the Atom-bond Connectivity (ABC) index for the inner dual graph of the 2D graphene network.

Theorem 4.8. *Let $GID(r, s)$ be the inner dual graph of 2D graphene network with r rows of hexagons and s hexagons in each row, for $r, s \geq 3$ its Atom-bond Connectivity (ABC) index is equal to*

$$\begin{aligned} ABC(GID(r, s)) = & (\sqrt{\frac{7}{18}} + 2\sqrt{\frac{2}{5}} - 8\frac{\sqrt{10}}{6} + 9\sqrt{\frac{1}{30}})r + rs\frac{\sqrt{10}}{2} + (\frac{\sqrt{6}}{2} - 4\frac{\sqrt{10}}{3} + 4\frac{\sqrt{3}}{3})s \\ & + (\frac{\sqrt{35}}{5} - 3\frac{\sqrt{6}}{2} - 4\sqrt{2} + \frac{4}{3} + \frac{\sqrt{15}}{3} + 7\frac{\sqrt{10}}{2} - 4\frac{\sqrt{30}}{5} - 10\frac{\sqrt{3}}{3}) \end{aligned}$$

Proof. As we know that $ABC(G)$ is the Atom-bond Connectivity index, from Table 1 for $GID(r, s)$, we have

$$ABC(GID(r, s)) = \sum_{pq \in E(GID(r, s))} \sqrt{\frac{(d_p + d_q) - 2}{d_p d_q}}$$

For $r, s \geq 3$

Using edge types and total number of edges from the Table 3, we get

$$\begin{aligned} ABC(GID(r, s)) &= r\sqrt{\frac{(3+6)-2}{3*6}} + 2\sqrt{\frac{(4+5)-2}{4*5}} + (2r-6)\sqrt{\frac{(3+5)-2}{3*5}} + (2s-6)\sqrt{\frac{(4+4)-2}{4*4}} \\ &\quad + 2\sqrt{\frac{(2+5)-2}{2*5}} + 2\sqrt{\frac{(3+4)-2}{3*4}} + 2\sqrt{\frac{(3+3)-2}{3*3}} + 2\sqrt{\frac{(2+4)-2}{2*4}} \\ &\quad + [(3r-8)s - (8r-21)]\sqrt{\frac{(6+6)-2}{6*6}} + (3r-8)\sqrt{\frac{(5+6)-2}{5*6}} + (4s-10)\sqrt{\frac{(4+6)-2}{4*6}} \end{aligned}$$

So ABC index for $r, s \geq 3$ is

$$\begin{aligned} ABC(GID(r, s)) &= \left(\frac{\sqrt{14}}{6} + 2\frac{\sqrt{10}}{5} - 4\frac{\sqrt{10}}{3} + 3\frac{\sqrt{30}}{10}\right)r + rs\frac{\sqrt{10}}{2} + \left(\frac{\sqrt{6}}{2} - 4\frac{\sqrt{10}}{3} + 4\frac{\sqrt{3}}{3}\right)s \\ &\quad + \left(\frac{\sqrt{35}}{5} - 3\frac{\sqrt{6}}{2} - 4\sqrt{2} + \frac{4}{3} + \frac{\sqrt{15}}{3} + 7\frac{\sqrt{10}}{2} - 4\frac{\sqrt{30}}{5} - 10\frac{\sqrt{3}}{3}\right) \end{aligned}$$

□

Now, we compute the Geometric-arithmetic (GA) index for the inner dual graph of the 2D graphene network.

Theorem 4.9. Let $GID(r, s)$ be the inner dual graph of 2D graphene network with r rows of hexagons and s hexagons in each row, for $r, s \geq 3$ its Geometric-arithmetic (GA) index is equal to

$$\begin{aligned} GA(GID(r, s)) &= \left(\frac{2\sqrt{2}}{3} + \frac{\sqrt{15}}{2} - 8 + \frac{6\sqrt{30}}{11}\right)r + \left(\frac{8\sqrt{6}}{5} - 6\right)s + 3rs + \left(\frac{8\sqrt{5}}{9} - \frac{3\sqrt{15}}{2} + \frac{4\sqrt{10}}{7}\right) \\ &\quad + \frac{8\sqrt{3}}{7} + \frac{4\sqrt{2}}{3} + 17 - \frac{16\sqrt{30}}{11} - 4\sqrt{6} \end{aligned}$$

Proof. As we know that $GA(G)$ is the Geometric-arithmetic index, from Table 1 for $GID(r, s)$, we have

$$GA(GID(r, s)) = \sum_{pq \in E(GID(r, s))} \frac{2\sqrt{(d_p * d_q)}}{d_p + d_q}$$

Where d_p and d_q are the end vertices degrees of an edge.

For $r, s \geq 3$

Using edge types and total number of edges from the Table 3, we get

$$\begin{aligned} GA(GID(r, s)) &= r\left(\frac{2\sqrt{3*6}}{3+6}\right) + 2\left(\frac{2\sqrt{4*5}}{4+5}\right) + (2r-6)\left(\frac{2\sqrt{3*5}}{3+5}\right) + (2s-6)\left(\frac{2\sqrt{4*4}}{4+4}\right) + 2\left(\frac{2\sqrt{2*5}}{2+5}\right) + 2\left(\frac{2\sqrt{3*4}}{3+4}\right) \\ &\quad + 2\left(\frac{2\sqrt{3*3}}{3+3}\right) + 2\left(\frac{2\sqrt{2*4}}{2+4}\right) + [(3r-8)s - (8r-21)]\left(\frac{2\sqrt{6*6}}{6+6}\right) + (3r-8)\left(\frac{2\sqrt{5*6}}{5+6}\right) + (4s-10)\left(\frac{2\sqrt{4*6}}{4+6}\right) \end{aligned}$$

So GA index for $GID(r, s)$ for $r, s \geq 3$ is

$$GA(GID(r, s)) = \left(\frac{2\sqrt{2}}{3} + \frac{\sqrt{15}}{2} - 8 + \frac{6\sqrt{30}}{11}\right)r + \left(\frac{8\sqrt{6}}{5} - 6\right)s + 3rs + \left(\frac{8\sqrt{5}}{9} - \frac{3\sqrt{15}}{2} + \frac{4\sqrt{10}}{7} + \frac{8\sqrt{3}}{7} + \frac{4\sqrt{2}}{3} + 17 - \frac{16\sqrt{30}}{11} - 4\sqrt{6}\right)$$

□

In the next theorem, Randić index of inner dual graph of 2D graphene network is computed.

Theorem 4.10. *Let $GID(r, s)$ be the inner dual graph of 2D graphene network with r rows of hexagons and s hexagons in each row, for $r, s \geq 3$.*

a) *The Randić index is equal to*

$$R_{-1/2}(GID(r, s)) = \left(\frac{\sqrt{2}}{6} + \frac{2}{\sqrt{15}} - \frac{4}{3} + \frac{3}{\sqrt{30}}\right)r + \left(\frac{\sqrt{6}}{3} - \frac{5}{6}\right)s + \left(\frac{\sqrt{5}}{5} - \frac{6}{\sqrt{15}} + \frac{2}{\sqrt{10}} + \frac{\sqrt{3}}{3} + \frac{8}{3} + \frac{\sqrt{2}}{2} - \frac{8}{\sqrt{30}} - \frac{5\sqrt{6}}{6}\right) + \left(\frac{1}{2}\right)rs$$

b) *The general Randić connectivity index is equal to*

$$R_{\alpha}(GID(r, s)) = r * 18^{\alpha} + 2 * 20^{\alpha} + (2r - 6)15^{\alpha} + (2s - 6)4^{2\alpha} + 2 * 10^{\alpha} + 2 * 12^{\alpha} + 2 * 3^{2\alpha} + 2 * 8^{\alpha} + [(3r - 8)s - (8r - 21)]6^{2\alpha} + (3r - 8)30^{\alpha} + (4s - 10)24^{\alpha}$$

where α is a real number.

Proof. b) As we know that $R_{\alpha}(G)$ is the general Randić index, from Table 1 for $GID(r, s)$, we have

$$R_{\alpha}(GID(r, s)) = \sum_{pq \in E(GID(r, s))} (d_p d_q)^{\alpha}$$

For $r, s \geq 3$

Using edge types and the total number of edges from the Table 3, we get

$$R_{\alpha}(GID(r, s)) = r(3 * 6)^{\alpha} + 2(4 * 5)^{\alpha} + (2r - 6)(3 * 5)^{\alpha} + (2s - 6)(4 * 4)^{\alpha} + 2(2 * 5)^{\alpha} + 2(3 * 4)^{\alpha} + 2(3 * 3)^{\alpha} + 2(2 * 4)^{\alpha} + [(3r - 8)s - (8r - 21)](6 * 6)^{\alpha} + (3r - 8)(5 * 6)^{\alpha} + (4s - 10)(4 * 6)^{\alpha}$$

So general Randić connectivity index for $r, s \geq 3$ is

$$R_{\alpha}(GID(r, s)) = r * 18^{\alpha} + 2 * 20^{\alpha} + (2r - 6)15^{\alpha} + (2s - 6)4^{2\alpha} + 2 * 10^{\alpha} + 2 * 12^{\alpha} + 2 * 3^{2\alpha} + 2 * 8^{\alpha} + [(3r - 8)s - (8r - 21)]6^{2\alpha} + (3r - 8)30^{\alpha} + (4s - 10)24^{\alpha}$$

□

In the following theorem, we calculate the Zagreb index for the inner dual graph of the 2D graphene network.

Theorem 4.11. *Let $GID(r, s)$ be the inner dual graph of 2D graphene network with r rows of hexagons and s hexagons in each row, for $r, s \geq 3$*

a) The first Zagreb index is equal to

$$M_1(GID(r, s)) = 36rs - 38r - 40s + 38$$

b) The second Zagreb index is equal to

$$M_2(GID(r, s)) = 108rs - 150r - 160s + 208$$

where α is a real number.

Proof. a) the first Zagreb index for $GID(r, s)$ is expressed as

$$M_1(GID(r, s)) = \sum_{pq \in E(GID(r, s))} (d_p + d_q)$$

For $r, s \geq 3$

Using edge types and total number of edges in each type from the Table 3, we get

$$\begin{aligned} M_1(GID(r, s)) &= r(3 + 6) + 2(4 + 5) + (2r - 6)(3 + 5) + (2s - 6)(4 + 4) + 2(2 + 5) + 2(3 + 4) \\ &\quad + 2(3 + 3) + 2(2 + 4) + [(3r - 8)s - (8r - 21)](6 + 6) + (3r - 8)(5 + 6) + (4s - 10)(4 + 6) \end{aligned}$$

So first Zagreb index for $r, s \geq 3$ is

$$M_1(GID(r, s)) = 36rs - 38r - 40s + 38$$

□

5. Conclusions

In this paper, we use the inner dual graph of the honeycomb network and 2D graphene network named $HcID(n)$ and $GID(r, s)$, respectively. We discuss some structural properties of these graphs. Structural properties deal with the graph structure in which various properties like vertices, edges, and degrees are used to establish results. We constructed tables to discuss edge types and the total number of edges in all types in the honeycomb and graphene network's inner dual graphs. We also discuss the total number of vertices and edges in these graphs. The generalized formulas for calculating the general Randić connectivity index, general sum-connectivity index, first general Zagreb index, Randić index, first Zagreb index, Second Zagreb index, Atom-bond Connectivity (ABC) index, and Geometric-Arithmetic (GA) index of inner dual graphs of honeycomb network and graphene network are computed.

References

- [1] Akhter, S., Imran, M., Wei, G.A.O. and Farahani, M.R.,(2018) On topological indices of honeycomb networks and graphene networks. *Hacetatepe Journal of Mathematics and Statistics*, 47(1), pp.19-35.
- [2] Amic D., Belso D., Lucic B., Nikolic S.,Trinajstic N.,(1998) 'The vertexconnectivity index revisited, *J. Chem. Inf. Comput. Sci.* 38, 819–822.
- [3] B.; Zhou and N.; Trinajstic (2009) "On a novel connectivity index", *J. Math. Chem.*, 46, 1252–1270.
- [4] B.; Zhou and N.; Trinajstic,(2010) "On general sum-connectivity index", *J. Math. Chem.*, 47,210–218.
- [5] Bharati Rajan, A.W., Grigorious, C. and Stephen, S.(2012) . On certain topological indices of silicate, honeycomb and hexagonal networks. *Journal of Computer and Mathematical Sciences* Vol, 3(5), pp.498-556.
- [6] Bollobas B., Erd'os P.(1998), Graphs of extremal weights, *Ars Combinatoria* 50, 225–233.
- [7] Das, K. C., Bhatti, F. M., Lee, S. G., & Gutman, I.(2011) . Spectral properties of the He matrix of hexagonal systems. *MATCH Commun. Math. Comput. Chem*, 65, 753-774.
- [8] Das, K.C. and Gutman, I.,(2004) . Some properties of the second Zagreb index. *MATCH Commun. Math. Comput. Chem*, 52(1), pp.3-1

- [9] D.; Vukic'evic' and B.; Furtula (2009), "Topological index based on the ratios of geometrical and arithmetical mmeans of end-vertex degrees of edges" *J. Math. Chem.*, 46, 1369–1376.
- [10] E.; Estrada, L.; Torres, L.; Rodriguez and I.; Gutman,(1998) "An atom-bond connectivity index: modelling the enthalpy of formation of alkanes", *Ind. J. Chem.*, 37A, 849–855.
- [11] Gutman I., Trinajstic N.(1972), Graph theory and molecular orbitals, Total π -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, 17, 535–538.
- [12] G. Sridhara, M. R. Rajesh Kanna, R. S. Indumathi,(2015) "Computation of Topological Indices of Graphene", *Journal of Nanomaterials*, vol. 2015, Article ID 969348, 8 pages, . <https://doi.org/10.1155/2015/969348>
- [13] Hayat, S. and Imran, M.,(2014) . Computation of topological indices of certain networks. *Applied Mathematics and Computation*, 240, pp.213-228.
- [14] Hayat, S., Malik, M.A. and Imran, M.(2015). Computing topological indices of honeycomb derived networks. *Romanian journal of Information science and technology*, 18, pp.144-165.
- [15] M.; Randic,(1975) "On characterization of molecular branching", *J. Am. Chem. Soc.*, 97, 6609–6615.
- [16] W.C. He, W.J. He (1989), A complete set of combination invariants of plane hexagonal graphs and its applications in chemistry, in: M.F. Capobiano, M.Guan, D.F. Hsu, F. Tian (Eds), *Graph Theory and its Application: East and West, New York Acad. Sci., New York* , pp.226-234.
- [17] Wiener H.(1947), Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* 69, 17–20.
- [18] X.; Li and H.; Zhao,(2004) "Trees with the first three smallest and largest generalized topological indices", *MATCH Commun. Math. Comput. Chem.*, 50, 57–62.