On molecular topological properties of benzenoid structures

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Abstract. The degree-based topological indices correlate certain physico-chemical properties such as boiling point, strain energy and the stability etc. of certain chemical compounds. Among the major classes of topological indices are the distance based topological indices, the degree-based topological indices and counting related polynomials and corresponding indices of graphs. Among all the degree based indices, namely first general Zagreb index, general Randić connectivity index, general sum-connectivity index, atom-bond connectivity index (ABC) and geometric-arithmetic index (GA) are most important due to their chemical significance.

In this paper, we compute the first general Zagreb index, general Randić connectivity index, general sum-connectivity index, ABC , GA , ABC_4 and GA_5 indices of hexagonal parallelogram $P(m, n)$ nanotube, triangular benzenoid G_n and zigzag-edge coronoid fused with starphene $ZCS(k, l, m)$ nanotubes by using the line graphs of subdivision of these chemical graphs.

Keywords: Topological indices, ABC index, GA index, hexagonal parallelogram $P(m, n)$ nanotube, triangular benzenoid, $ZCS(k, l, m)$ nanotube.

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1 Introduction and preliminary results

Let G be a simple connected graph having the vertex set $V(G)$ and the edge set $E(G)$. Two vertices in G are *adjacent* if and only if they are end vertices of an edge and two edges are *incident* to each other if and only if they share a common vertex. The *degree* of a vertex $u \in V(G)$ is denoted by d_u and s_u is the sum of the degrees of all neighbors of vertex u . In other words, we say $s_u = \sum_{v \in N_u} d_v$, where $N_u = \{u \in V(G) | uv \in E(G)\}$ that is known as the set of neighbor vertices of u . The *subdivision graph* denoted by $S(G)$ is the graph obtained from graph G by replacing each of its edges by a path of length two. The line graph denoted by $L(G)$ of a graph G is the graph whose vertices are the edges of existing graph G ; two vertices f and g are incident if and only if they have a common end vertex in graph G .

Cheminformatics is new subject which is a combination of chemistry, mathematics and information science. In the last decades, there is a lot of research which is done in this area. Graph theory has provided to the theoretical chemists with a variety of useful tools, such as topological matrices, topological polynomials and topological indices. A structural formula of a chemical compounds is represented by a *molecular graph* in terms of graph theory. The vertices and edges of molecular graphs are corresponding to the atoms of the compounds and chemical bonds, respectively.

A *topological index* is actually an invariant number associated with a given graph. In the QSAR/QSPR study, physico-chemical properties and topological indices such as Wiener index, Szeged index, Randić index, Zagreb indices and ABC index are used to predict the bioactivity of the chemical compounds. There are many classes of topological indices, some of them are distance based topological indices, degree based topological indices and counting related polynomials and indices of graphs. Among all these topological indices, the degree based topological indices play an important role in chemical graph theory and particularly in theoretical chemistry due to their chemical applications.

The topological index of any two graphs G and H are equal if they are isomorphic. The Wiener index in the theoretical point of view and applications, is the first and most studied topological indices. Firstly, Wiener index was as a path index but later on it was renamed as Wiener index.

In 1975, the *Randić connectivity index*¹ was defined as follows:

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

The generalization of Randić index is known as *general Randić connectivity index* or *general product-connectivity index* and that is defined as follows:

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha,$$

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where α is a real number. Then $R_{-1/2}$ is the *classical Randić connectivity index*. The *sum-connectivity index* of a graph G was proposed in². The concept of sum-connectivity index was extended to the *general sum-connectivity index* in³, which is defined as:

$$\chi_{\alpha}(G) = \sum_{uv \in E(G)} (deg(u) + deg(v))^{\alpha},$$

where α is a real number. If $\alpha = -1/2$, then this is the classical sum-connectivity index. The *sum-connectivity index* and *product-connectivity index* correlate well with the π -electron energy of benzenoid hydrocarbons⁴. Li and Zhao introduced the first general Zagreb index in⁵:

$$M_{\alpha}(G) = \sum_{u \in V(G)} (d_u)^{\alpha},$$

where α is a real number. The atom-bond Connectivity *ABC* index was introduced by Estrada et al.⁶ and is defined as:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

D. Vukičević introduced the geometric-arithmetic (*GA*) index in⁷, that is defined as:

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

The fourth member of the class of *ABC* index was introduced by Ghorbani and Hosseinzadeh⁸ in 2010 and defined as:

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}}.$$

Recently, the fifth version of (*GA*) index (GA_5) was proposed by Graovac⁹ in 2011 and was defined as:

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{s_u s_v}}{s_u + s_v}.$$

For further study of these topological indices, we refer the readers to consult^{10–19}. Carbon nanotubes are types of nanostructure which are allotropes of carbon and having a cylindrical shape. Carbon nanotubes, a type of fullerene, have potential in fields such as nanotechnology, electronics, optics, materials science, and architecture. Baig et al. [20] determined the Omega polynomials of hexagonal parallelogram $P(m, n)$ nanotube and zigzag-edge coronoid fused with starphene $ZCS(k, l, m)$ nanotube and thier result is described in the following theorem.

Theorem 1.0.1. [20] The Omega polynomial of $P(m, n)$ nanotube $\forall m, n \in \mathbb{N}$ is as follows:

$$\Omega(P(m, n), x) = \begin{cases} (n+1)x^{m+1} + mx^{n+1} + 2x^{\sum_{i=1}^{m-1} (i+1)}, & m = n \\ nx^{m+1} + (m+1)x^{n+1} + 2x^{\sum_{i=1}^n (i+1)}, & m > n \\ (n+1)x^{m+1} + mx^{n+1} + 2x^{\sum_{i=1}^m (i+1)}, & m < n. \end{cases}$$

Theorem 1.0.2. [20] The Omega polynomial of nanotube $ZCS(k, l, m)$ for $k = l = m \geq 4$ is equal to:

$$\Omega(ZCS(k, l, m), x) = (k^2 + 9)x^{15k-21} + (l^2 + 9)x^{15l-21} + (m^2 + 9)x^{15m-21}.$$

Farahani et al. [21] determined the Omega polynomial of triangular benzenoid G_n in the theorem stated below.

Theorem 1.0.3. [21] Let G_n be the triangular benzenoid $\forall n \in \mathbb{N}$, then the Omega polynomial of G_n is equal to

$$\Omega(G_n, x) = 3x^2 + 3x^3 + \dots + 3x^{n+1}.$$

In this paper, we extend this study and compute the first general Zagreb index, general Randić connectivity index, general sum-connectivity index, ABC , GA , ABC_4 and GA_5 indices of hexagonal parallelogram $P(m, n)$ nanotube, triangular benzenoid G_n and zigzag-edge coronoid fused with starphene $ZCS(k, l, m)$ nanotubes by using the line graphs of subdivision of these chemical graphs.

2 Topological indices of $L(S(G))$

In 2011, Su and Xu²² calculated the general sum-connectivity indices and co-indices of the line graphs of the tadpole, wheel and ladder graphs by using the subdivision technique. They also computed the Zagreb indices of the line graphs of the tadpole, wheel and ladder graphs with subdivision in²³. Ranjini et al.²⁴ in 2011 calculated the explicit expressions for the Shultz indices of the subdivision graphs of the tadpole, wheel, helm and ladder graphs. In 2015, Nadeem et al.²⁵ computed the ABC_4 and GA_5 indices of the line graphs of the tadpole, wheel and ladder graphs by using the notion of subdivision. M. Nadeem et al.²⁶ also calculated topological properties of the line graphs of subdivision graphs of certain nanostructures in 2016. In this paper, we apply this technique to hexagonal parallelogram, triangular benzenoid and zigzag-edge coronoid fused with starphene to compute their topological indices in the next subsections.

2.1 Hexagonal Parallelogram $P(m, n)$, $\forall m, n \in \mathbb{N}$ nanotubs

Hexagonal parallelogram nanotube denoted by $P(m, n)$ consists of a hexagons arranged is a parallelogram fashion. In $P(m, n)$ nanotube, where m is the number of hexagons in any row and n is the number of

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hexagons in any column. The number of vertices in hexagonal parallelogram $P(m, n)$ are $2(m + n + mn)$ and the number of edges are $3mn + 2m + 2n - 1$, respectively.

The subdivision graph of hexagonal parallelogram $P(m, n)$ and its line graph is shown in Fig. 1(b) and Fig. 2. The number of vertices in the line graph of the subdivision graph of hexagonal parallelogram $P(m, n)$ are $2(3mn + 2m + 2n - 1)$ and number of edges are $9mn + 4m + 4n - 5$, respectively. In this section, we computed first general Zagreb index, general Randić connectivity index, general sum connectivity index, atom-bond connectivity ABC index, geometric-arithmetic GA index, the fourth version of ABC index (ABC_4) and the fifth version of GA index (GA_5) of the line graph of the subdivision graph of hexagonal parallelogram $P(m, n)$ nanotubes. In the next theorem, an exact expression for the first general Zagreb

Fig. 1. (a) A hexagonal parallelogram $P(4, 4)$ (b) A Subdivision of hexagonal parallelogram $P(4, 4)$.

Fig. 2. A line graph of subdivision graph of hexagonal parallelogram $P(4, 4)$.

Row	n_2	n_3
1	$2(m + 3)$	$4(2m - 1)$
2	4	$6m$
3	4	$6m$
4	4	$6m$
.	.	.
.	.	.
.	.	.
n	$2(m + 3)$	$2(2m - 1)$
Total	$4(m + n + 1)$	$6(mn - 1)$

Table 1. The vertex partition of graph G based on degree of vertices.

index of the line graph of the subdivision graph of hexagonal parallelogram $P(m, n)$ is computed.

Theorem 2.1.1. *The first general Zagreb index of the line graph of the subdivision graph G of hexagonal parallelogram $P(m, n)$, where m is the number of hexagons in any row and n is the number of hexagons in any column is given by*

$$M_{\alpha}(G) = \begin{cases} (m+2)2^{\alpha+2} + 2(m-1)3^{\alpha+1}, & n = 1; \\ (m+n+1)2^{\alpha+2} + 2(mn-1)3^{\alpha+1}, & n \neq 1. \end{cases}$$

Proof. We distinguish the following two cases.

Case 1. For $n \neq 1$,

The subdivision and the line graph G of hexagonal parallelogram $P(m, n)$ are shown in Fig. 1(b) and Fig. 2 respectively. In the graph G , there are total $2(3mn + 2m + 2n - 1)$ vertices among which $4(m + n + 1)$ vertices are of degree 2 and $6(mn - 1)$ vertices are of degree 3, by Table 1. Using these values in the formula of first general Zagreb index, we obtain the required result for $n \neq 1$.

Case 2. For $n = 1$,

The subdivision and the line graph G of hexagonal parallelogram $P(m, n)$ are shown in Fig. 1(b) and Fig. 2 respectively. In G there are total $2(5m + 1)$ vertices among which $4(m + 2)$ vertices are of degree 2 and $6(m - 1)$ vertices are of degree 3. Using these values in the formula of first general Zagreb index, we obtain the required result for $n = 1$, which completes the proof. $\square$

Row	$e_{2,2}$	$e_{2,3}$	$e_{3,3}$
1	$m + 6$	$2m$	$9m - 5$
2	2	4	$9m - 2$
3	2	4	$9m - 2$
4	2	4	$9m - 2$
.	.	.	.
.	.	.	.
.	.	.	.
n	$m + 6$	$2m$	$7m - 4$
Total	$2(m + n + 4)$	$4(m + n - 2)$	$9mn - 2m - 2n - 5$

Table 2. The edge partition of graph G based on degree of end vertices of each edge.

In the following theorem, we obtain a closed-form solution for the general Randić connectivity index for the line graph of the subdivision graph G of hexagonal parallelogram $P(m, n)$.

Theorem 2.1.2. *Let the line graph of the subdivision graph G of hexagonal parallelogram $P(m, n)$, where m is the number of hexagons in any row and n is the number of hexagons in any column. Then the general*

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Randić connectivity index is given as follows

$$R_{\alpha}(G) = (m + n + 4)2^{2\alpha+1} + 4(m + n - 2)6^{\alpha} + (9mn - 2m - 2n - 5)9^{\alpha}.$$

where α denotes real number and $n \neq 1$ is an integer.

Proof. We first find the edge partition of the line graph of the subdivision graph of hexagonal parallelogram $P(m, n)$ based on the degree of end vertices of each edge in the Table 2. Now we can apply the formula of general Randić connectivity index. Since we have

$$R_{\alpha}(G) = \sum_{uv \in E(G)} (d_u d_v)^{\alpha}.$$

This implies that

$$R_{\alpha}(G) = e_{2,2}(2 \times 2)^{\alpha} + e_{2,3}(2 \times 3)^{\alpha} + e_{3,3}(3 \times 3)^{\alpha}.$$

By using the edge partition given in Table 2 and after some simple calculation, we get the following expression

$$R_{\alpha}(G) = (m + n + 4)2^{2\alpha+1} + 4(m + n - 2)6^{\alpha} + (9mn - 2m - 2n - 5)9^{\alpha}.$$

□

In the next theorem, we compute the exact expression for the general sum-connectivity index of the line graph of the subdivision graph of hexagonal parallelogram $P(m, n)$.

Theorem 2.1.3. *Let the line graph of the subdivision graph G of hexagonal parallelogram $P(m, n)$ with m is the number of hexagons in any row and n is the number of hexagons in any column. Then the general sum-connectivity index is given by*

$$\chi_{\alpha}(G) = (m + n + 4)2^{2\alpha+1} + 4(m + n - 2)5^{\alpha} + (9mn - 2m - 2n - 5)6^{\alpha}.$$

where α is a real number and $n \neq 1$ is an integer.

Proof. We find the edge partition of the line graph of the subdivision graph of hexagonal parallelogram $P(m, n)$ based on the degree of end vertices of each edge in the Table 2. Now we can apply formula of general sum-connectivity index. Since we have

$$\chi_{\alpha}(G) = \sum_{uv \in E(G)} (d_u + d_v)^{\alpha}.$$

This implies that

$$\chi_{\alpha}(G) = e_{2,2}(2 + 2)^{\alpha} + e_{2,3}(2 + 3)^{\alpha} + e_{3,3}(3 + 3)^{\alpha}.$$

By using the edge partition given in Table 2 and after some simple calculation, we get

$$\chi_\alpha(G) = (m + n + 4)2^{2\alpha+1} + 4(m + n - 2)5^\alpha + (9mn - 2m - 2n - 5)6^\alpha.$$

□

In the following theorem, we compute the exact expression for atom-bound connectivity index of the line graph of the subdivision graph of hexagonal parallelogram $P(m, n)$.

Theorem 2.1.4. *For every $n \neq 1$, the atom-bound connectivity index ABC of the line graph of the subdivision graph G of hexagonal parallelogram $P(m, n)$, where m is the number of hexagons in any row and n is the number of hexagons in any column is given by*

$$ABC(G) = 6mn + \left(\frac{9\sqrt{2}-4}{3}\right)m + \left(\frac{9\sqrt{2}-4}{3}\right)n - \frac{10}{3}.$$

Proof. Consider the line graph of the subdivision graph of hexagonal parallelogram $P(m, n)$ where m is the number of hexagons in any row and n is the number of hexagons in any column. Let $e_{i,j}$ denotes the number of edges connecting the vertices of degrees d_i and d_j . The two-dimensional structure of the line graph of the subdivision graph of hexagonal parallelogram $P(m, n)$ contains only $e_{2,2}$, $e_{2,3}$ and $e_{3,3}$ edges. The number of $e_{2,2}$, $e_{2,3}$ and $e_{3,3}$ edges in each row is mentioned in Table 2. Since we have

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

This implies that

$$ABC(G) = e_{2,2} \sqrt{\frac{2+2-2}{2 \times 2}} + e_{2,3} \sqrt{\frac{2+3-2}{2 \times 3}} + e_{3,3} \sqrt{\frac{3+3-2}{3 \times 3}}.$$

By using the edge partition given in Table 2, we get the followings

$$ABC(G) = 2(m + n + 4) \frac{1}{\sqrt{2}} + 4(m + n - 2) \frac{1}{\sqrt{2}} + (9mn - 2m - 2n - 5) \frac{2}{3}.$$

After an easy simplification, we ge

$$ABC(G) = 6mn + \left(\frac{9\sqrt{2}-4}{3}\right)m + \left(\frac{9\sqrt{2}-4}{3}\right)n - \frac{10}{3}.$$

□

In the following theorem, we compute the closed-form solution for the geometric-arithmetic index of the line graph of the subdivision graph of hexagonal parallelogram $P(m, n)$.

Theorem 2.1.5. For every $n \neq 1$, the geometric-arithmetic index GA of the line graph of the subdivision graph G of hexagonal parallelogram $P(m, n)$, where m is the number of hexagons in any row and n is the number of hexagons in any column is given by

$$GA(G) = \frac{45mn + 8\sqrt{6}m + 8\sqrt{6}n + 15 - 16\sqrt{6}}{5}.$$

Proof. The geometric-arithmetic GA index of the line graph of the subdivision graph of hexagonal parallelogram $P(m, n)$ for $n \neq 1$ is given by

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

This implies that

$$GA(G) = e_{2,2}(\frac{2\sqrt{2 \times 2}}{2+2}) + e_{2,3}(\frac{2\sqrt{2 \times 3}}{2+3}) + e_{3,3}(\frac{2\sqrt{3 \times 3}}{3+3}).$$

By using the edge partition given in Table 2, we get

$$GA(G) = 2(m+n+4)(\frac{2 \times 2}{4}) + 4(m+n-2)(\frac{2\sqrt{6}}{5}) + (9mn - 2m - 2n - 5)(\frac{2 \times 3}{6}).$$

After an easy simplification, we get

$$GA(G) = \frac{45mn + 8\sqrt{6}m + 8\sqrt{6}n + 15 - 16\sqrt{6}}{5}.$$

□

Row	$e_{4,4}$	$e_{4,5}$	$e_{5,5}$	$e_{5,8}$	$e_{8,8}$	$e_{8,9}$	$e_{9,9}$
1	4	4	$m-2$	$2m$	m	$2m$	$6m-5$
2	0	0	2	4	2	4	$9m-8$
3	0	0	2	4	2	4	$9m-8$
4	0	0	2	4	2	4	$9m-8$
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
n	4	4	$m-2$	$2m$	m	$2m$	$4(m-1)$
Total	8	8	$2(m+n-4)$	$4(m+n-2)$	$2(m+n-2)$	$4(m+n-2)$	$9mn-8(m+n)+7$

Table 3. The edge partition of graph G based on degree sum of neighbor vertices of end vertices of each edge.

In the following two theorems, we obtain analytical closed formulas for the fourth version of atom-bond connectivity index and fifth version of geometric-arithmetic index for the line graph of the subdivision graph G of hexagonal parallelogram $P(m, n)$

Row	$e_{4,4}$	$e_{4,5}$	$e_{5,5}$	$e_{5,8}$	$e_{8,8}$	$e_{8,9}$	$e_{9,9}$
1	5	2	0	2	1	2	1
2	0	0	2	4	2	4	1
3	0	2	2	4	2	4	1
4	0	2	2	4	2	4	.
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
n	5	2	0	2	1	2	1
Total	10	4	$2(n-2)$	$4(n-1)$	$2(n-1)$	$4(n-1)$	$n-1$

Table 4. The edge partition of graph G based on degree sum of neighbor vertices of end vertices of each edge, when $m = 1$.

Theorem 2.1.6. *The fourth atom-bond connectivity index of the line graph of the subdivision graph G of hexagonal parallelogram $P(m, n)$, where m is the number of hexagons in any row and n is the number of hexagons in any column is given by*

$$ABC_4(G) = \begin{cases} \left(\frac{4\sqrt{2}}{5} + \frac{2\sqrt{11}}{\sqrt{10}} + \frac{\sqrt{14}}{4} + \frac{\sqrt{30}}{3} + \frac{4}{9} \right)n + \left(\frac{5\sqrt{6}}{2} + \frac{2\sqrt{7}}{\sqrt{5}} - \frac{8\sqrt{2}}{5} - \frac{2\sqrt{11}}{\sqrt{10}} - \frac{\sqrt{14}}{4} - \frac{\sqrt{30}}{3} - \frac{4}{9} \right), & n \neq 1, m = 1; \\ 4mn + \left(\frac{4\sqrt{2}}{5} + \frac{2\sqrt{11}}{\sqrt{10}} + \frac{\sqrt{14}}{4} + \frac{\sqrt{30}}{3} - \frac{8}{9} \right)m + \left(\frac{\sqrt{14}}{4} + \frac{2\sqrt{11}}{\sqrt{10}} + \frac{\sqrt{30}}{3} - \frac{8}{9} + \frac{4\sqrt{2}}{5} \right)n + 2\sqrt{6} + \frac{4\sqrt{7}}{\sqrt{5}} - \frac{16\sqrt{2}}{5} \\ - \frac{4\sqrt{11}}{\sqrt{10}} - \frac{\sqrt{14}}{2} - \frac{2\sqrt{30}}{3} + \frac{28}{9}, & n \neq 1, m > 1. \end{cases}$$

Proof. Let $e_{i,j}$ denotes the number of edges of the line graph of the subdivision graph of hexagonal parallelogram $P(m, n)$ with $i = s_u$ and $j = s_v$. It is easy to see that the summation of degree of edge endpoints of hexagonal parallelogram has seven edge types $e_{4,4}$, $e_{4,5}$, $e_{5,5}$, $e_{5,8}$, $e_{8,8}$, $e_{8,9}$ and $e_{9,9}$, respectively that are shown in Table 4.

Case 1. The fourth atom-bond connectivity index of the line graph of the subdivision graph of hexagonal parallelogram for $n \neq 1$ and $m = 1$, Since we have

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}}.$$

This implies that

$$ABC_4(G) = e_{4,4} \sqrt{\frac{4+4-2}{4 \times 4}} + e_{4,5} \sqrt{\frac{4+5-2}{4 \times 5}} + e_{5,5} \sqrt{\frac{5+5-2}{5 \times 5}} + e_{5,8} \sqrt{\frac{5+8-2}{5 \times 8}} \\ + e_{8,8} \sqrt{\frac{8+8-2}{8 \times 8}} + e_{8,9} \sqrt{\frac{8+9-2}{8 \times 9}} + e_{9,9} \sqrt{\frac{9+9-2}{9 \times 9}}.$$

By using Table 4, we get

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$$ABC_4(G) = 10\frac{\sqrt{6}}{4} + 4\left(\frac{\sqrt{7}}{2\sqrt{5}}\right) + 2(n-2)\frac{2\sqrt{2}}{5} + 4(n-1)\frac{\sqrt{11}}{2\sqrt{10}} + 2(n-1)\frac{\sqrt{14}}{8} \\ + 4(n-1)\frac{\sqrt{15}}{6\sqrt{2}} + (n-1)\frac{4}{9}.$$

After an easy simplification we get,

$$ABC_4(G) = \left(\frac{4\sqrt{2}}{5} + \frac{2\sqrt{11}}{\sqrt{10}} + \frac{\sqrt{14}}{4} + \frac{\sqrt{30}}{3} + \frac{4}{9}\right)n + \left(\frac{5\sqrt{6}}{2} + \frac{2\sqrt{7}}{\sqrt{5}} - \frac{8\sqrt{2}}{5} - \frac{2\sqrt{11}}{\sqrt{10}} \right. \\ \left. - \frac{14}{4} - \frac{\sqrt{30}}{3} - \frac{4}{9}\right).$$

Case 2. For $n \neq 1$ and $m > 1$, the line graph of the subdivision graph of hexagonal parallelogram has seven types of edges, namely $e_{4,4}$, $e_{4,5}$, $e_{5,5}$, $e_{5,8}$, $e_{8,8}$, $e_{8,9}$ and $e_{9,9}$. The number of edges of these types is shown in Table 3. Since we have

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}}.$$

This implies that

$$ABC_4(G) = e_{4,4}\sqrt{\frac{4+4-2}{4 \times 4}} + e_{4,5}\sqrt{\frac{4+5-2}{4 \times 5}} + e_{5,5}\sqrt{\frac{5+5-2}{5 \times 5}} + e_{5,8}\sqrt{\frac{5+8-2}{5 \times 8}} \\ + e_{8,8}\sqrt{\frac{8+8-2}{8 \times 8}} + e_{8,9}\sqrt{\frac{8+9-2}{8 \times 9}} + e_{9,9}\sqrt{\frac{9+9-2}{9 \times 9}}.$$

By using Table 3, we get

$$ABC_4(G) = 8\left(\frac{\sqrt{6}}{4}\right) + 8\left(\frac{\sqrt{7}}{2\sqrt{5}}\right) + 2(m+n-4)\frac{2\sqrt{2}}{5} + 4(m+n-2)\frac{\sqrt{11}}{2\sqrt{10}} + 2(m+n-2)\frac{\sqrt{14}}{8} \\ + 4(m+n-2)\frac{\sqrt{15}}{6\sqrt{2}} + (9mn - 2m - 2n + 7)\frac{4}{9}.$$

After easy simplification we get

$$ABC_4(G) = 4mn + \left(\frac{4\sqrt{2}}{5} + \frac{2\sqrt{11}}{\sqrt{10}} + \frac{\sqrt{14}}{4} + \frac{\sqrt{30}}{3} - \frac{8}{9}\right)m + \left(\frac{\sqrt{14}}{4} + \frac{2\sqrt{11}}{\sqrt{10}} + \frac{\sqrt{30}}{3} - \frac{8}{9} \right. \\ \left. + \frac{4\sqrt{2}}{5}\right)n + 2\sqrt{6} + \frac{4\sqrt{7}}{\sqrt{5}} - \frac{16\sqrt{2}}{5} - \frac{4\sqrt{11}}{\sqrt{10}} - \frac{\sqrt{14}}{2} - \frac{2\sqrt{30}}{3} + \frac{28}{9}. \quad \square$$

Theorem 2.1.7. The fifth geometric-arithmetic index of the line graph of the subdivision graph G of hexagonal parallelogram $P(m, n)$, where m is the number of hexagons in any row and n is the number of

hexagons in any column is given by

$$GA_5(G) = \begin{cases} (5 + \frac{16\sqrt{10}}{13} + \frac{48\sqrt{2}}{17})n + 3 + \frac{16\sqrt{5}}{9} - \frac{16\sqrt{10}}{13} - \frac{48\sqrt{2}}{17}, & n \neq 1, m = 1; \\ 9mn + (\frac{16\sqrt{10}}{13} + \frac{48\sqrt{2}}{17} - 4)m + (\frac{16\sqrt{10}}{13} + \frac{48\sqrt{2}}{17} - 4)n + 3 + \frac{32\sqrt{5}}{9} - \frac{32\sqrt{10}}{13} - \frac{96\sqrt{2}}{17}, & n \neq 1, m > 1; \end{cases}$$

Proof. Let $e_{i,j}$ denotes the number of edges of the line graph of the subdivision graph of hexagonal parallelogram with $i = s_u$ and $j = s_v$. It is easy to see that the summation of degree of edge endpoints of hexagonal parallelogram has seven edge types $e_{4,4}$, $e_{4,5}$, $e_{5,5}$, $e_{5,8}$, $e_{8,8}$, $e_{8,9}$ and $e_{9,9}$ that are shown in Table 4.

Case 1. The fifth geometric-arithmetic index of the line graph of the subdivision graph of hexagonal parallelogram for $n \neq 1$ and $m = 1$, Since we have

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{s_u s_v}}{s_u + s_v}.$$

This implies that

$$GA_5(G) = e_{4,4}(\frac{2\sqrt{4 \times 4}}{4+4}) + e_{4,5}(\frac{2\sqrt{4 \times 5}}{4+5}) + e_{5,5}(\frac{2\sqrt{5 \times 5}}{5+5}) + e_{5,8}(\frac{2\sqrt{5 \times 8}}{5+8}) + e_{8,8}(\frac{2\sqrt{8 \times 8}}{8+8}) \\ + e_{8,9}(\frac{2\sqrt{8 \times 9}}{8+9}) + e_{9,9}(\frac{2\sqrt{9 \times 9}}{9+9}).$$

By using Table 4, we get

$$GA_5(G) = 10(\frac{2 \times 2 \times 2}{8}) + 4(\frac{2 \times 2 \times \sqrt{5}}{9}) + 2(n-2)(\frac{2 \times 5}{10}) + 4(n-1)(\frac{2 \times 2 \times \sqrt{10}}{13}) + 2(n-1)(\frac{2 \times 8}{16}) \\ + 4(n-1)(\frac{2 \times 2 \times 3 \times \sqrt{2}}{17}) + (n-1)(\frac{2 \times 9}{18}).$$

After some calculation we get,

$$GA_5(G) = (5 + \frac{16\sqrt{10}}{13} + \frac{48\sqrt{2}}{17})n + 3 + \frac{16\sqrt{5}}{9} - \frac{16\sqrt{10}}{13} - \frac{48\sqrt{2}}{17}.$$

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Case 2. For $n \neq 1$ and $m > 1$, then the geometric-arithmetic index of the line graph of the subdivision graph of hexagonal parallelogram is

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{s_u s_v}}{s_u + s_v}.$$

This implies that

$$\begin{aligned} GA_5(G) = & e_{4,4}\left(\frac{2\sqrt{4 \times 4}}{4+4}\right) + e_{4,5}\left(\frac{2\sqrt{4 \times 5}}{4+5}\right) + e_{5,5}\left(\frac{2\sqrt{5 \times 5}}{5+5}\right) + e_{5,8}\left(\frac{2\sqrt{5 \times 8}}{5+8}\right) + e_{8,8}\left(\frac{2\sqrt{8 \times 8}}{8+8}\right) \\ & + e_{8,9}\left(\frac{2\sqrt{8 \times 9}}{8+9}\right) + e_{9,9}\left(\frac{2\sqrt{9 \times 9}}{9+9}\right). \end{aligned}$$

By using Table 3, we get

$$\begin{aligned} GA_5(G) = & 8\left(\frac{2 \times 2 \times 2}{8}\right) + 8\left(\frac{2 \times 2 \times \sqrt{5}}{9}\right) + 2(m+n-4)\left(\frac{2 \times 5}{10}\right) + 4(m+n-2)\left(\frac{2 \times 2 \times \sqrt{10}}{13}\right) \\ & + 2(m+n-2)\left(\frac{2 \times 8}{16}\right) + 4(m+n-2)\left(\frac{2 \times 2 \times 3 \times \sqrt{2}}{17}\right) + (9mn - 8m - 8n + 7)\left(\frac{2 \times 9}{18}\right). \end{aligned}$$

After some calculation we get,

$$\begin{aligned} GA_5(G) = & 9mn + \left(\frac{16\sqrt{10}}{13} + \frac{48\sqrt{2}}{17} - 4\right)m + \left(\frac{16\sqrt{10}}{13} + \frac{48\sqrt{2}}{17} - 4\right)n + 3 + \frac{32\sqrt{5}}{9} \\ & - \frac{32\sqrt{10}}{13} - \frac{96\sqrt{2}}{17}. \end{aligned}$$

□

2.2 Triangular benzenoids G_n , $\forall n \in \mathbb{N}$

Triangular benzenoids denoted by G_n is a family of benzenoid molecular graphs, which is the generalizations of benzene molecule C_6H_6 in which benzene rings form a triangular shape. The benzene molecule is a usual molecule in chemistry, physics and nano-sciences and is very useful to synthesize aromatic compounds. These graphs consists of a hexagonal arranged in rows and in each row one hexagon increases. The numbers of vertices in triangular benzenoid G_n are $n^2 + 4n + 1$ and the number of edges are $\frac{3}{2}n(n+3)$.

The subdivision graph of triangular benzenoid G_n and its line graph are shown in Fig. 3(b) and Fig. 4. The number of vertices in the line graph of the subdivision graph of triangular benzenoid G_n are $3n(n+3)$ and number of edges are $\frac{3}{2}(3n^2 + 7n - 2)$. In this section, we computed first general Zagreb index M_α , general Randić connectivity index R_α , general sum-connectivity index χ_α , atom-bond connectivity ABC index, geometric-arithmetic GA index, ABC_4 index and GA_5 index of the line graph of the subdivision graph of triangular benzenoid G_n . In the next theorem, we compute the exact expression for the first

Fig. 3. (a) A triangular benzenoid G_5 (b) A Subdivision of triangular benzenoid G_5 .

Fig. 4. A line graph of subdivision graph of triangular benzenoid G_5 .

m_{d_u, d_v} where $uv \in E(G)$	$m_{2,2}$	$m_{2,3}$	$m_{3,3}$
Number of edges	$3(n+3)$	$6(n-1)$	$\frac{3}{2}(3n^2+n-4)$

Table 5. The edge partition of graph G based on degree of end vertices of each edge.

general Zagreb index, general Randić connectivity index, and general sum-connectivity index of the line graph of the subdivision graph of triangular benzenoid G_n .

Theorem 2.2.1. *Let G denotes the line graph of the subdivision graph of triangular benzenoid G_n , for every $n \in \mathbb{N}$. Then we have*

1. $M_\alpha(G) = 3(n+1).2^{\alpha+1} + (n-1)(n+2).3^{\alpha+1}$.
2. $R_\alpha(G) = 3(n+3).4^\alpha + (n-1).6^{\alpha+1} + \frac{1}{2}(3n^2+n-4).3^{2\alpha+1}$.
3. $\chi_\alpha(G) = 3(n+3).4^\alpha + 6(n-1).5^\alpha + \frac{3}{2}(3n^2+n-4).6^\alpha$.

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where α is a real number.

Proof. The subdivision graph and the line graph G of triangular benzenoid are shown in Fig. 3(b) and Fig. 4 respectively. In graph G , there are total $3n(n+3)$ vertices among which $3(n-1)(n+2)$ vertices are of degree 3 and $6(n+1)$ vertices are of degree 2. Using these values in the formula of first general Zagreb index, we may obtain the required result.

The total number of edges of the line graph of the subdivision graph of triangular benzenoid G_n is $\frac{3}{2}(3n^2 + 7n - 2)$. Therefore we get the edge-partition based on the degree of the end vertices of each edge as shown in Table 5. We use the edge partition given in Table 5 in the formulas of general Randić index and general sum-connectivity index, respectively.

Case 1. Since we have

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha.$$

This implies that

$$R_\alpha(G) = m_{2,2}(2 \times 2)^\alpha + m_{2,3}(2 \times 3)^\alpha + m_{3,3}(3 \times 3)^\alpha.$$

By using the edge-partition given in Table 5 and after an easy simplification, we get

$$R_\alpha(G) = 3(n+3)4^\alpha + 6(n-1)6^\alpha + \frac{1}{2}(3n^2 + n - 4)3^{2\alpha+1}.$$

Case 2. Since we have

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha.$$

This implies that

$$\chi_\alpha(G) = m_{2,2}(2+2)^\alpha + m_{2,3}(2+3)^\alpha + m_{3,3}(3+3)^\alpha.$$

By using the edge-partition given in Table 5, we get

$$\chi_\alpha(G) = 3(n+3)4^\alpha + 6(n-1)5^\alpha + \frac{3}{2}(3n^2 + n - 4)6^\alpha.$$

□

In the next theorem, we compute the analytical closed form expression for atom-bond connectivity index of the line graph of the subdivision graph of triangular benzenoid G_n .

Theorem 2.2.2. Let G denotes the line graph of the subdivision graph of triangular benzenoid G_n , for every $n \in \mathbb{N}$. Then its atom-bond connectivity index ABC index is equal to

$$ABC(G) = 3n^2 + \left(\frac{9+\sqrt{2}}{\sqrt{2}}\right)n + \frac{3-4\sqrt{2}}{\sqrt{2}}.$$

Proof. We use the edge-partition based on the degree of end vertices of each edge of the line graph of the subdivision graph of triangular benzenoid given in Table 5. Then we may compute the ABC index. Since we have

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

This implies that

$$ABC(G) = m_{2,2} \sqrt{\frac{2+2-2}{2 \times 2}} + m_{2,3} \sqrt{\frac{2+3-2}{2 \times 3}} + m_{3,3} \sqrt{\frac{3+3-2}{3 \times 3}}.$$

By using the edge-partition given in Table 5, we get

$$ABC(G) = 3(n+3) \frac{1}{\sqrt{2}} + 6(n-1) \frac{1}{\sqrt{2}} + \frac{3}{2} (3n^2 + n - 4) \frac{2}{3}.$$

After some easy simplification, we get

$$ABC(G) = 3n^2 + \left(\frac{9 + \sqrt{2}}{\sqrt{2}}\right)n + \frac{3 - 4\sqrt{2}}{\sqrt{2}}.$$

□

In the following theorem, we compute the analytical closed form expression for geometric-arithmetic index of the line graph of the subdivision graph of triangular benzenoid G_n .

Theorem 2.2.3. *Let G be the line graph of the subdivision graph of triangular benzenoid G_n , for every $n \in \mathbb{N}$. Then its geometric-arithmetic GA index is equal to*

$$GA(G) = \frac{9}{2}n^2 + \left(\frac{24\sqrt{6} + 45}{10}\right)n + \frac{15 - 12\sqrt{6}}{5}.$$

Proof. We use the edge partition based on the degree of end vertices of each edge of the line graph of the subdivision graph of triangular benzenoid given in Table 5 to compute the GA index of G . Since we have

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

This implies that

$$GA(G) = m_{2,2} \frac{2\sqrt{2 \times 2}}{2 + 2} + m_{2,3} \frac{2\sqrt{2 \times 3}}{2 + 3} + m_{3,3} \frac{2\sqrt{3 \times 3}}{3 + 3}.$$

By using the edge-partition given in Table 5, we get

$$GA(G) = 3(n+3) \frac{2 \times 2}{4} + 6(n-1) \frac{2\sqrt{6}}{5} + \frac{3}{2} (3n^2 + n - 4) \frac{2 \times 3}{6}.$$

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After some easy simplification, we get

$$GA(G) = \frac{9}{2}n^2 + \left(\frac{24\sqrt{6} + 45}{10}\right)n + \frac{15 - 12\sqrt{6}}{5}.$$

□

In the next two theorems, we calculated the ABC_4 and GA_5 index of G . There are seven types of edges on degree based sum of neighbors vertices of each edge in the line graph of the subdivision graph G of triangular benzinoid. We use this partition of edges to calculate ABC_4 and GA_5 indices. Table 6 gives such types of edges of the line graph of the subdivision graph G of triangular benzenoid G_n .

m_{s_u, s_v} where $uv \in E(G)$	Number of edges
(4, 4)	9
(4, 5)	6
(5, 5)	$3(n - 2)$
(5, 8)	$6(n - 1)$
(8, 8)	$3(n - 1)$
(8, 9)	$6(n - 1)$
(9, 9)	$\frac{3}{2}(3n^2 - 5n + 2)$

Table 6. The edge partition of graph G based on degree sum of neighbor vertices of end vertices of each edge.

Theorem 2.2.4. Consider the line graph of the subdivision graph G of triangular benzenoid G_n , for every $n \in \mathbb{N}$. Then the ABC_4 index is

$$ABC_4(G) = \begin{cases} \frac{9\sqrt{6}}{4}, & n = 1; \\ 2n^2 + \left(\frac{6\sqrt{2}}{5} + \frac{3\sqrt{14}}{8} + \frac{3\sqrt{11}}{\sqrt{10}} + \frac{\sqrt{15}}{\sqrt{2}} - \frac{10}{3}\right)n \\ + \frac{9\sqrt{6}}{4} - \frac{12\sqrt{2}}{5} - \frac{3\sqrt{14}}{8} + \frac{3\sqrt{7}}{\sqrt{5}} - \frac{3\sqrt{11}}{\sqrt{10}} - \frac{\sqrt{15}}{\sqrt{2}} + \frac{4}{3}, & n \neq 1. \end{cases}$$

Proof. We find the edge partition of the line graph of the subdivision graph of triangular benzenoid G_n based on degree sum of vertices lying at unit distance from end vertices of each edge. Now we can apply formula of ABC_4 index.

Case 1. For $n \neq 1$, Since we have

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}}.$$

Then,

$$ABC_4(G) = e_{4,4}\sqrt{\frac{4+4-2}{4 \times 4}} + e_{4,5}\sqrt{\frac{4+5-2}{4 \times 5}} + e_{5,5}\sqrt{\frac{5+5-2}{5 \times 5}} + e_{5,8}\sqrt{\frac{5+8-2}{5 \times 8}}$$

$$+ e_{8,8}\sqrt{\frac{8+8-2}{8 \times 8}} + e_{8,9}\sqrt{\frac{8+9-2}{8 \times 9}} + e_{9,9}\sqrt{\frac{9+9-2}{9 \times 9}}.$$

By using the edge-partition given in Table 6, we get

$$\begin{aligned} ABC_4(G) &= 9\frac{\sqrt{6}}{4} + 6\frac{\sqrt{7}}{2\sqrt{5}} + 3(n-2)\frac{2\sqrt{2}}{5} + 6(n-1)\frac{\sqrt{11}}{2\sqrt{10}} + 3(n-1)\frac{\sqrt{14}}{8} \\ &\quad + 6(n-1)\frac{\sqrt{15}}{6\sqrt{2}} + \frac{3}{2}(3n^2 - 5n + 2)\frac{4}{9}. \end{aligned}$$

After some calculation, we get

$$\begin{aligned} ABC_4(G) &= 2n^2 + \left(\frac{6\sqrt{2}}{5} + \frac{3\sqrt{14}}{8} + \frac{3\sqrt{11}}{\sqrt{10}} + \frac{\sqrt{15}}{\sqrt{2}} - \frac{10}{3}\right)n + \frac{9\sqrt{6}}{4} - \frac{12\sqrt{2}}{5} - \frac{3\sqrt{14}}{8} + \frac{3\sqrt{7}}{\sqrt{5}} \\ &\quad - \frac{3\sqrt{11}}{\sqrt{10}} - \frac{\sqrt{15}}{\sqrt{2}} + \frac{4}{3}. \end{aligned}$$

Case 2. For $n = 1$, Since we have

$$\begin{aligned} ABC_4(G) &= \sum_{uv \in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}}. \\ ABC_4 &= 9 \times \sqrt{\frac{4 + 4 - 2}{4 \times 4}}. \end{aligned}$$

After simple calculation we get,

$$ABC_4(G) = \frac{9\sqrt{6}}{4}.$$

□

Theorem 2.2.5. Consider the line graph of the subdivision graph G of triangular benzenoid G_n , $n \in \mathbb{N}$. Then the GA_5 index is

$$GA_5(G) = \begin{cases} 9, & n = 1; \\ \frac{9}{2}n^2 + \left(\frac{24\sqrt{10}}{13} + \frac{72\sqrt{2}}{17} - \frac{3}{2}\right)n + \frac{8\sqrt{5}}{3} - \frac{24\sqrt{10}}{13} + \frac{72\sqrt{2}}{17} + 3, & n \neq 1. \end{cases}$$

Proof. We find the edge partition of the line graph of the subdivision graph G of triangular benzenoid G_n based on degree sum of vertices lying at unit distance from end vertices of each edge. Now we can apply formula of GA_5 index.

Case 1. For $n \neq 1$, Since we have

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{s_u s_v}}{s_u + s_v}.$$

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Then,

$$GA_5(G) = m_{4,4}\left(\frac{2\sqrt{4 \times 4}}{4+4}\right) + m_{4,5}\left(\frac{2\sqrt{4 \times 5}}{4+5}\right) + m_{5,5}\left(\frac{2\sqrt{5 \times 5}}{5+5}\right) + m_{5,8}\left(\frac{2\sqrt{5 \times 8}}{5+8}\right) \\ + m_{8,8}\left(\frac{2\sqrt{8 \times 8}}{8+8}\right) + m_{8,9}\left(\frac{2\sqrt{8 \times 9}}{8+9}\right) + m_{9,9}\left(\frac{2\sqrt{9 \times 9}}{9+9}\right).$$

By using the edge-partition given in Table 6, we have

$$GA_5(G) = 9\left(\frac{2 \times 4}{8}\right) + 6\left(\frac{4 \times 5}{9}\right) + 3(n-2)\left(\frac{2 \times 5}{10}\right) + 6(n-1)\left(\frac{4 \times 10}{13}\right) + 3(n-1)\left(\frac{2 \times 8}{16}\right) \\ + 6(n-1)\left(\frac{12 \times 2}{17}\right) + \frac{3}{2}(3n^2 - 5n + 2)\left(\frac{2 \times 9}{18}\right).$$

After some calculation we get,

$$GA_5(G) = \frac{9}{2}n^2 + \left(\frac{24\sqrt{10}}{13} + \frac{72\sqrt{2}}{17} - \frac{3}{2}\right)n + \frac{8\sqrt{5}}{3} - \frac{24\sqrt{10}}{13} + \frac{72\sqrt{2}}{17} + 3.$$

Case 2. For $n = 1$, Since we have

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{s_u s_v}}{s_u + s_v}.$$

$$GA_5 = 9 \times \frac{2\sqrt{4 \times 4}}{4 + 4}.$$

After simple calculation we get,

$$GA_5(G) = 9.$$

□

2.3 Zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$

This system considered in this work is a composite benzenoid obtained by fusing a zigzag-edge coronoid $ZC(k, l, m)$ with a starphene denoted by $St(k, l, m)$. The numbers of vertices in Zigzag-edge Coronoid fused with starphene nanotubes $ZCS(k, l, m)$ are $36k - 54$ and the number of edges are $15(k + l + m) - 63$. The subdivision graph of zigzag-edge Coronoid fused with starphene nanotubes $ZCS(k, l, m)$ and its line graph are shown in Fig. 5(b) and Fig. 6. The number of vertices in the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$ are $30(k + l + m) - 126$ and number of edges are $39(k + l + m) - 153$. In this section, we computed the first general Zagreb index M_α , general Randić connectivity index R_α , general sum-connectivity index χ_α , atom-bond connectivity ABC index,

geometric-arithmetic GA index, ABC_4 index and GA_5 index of the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$. In the next theorem, we compute the

Fig. 5. (a) A zigzag-edge coronoid fused with starphene nanotubes $ZCS(4, 4, 4)$. (b) A subdivision of zigzag-edge coronoid fused with starphene nanotubes $ZCS(4, 4, 4)$.

Fig. 6. A line graph of subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(4, 4, 4)$.

m_{d_u, d_v} where $uv \in E(G)$	$m_{2,2}$	$m_{2,3}$	$m_{3,3}$
Number of edges	$6(k + l + m - 5)$	$12(k + l + m - 7)$	$21(k + l + m) - 39$

Table 7. The edge partition of graph G based on degree of end vertices of each edge.

analytical closed form expression for the first general Zagreb index, general Randić connectivity index, and general sum-connectivity index of the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$.

Theorem 2.3.1. Let G be the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$ for every $k = l = m \geq 4$. Then we have

1. $M_\alpha(G) = 3(k + l + m).2^{\alpha+2} + 2(k + l + m - 3).3^{\alpha+2}.$
2. $R_\alpha(G) = 3(k + l + m - 5).2^{2\alpha+1} + 2(k + l + m - 7).6^{\alpha+1} + \{21(k + l + m) - 39\}.3^{2\alpha}.$
3. $\chi_\alpha(G) = 3(k + l + m - 5).2^{2\alpha+1} + 12(k + l + m - 7).5^\alpha + \{21(k + l + m) - 39\}.6^\alpha.$

where α is a real number.

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Proof. The subdivision graph and the line graph G of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$ are shown in Fig. 5(b) and Fig. 6 respectively. In graph G , there are total $30(k + l + m) - 126$ vertices among which $18(k + l + m - 3)$ vertices are of degree 3 and $12(k + l + m - 6)$ vertices are of degree 2. Using these values in the formula of first general Zagreb index we obtain the required result.

The total number of edges of the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$ is $39(k + l + m) - 153$. Therefore we get the edge-partition based on the degree of the vertices as shown in Table 7. Using the edge-partition given in Table 7 in the formulas of general Randić index and general sum-connectivity index, respectively, we can get the required expression.

Case 1. Since we have

$$R_{\alpha}(G) = \sum_{uv \in E(G)} (d_u d_v)^{\alpha}.$$

This implies that

$$R_{\alpha}(G) = m_{2,2}(2 \times 2)^{\alpha} + m_{2,3}(2 \times 3)^{\alpha} + m_{3,3}(3 \times 3)^{\alpha}.$$

By using the edge-partition given in Table 7 and after an easy simplification, we get

$$R_{\alpha}(G) = 3(k + l + m - 5).2^{2\alpha+1} + 2(k + l + m - 7).6^{\alpha+1} + \{21(k + l + m) - 39\}.3^{2\alpha}.$$

Case 2. Since we have

$$\chi_{\alpha}(G) = \sum_{uv \in E(G)} (d_u + d_v)^{\alpha}.$$

This implies that

$$\chi_{\alpha}(G) = m_{2,2}(2 + 2)^{\alpha} + m_{2,3}(2 + 3)^{\alpha} + m_{3,3}(3 + 3)^{\alpha}.$$

By using the edge-partition given in Table 7, we get

$$\chi_{\alpha}(G) = 3(k + l + m - 5).2^{2\alpha+1} + 12(k + l + m - 7).5^{\alpha} + \{21(k + l + m) - 39\}.6^{\alpha}.$$

□

In the following theorem, we compute the analytical closed form expression for atom-bond connectivity index of the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$.

Theorem 2.3.2. *Let G be the line graph of the subdivision graph of Zigzag-edge Coronoid fused with Starphene nanotubes $ZCS(k, l, m)$ for every $k = l = m \geq 4$. Then its atom-bond connectivity index ABC*

index is equal to

$$ABC(G) = (9\sqrt{2} + 14)(k + l + m) - 57\sqrt{2} - 26.$$

Proof. By using the edge-partition based on the degree of end vertices of each edge of the line graph of the subdivision graph G of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$, given in Table 1, we compute the ABC index. Since we have

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

This implies that

$$ABC(G) = m_{2,2} \sqrt{\frac{2+2-2}{2 \times 2}} + m_{2,3} \sqrt{\frac{2+3-2}{2 \times 3}} + m_{3,3} \sqrt{\frac{3+3-2}{3 \times 3}}.$$

By using the edge partition given in Table 7, we get

$$ABC(G) = \frac{6}{\sqrt{2}}(k + l + m - 5) + \frac{12}{\sqrt{2}}(k + l + m - 7) + \frac{2}{3}\{21(k + l + m) - 39\}.$$

After some easy simplification, we get

$$ABC(G) = (9\sqrt{2} + 14)(k + l + m) - 57\sqrt{2} - 26.$$

□

In the following theorem, we compute the closed-form expression for geometric-arithmetic index of the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$.

Theorem 2.3.3. *Let G be the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$ for $k = l = m \geq 4$. Then its geometric-arithmetic GA index is equal to*

$$GA(G) = (27 + \frac{24\sqrt{6}}{5})(k + l + m) - 69 - \frac{168\sqrt{6}}{5}.$$

Proof. By using the edge partition based on the degree of end vertices of each edge of the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$ given in Table 7, we compute the GA index of G . Since we have

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

This implies that

$$GA(G) = m_{2,2} \frac{2\sqrt{2 \times 2}}{2 + 2} + m_{2,3} \frac{2\sqrt{2 \times 3}}{2 + 3} + m_{3,3} \frac{2\sqrt{3 \times 3}}{3 + 3}.$$

$$GA(G) = 6(k+l+m-5)\frac{2 \times 2}{4} + 12(k+l+m)\frac{2\sqrt{6}}{5} + \{21(k+l+m) - 39\}\frac{2 \times 3}{6}.$$

After some easy simplification, we get

$$GA(G) = (27 + \frac{24\sqrt{6}}{5})(k+l+m) - 69 - \frac{168\sqrt{6}}{5}.$$

□

In the next two theorems, we have calculated the ABC_4 and GA_5 index of G . There are seven types of edges on degree based sum of neighbors vertices of each edge in the line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$ for every $k = l = m \geq 4$.

e_{s_u, s_v} where $uv \in E(G)$	Number of edges
$e_{4,4}$	6
$e_{4,5}$	12
$e_{5,5}$	$6(k+l+m-8)$
$e_{5,8}$	$12(k+l+m-7)$
$e_{8,8}$	$6(k+l+m-9)$
$e_{8,9}$	$12(k+l+m-5)$
$e_{9,9}$	$3(k+l+m+25)$

Table 8. The edge partition of graph G based on degree sum of neighbor vertices of end vertices of each edge.

Theorem 2.3.4. Consider the line graph of the subdivision graph G of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$ for every $k = l = m \geq 4$. Then the ABC_4 index is

$$ABC_4(G) = (\frac{12\sqrt{2}}{5} + \frac{3\sqrt{14}}{4} + \frac{6\sqrt{11}}{\sqrt{10}} + \sqrt{30} + \frac{4}{3})(k+l+m) + \frac{3\sqrt{6}}{2} - \frac{96\sqrt{2}}{5} + \frac{27\sqrt{14}}{4} + \frac{6\sqrt{7}}{\sqrt{5}} - \frac{42\sqrt{11}}{\sqrt{10}} - 5\sqrt{30} + \frac{100}{3}.$$

Proof. We find the edge partition of the line graph of the subdivision graph G of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$ based on degree sum of vertices lying at unit distance from end vertices of each edge in Table 8. Now we can apply formula of ABC_4 index. Since we have

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}}.$$

Then,

$$ABC_4(G) = e_{4,4}\sqrt{\frac{4+4-2}{4 \times 4}} + e_{4,5}\sqrt{\frac{4+5-2}{4 \times 5}} + e_{5,5}\sqrt{\frac{5+5-2}{5 \times 5}} + e_{5,8}\sqrt{\frac{5+8-2}{5 \times 8}}$$

$$+ e_{8,8}\sqrt{\frac{8+8-2}{8 \times 8}} + e_{8,9}\sqrt{\frac{8+9-2}{8 \times 9}} + e_{9,9}\sqrt{\frac{9+9-2}{9 \times 9}}.$$

By using the edge-partition given in Table 8, we get

$$\begin{aligned} ABC_4(G) &= 6\frac{\sqrt{6}}{4} + 12\frac{\sqrt{7}}{2\sqrt{5}} + 6(k+l+m-8)\frac{2\sqrt{2}}{5} + 12(k+l+m-7)\frac{\sqrt{11}}{2\sqrt{10}} \\ &\quad + 6(k+l+m-9)\frac{\sqrt{14}}{8} + 12(k+l+m-5)\frac{\sqrt{15}}{6\sqrt{2}} + 3(k+l+m+25)\frac{4}{9}. \end{aligned}$$

After some calculation we get

$$\begin{aligned} ABC_4(G) &= \left(\frac{12\sqrt{2}}{5} + \frac{3\sqrt{14}}{4} + \frac{6\sqrt{11}}{\sqrt{10}} + \sqrt{30} + \frac{4}{3}\right)(k+l+m) + \frac{3\sqrt{6}}{2} - \frac{96\sqrt{2}}{5} + \frac{27\sqrt{14}}{4} \\ &\quad + \frac{6\sqrt{7}}{\sqrt{5}} - \frac{42\sqrt{11}}{\sqrt{10}} - 5\sqrt{30} + \frac{100}{3}. \end{aligned}$$

□

Theorem 2.3.5. Consider the line graph of the subdivision graph G of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$ for every $k = l = m \geq 4$. Then the GA_5 index is given as

$$GA_5(G) = \left(\frac{48\sqrt{10}}{13} + \frac{144\sqrt{2}}{17} + 15\right)(k+l+m) + \frac{16\sqrt{5}}{3} - \frac{336\sqrt{10}}{13} - \frac{720\sqrt{2}}{17} + 3.$$

Proof. We find the edge-partition of the line graph of the subdivision graph G of zigzag-edge coronoid fused with starphene nanotubes $ZCS(k, l, m)$ based on degree-sum of vertices lying at unit distance from end vertices of each edge. Now we can apply formula of GA_5 index. Since we have

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{s_u s_v}}{s_u + s_v}.$$

Then,

$$\begin{aligned} GA_5(G) &= m_{4,4}\left(\frac{2\sqrt{4 \times 4}}{4+4}\right) + m_{4,5}\left(\frac{2\sqrt{4 \times 5}}{4+5}\right) + m_{5,5}\left(\frac{2\sqrt{5 \times 5}}{5+5}\right) + m_{5,8}\left(\frac{2\sqrt{5 \times 8}}{5+8}\right) \\ &\quad + m_{8,8}\left(\frac{2\sqrt{8 \times 8}}{8+8}\right) + m_{8,9}\left(\frac{2\sqrt{8 \times 9}}{8+9}\right) + m_{9,9}\left(\frac{2\sqrt{9 \times 9}}{9+9}\right). \end{aligned}$$

By using the edge-partition given in Table 8, we get

$$\begin{aligned} GA_5(G) &= 6\left(\frac{2 \times 4}{8}\right) + 12\left(\frac{4\sqrt{5}}{9}\right) + 6(k+l+m)\left(\frac{2 \times 5}{10}\right) + 12(k+l+m-7)\left(\frac{4\sqrt{10}}{13}\right) \\ &\quad + 6(k+l+m-5)\left(\frac{2 \times 8}{16}\right) + 12(k+l+m-5)\left(\frac{12\sqrt{2}}{17}\right) + 3(k+l+m+25)\left(\frac{2 \times 9}{18}\right). \end{aligned}$$

After some calculation we get,

$$GA_5(G) = \left(\frac{48\sqrt{10}}{13} + \frac{144\sqrt{2}}{17} + 15\right)(k + l + m) + \frac{16\sqrt{5}}{3} - \frac{336\sqrt{10}}{13} - \frac{720\sqrt{2}}{17} + 3.$$

□

3 Conclusion

In this paper, five important degree-based indices, namely first general Zagreb index M_α , general Randić connectivity index R_α , general sum-connectivity index χ_α , atom-bond connectivity index ABC , geometric-arithmetic index GA , ABC_4 index and GA_5 index are studied. These topological indices correlate certain physico-chemical properties such as boiling point, strain energy and stability etc. of chemical compounds. We compute these indices for the line graphs of subdivision graphs of hexagonal parallelogram $P(m, n)$ nanotube, triangular benzenoids G_n and zigzag-edge coronoid fused with starphene $ZCS(k, l, m)$ nanotube. This will start a new direction for researchers in this field. However, there are still open and challenging problems for researchers.

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