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# NEW AUGMENTED ZAGREB INDICES

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***ABSTRACT***

*We introduce some new augmented Zagreb indices: second, third and fourth augmented Zagreb indices of a molecular graph. A topological index is a numerical parameter mathematically derived from the graph structure. In this paper, we compute augmented zegreb index and Sanskruti index of triangular benzenoid $T_n$, hexagonal parallelogram nanotube P(m, n) and zigzag-edge coronoid fused with starphene nanotube ZCS(k, l, m) by using the line graphs of the subdivision graphs of these important chemical graphs.*

***Keywords:*** *augmented Zagreb index, triangular benzenoid, hexagonal parallelogram nanotube, zigzag-edge coronoid fused with starphene nanotube.*

***Mathematics Subject Classification:*** *05C05, 05C12, 05C35.*

## 1. INTRODUCTION

Let $G = (V, E)$ be a simple connected graph. The degree $d_G(v)$ of a vertex $v$ is the number of vertices adjacent to $v$. The edge connecting the vertices $u$ and $v$ will be denoted by $uv$. Let $S_G(v)$ denote the sum of the degrees of all vertices adjacent to a vertex $v$. We refer to [1] for undefined term and notation.

A molecular graph or a chemical graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule and its edges to the bonds between atoms. A topological index is a numerical parameter mathematically derived from the graph structure. These topological indices are useful for establishing correlations between the structure of a molecular compound and its physico-chemical properties, see [2].

In [3], Furtula *et al.* introduced the augmented Zagreb index of a graph. The augmented Zagreb index of a graph $G$ is defined as

$$AZI(G) = \sum_{uv \in E(G)} \left( \frac{d_G(u) d_G(v)}{d_G(u) + d_G(v) - 2} \right)^3.$$

This topological index has proved to a valuable predictive index in the study of the heat formation in octanes, and heptanes, whose prediction power is better than atom bond connectivity index, see [3]. This index was also studied, for example, in [4, 5].

Motivated by the previous research in augmented Zagreb index and its wide applications, we now introduce the second, third and fourth augmented Zagreb indices of the molecular graph as follows:

The second augmented Zagreb index of a molecular graph $G$ is defined as

$$AZI_2(G) = \sum_{uv \in E(G)} \left( \frac{n_u n_v}{n_u + n_v - 2} \right)^3$$

where the number $n_u$ of vertices of $G$ lying closer to the vertex $u$ than to the vertex $v$ for the edge $uv$ of a graph $G$.

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The third augmented Zagreb index of a molecular graph $G$ is defined as

$$AZI_3(G) = \sum_{uv \in E(G)} \left( \frac{m_u m_v}{m_u + m_v - 2} \right)^3$$

where the number $m_u$ of edges of $G$ lying closer to the vertex $u$ than to the vertex $v$ for the edge $uv$ of a graph $G$.

The fourth augmented Zagreb index of a molecular graph $G$ is defined as

$$AZI_4(G) = \sum_{uv \in E(G)} \left( \frac{\varepsilon(u)\varepsilon(v)}{\varepsilon(u) + \varepsilon(v) - 2} \right)^3$$

where the number $\varepsilon(u)$ is the eccentricity of all vertices adjacent to a vertex $u$.

In [6], the Sanskruti index of a graph $G$ is introduced by Hosamani and it is defined as

$$S(G) = \sum_{uv \in E(G)} \left( \frac{S_G(u) S_G(v)}{S_G(u) + S_G(v) - 2} \right)^3.$$

In this paper, we compute the augmented Zagreb index and Sanskruti index of line graphs of subdivision graphs of triangular benzenoid $T_n$, hexagonal parallelogram nanotube $P(m, n)$ and zigzag-edge coronoid fused with starphene nanotube $ZCS(k, l, m)$. For benzenoid structures, see [7].

Recently, some topological indices were studied, for example, in [7, 8, 9, 10, 11, 12, 13, 14].

The line graph $L(G)$ of a graph $G$ is the graph whose vertex set corresponds to the edges of $G$ such that two vertices of $L(G)$ are adjacent if the corresponding edges of $G$ are adjacent. The subdivision graph $S(G)$ of a graph $G$ is the graph obtained from $G$ by replacing each of its edges by a path of length two.

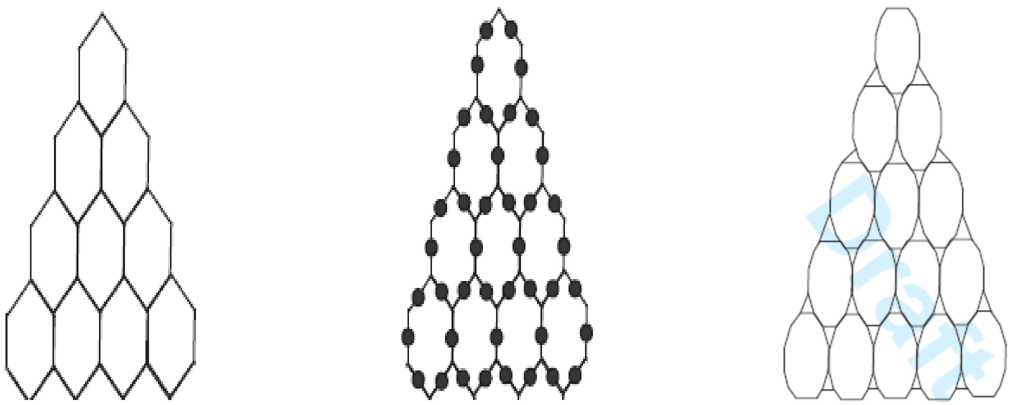
We need the following results.

**Lemma 1 [1]:** Let $G$ be a $(p, q)$ graph. Then $L(G)$ has $q$ vertices and $\frac{1}{2}\sum_{i=1}^{p} d_G(u_i)^2 - q$ edges.

**Lemma 2:** Let $G$ be a $(p, q)$ graph. Then $S(G)$ has $p+q$ vertices and $2q$ edges.

## 2. RESULTS FOR TRIANGULAR BENZENOIDS $T_n$, $n \in N$

In this section, we consider triangular benzenoids which is a family of benzenoid molecular graphs. We denote the triangular benzenoid molecular graph by $T_n$ in which $n$ is the number of hexagons in the base of a graph, as shown in Figure 1(a). We see that a triangular benzenoid $T_n$ has $n^2 + 4n + 1$ vertices and $\frac{3}{2}n\,(n+3)$ edges.



(a) (b) (c)

**Figure-1:** (a) triangular benzenoid $T_4$, (b) subdivision graph of $T_4$, (c) Line graph of the subdivision graph of $T_4$.

The line graph of the subdivision graph of triangular bonzenoid $T_4$ is shown in Figure 1(c).

We compute augmented Zagreb index of the line graph of the subdivision graph of a triangular benzenoid.

**Theorem 2.1:** Let $G$ be the line graph of the subdivision graph of a triangular benzenoid $T_n$, $n \in N$. Then
$AZI(G) = 51.2578125\, n^2 + 89.0859375n - 44.34375$.

**Proof:** The graph of a triangular benzenoid $T_n$ has $n^2+4n+1$ vertices and $\frac{3}{2}n\,(n+3)$ edges. By Lemma 2 and Lemma 1, the line graph of the subdivision graph $G$ has $3n(n+3)$ vertices and $\frac{3}{2}(3n^2+7n-2)$ edges. Further, the edge partition of $G$ based on degree of end vertices of each edge is given in Table 1.

| $d_G(u), d_G(v)\backslash uv\in E(G)$ | (2, 2) | (2, 3) | (3,3) |
|---|---|---|---|
| Number of edges | $3(n+3)$ | $6(n-1)$ | $\frac{3}{2}\left(3n^2+n-4\right)$ |

**Table-1:** Edge partition of $G$

To compute $AZI(G)$, we see that

$$AZI(G)=\sum_{uv\in E(G)}\left(\frac{d_G(u)d_G(v)}{d_G(u)+d_G(v)-2}\right)^3.$$

$$=3(n+3)\left(\frac{2\times 2}{2+2-2}\right)^3+6(n-1)\left(\frac{2\times 3}{2+3-2}\right)^3+\frac{3}{2}(3n^2+n-4)\left(\frac{3\times 3}{3+3-2}\right)^3$$

$$= 51.2578125n^2 + 89.0859375n - 44.34375.$$

In the following theorem, we compute Sanskruti index of the line graph of the subdivision graph of a triangular benzenoid.

**Theorem 2.2:** Let $G$ be the line graph of the subdivision graph of a triangular benzenoid $T_n$, $n\in N$. Then

$$S(G)=\frac{9}{2}\left(\frac{81}{16}\right)^3 n^2+\left[3\left(\frac{25}{8}\right)^3+6\left(\frac{40}{11}\right)^3+3\left(\frac{32}{7}\right)^3+6\left(\frac{72}{15}\right)^3-\frac{15}{2}\left(\frac{81}{16}\right)^3\right]n$$

$$+9\left(\frac{8}{3}\right)^3+6\left(\frac{20}{7}\right)^3-6\left(\frac{25}{8}\right)^3-6\left(\frac{40}{11}\right)^3-3\left(\frac{32}{7}\right)^3+3\left(\frac{81}{16}\right)^3,\quad \text{if } n\neq 1,$$

$$=\frac{256}{3}, \text{ if } n=1,$$

**Proof:** The edge partition based on the degree sum of neighbor vertices of each edge of $G$ is obtained, as given in Table 2.

| $S_G(u), S_G(v) \setminus uv \in E(G)$ | (4,4) | (4,5) | (5,5) | (5, 8) | (8, 8) | (8, 9) | (9, 9) |
|---|---|---|---|---|---|---|---|
| Number of edges | 9 | 6 | $3(n-2)$ | $6(n-1)$ | $3(n-1)$ | $6(n-1)$ | $\frac{3}{2}(3n^2-5n+2)$ |

**Table-2:** Edge partition of $G$

**Case-1:** Suppose $n \neq 1$.

To compute $S(G)$, we see that

$$S(G)=\sum_{uv\in E(G)}\left(\frac{S_G(u)S_G(v)}{S_G(u)+S_G(v)-2}\right)^3.$$

$$=9\left(\frac{4\times 4}{4+4-2}\right)^3+6\left(\frac{4\times 5}{4+5-2}\right)^3+3(n-2)\left(\frac{5\times 5}{5+5-2}\right)^3+6(n-1)\left(\frac{5\times 8}{5+8-2}\right)^3$$

$$+3(n-1)\left(\frac{8\times 8}{8+8-2}\right)^3+6(n-1)\left(\frac{8\times 9}{8+9-2}\right)^3+\frac{3}{2}(3n^2-5n+2)\left(\frac{9\times 9}{9+9-2}\right)^3$$

$$=\frac{9}{2}\left(\frac{81}{16}\right)^3 n^2+\left[3\left(\frac{25}{8}\right)^3+6\left(\frac{40}{11}\right)^3+3\left(\frac{32}{7}\right)^3+6\left(\frac{72}{15}\right)^3-\frac{15}{2}\left(\frac{81}{16}\right)^3\right]n$$

$$+9\left(\frac{8}{3}\right)^3+6\left(\frac{20}{7}\right)^3-6\left(\frac{25}{8}\right)^3-6\left(\frac{40}{11}\right)^3-3\left(\frac{32}{7}\right)^3+3\left(\frac{81}{16}\right)^3.$$

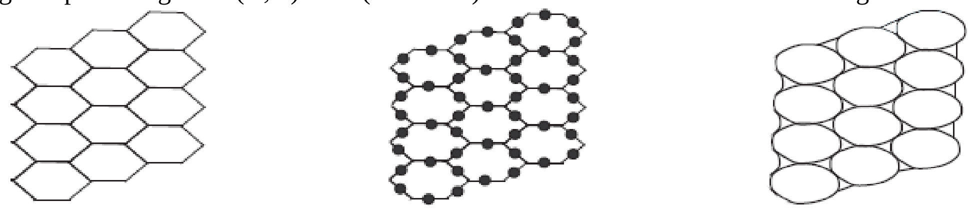
**Case-2:** Suppose $n = 1$.

To compute *S(G)*, we see that

$$S(G)=\sum_{uv\in E(G)}\left(\frac{S_G(u)S_G(v)}{S_G(u)+S_G(v)-2}\right)^3=9\left(\frac{4\times4}{4+4-2}\right)^3=\frac{256}{3}.$$

## 3. RESULTS FOR HEXAGONAL PARALLELOGRAM *P*(*m, n*) FOR ANY *m* , *n* ∈ *N* NANOTUBES

In this section, we consider hexagonal parallelogram nanotubes. These nanotubes usually symbolized as $P(m, n)$ for any $m, n \in N$ in which m is the number of hexagons in any row and $n$ is the number hexagons in any column, see Figure 2(a). A hexagonal parallelogram $P(m, n)$ has $2(m+n+mn)$ vertices and $3mn + 2m + 2n – 1$ edges.



(a) (b) (c)

**Figure-2:** (a) hexagonal parallelogram $P(3, 4)$ (b) subdivision graph of $P(3, 4)$ (c) line graph of the subdivision graph of $P(3,4)$

The line graph of the subdivision graph of hexagonal parallelogram $P(3,4)$ is depicted in Figure 2(c).

In the following theorem, we compute augmented Zagreb index of the line graph of the subdivision graph of a hexagonal parallelogram.

**Theorem 3.1:** Let $G$ be the line graph of the subdivision graph of a hexagonal parallelogram $P(m, n)$ for any $m, n \in N$. Then

$$AZI(G) = 102.515625\, mn + 25.21875m + 25.21875n – 56.953125.$$

**Proof:** The graph of a hexagonal parallelogram $P(m, n)$ has $2(m + n + mn)$ vertices and $3mn + 2m + 2n – 1$ edges. By Lemma 2 and Lemma 1, the line graph of the subdivision graph $G$ has $2(3mn+2m+2n – 1)$ vertices and $9mn + 4m + 4n – 5$ edges. Further, the edge partition of $G$ based on degree of end vertices of each edge is given in Table 3.

| $d_G(u), d_G(v)\backslash e = uv\in E(G)$ | (2, 2) | (2, 3) | (3,3) |
|---|---|---|---|
| Number of edges | $2(m + n + 4)$ | $4(m + n – 2)$ | $9mn –2m – 2n – 5$ |

**Table-3:** Edge degree partition of $G$

To compute *AZI(G)*, we see that

$$AZI(G)=\sum_{uv\in E(G)}\left(\frac{d_G(u)d_G(v)}{d_G(u)+d_G(v)-2}\right)^3.$$

$$=2(m+n+4)\left(\frac{2\times2}{2+2-2}\right)^3+4(m+n-2)\left(\frac{2\times3}{2+3-2}\right)^3+(9mn-2m-2n-5)\left(\frac{3\times3}{3+3-2}\right)^3$$

$$= 102.515625mn + 25.21875m + 25.21875n – 56.953125.$$

In the following theorem, we compute Sanskruti index of the line graph of the subdivision graph of a hexagonal parallelogram.

**Theorem 3.2:** Let $G$ be the line graph of the subdivision graph of a hexagonal parallelogram $P(m, n)$ for any $m, n \in N$. Then

$$S(G)=\left[2\left(\frac{25}{8}\right)^3+4\left(\frac{40}{11}\right)^3+2\left(\frac{32}{7}\right)^3+4\left(\frac{72}{15}\right)^3+\left(\frac{81}{16}\right)^3\right]n$$

$$+10\left(\frac{8}{3}\right)^3+4\left(\frac{20}{7}\right)^3-4\left(\frac{25}{8}\right)^3-4\left(\frac{40}{11}\right)^3-2\left(\frac{32}{7}\right)^3-4\left(\frac{72}{15}\right)^3-\left(\frac{81}{16}\right)^3, \qquad \text{if } n\neq1,\ m=1,$$

$$=9\left(\frac{81}{16}\right)^3 mn+\left[2\left(\frac{25}{8}\right)^3+4\left(\frac{40}{11}\right)^3+2\left(\frac{32}{7}\right)^3+4\left(\frac{72}{15}\right)^3-8\left(\frac{81}{16}\right)^3\right](m+n)$$
$$+8\left(\frac{8}{3}\right)^3+8\left(\frac{20}{7}\right)^3-8\left(\frac{25}{8}\right)^3-8\left(\frac{40}{11}\right)^3-4\left(\frac{32}{7}\right)^3-8\left(\frac{72}{15}\right)^3+7\left(\frac{81}{16}\right)^3, \qquad \text{if } n\neq 1,\ m>1.$$

**Proof: Case 1.** The edge partition based on the degree sum of neighbor vertices of each edge of $G$ is obtained, as given Table 4.

| $S_G(u), S_G(v)\backslash uv\in E(G)$ | (4,4) | (4,5) | (5,5) | (5, 8) | (8, 8) | (8, 9) | (9,9) |
|---|---|---|---|---|---|---|---|
| Number of edges | 10 | 4 | 2(*n*–2) | 4(*n*–1) | 2(*n*–1) | 4(*n*–1) | *n*–1 |

**Table-4:** Edge partition of $G$

Suppose $n \neq 1$ and $m = 1$.

To compute *S(G)*, we see that

$$S(G)=\sum_{uv\in E(G)}\left(\frac{S_G(u)S_G(v)}{S_G(u)+S_G(v)-2}\right)^3$$
$$=10\left(\frac{4\times4}{4+4-2}\right)^3+4\left(\frac{4\times5}{4+5-2}\right)^3+2(n-2)\left(\frac{5\times5}{5+5-2}\right)^3+4(n-1)\left(\frac{5\times8}{5+8-2}\right)^3$$
$$+2(n-1)\left(\frac{8\times8}{8+8-2}\right)^3+4(n-1)\left(\frac{8\times9}{8+9-2}\right)^3+(n-1)\left(\frac{9\times9}{9+9-2}\right)^3$$
$$=\left[2\left(\frac{25}{8}\right)^3+4\left(\frac{40}{11}\right)^3+2\left(\frac{32}{7}\right)^3+4\left(\frac{72}{15}\right)^3+\left(\frac{81}{16}\right)^3\right]n$$
$$+10\left(\frac{8}{3}\right)^3+4\left(\frac{20}{7}\right)^3-4\left(\frac{25}{8}\right)^3-4\left(\frac{40}{11}\right)^3-2\left(\frac{32}{7}\right)^3-4\left(\frac{72}{15}\right)^3-\left(\frac{81}{16}\right)^3.$$

**Case-2:** The edge partition based on the degree sum of neighbor vertices of each edge of $G$ is obtained, as given in Table 5.

| $S_G(u), S_G(v)\backslash uv\in E(G)$ | (4,4) | (4,5) | (5,5) | (5, 8) | (8, 8) | (8, 9) | (9,9) |
|---|---|---|---|---|---|---|---|
| Number of edges | 8 | 8 | 2(m+*n*–4) | 4(m+*n*–2) | 2(m+*n*–2) | 4(m+*n*–2) | 9*mn*–8(*m*+*n*)+7 |

**Table-5:** Edge partition of $G$

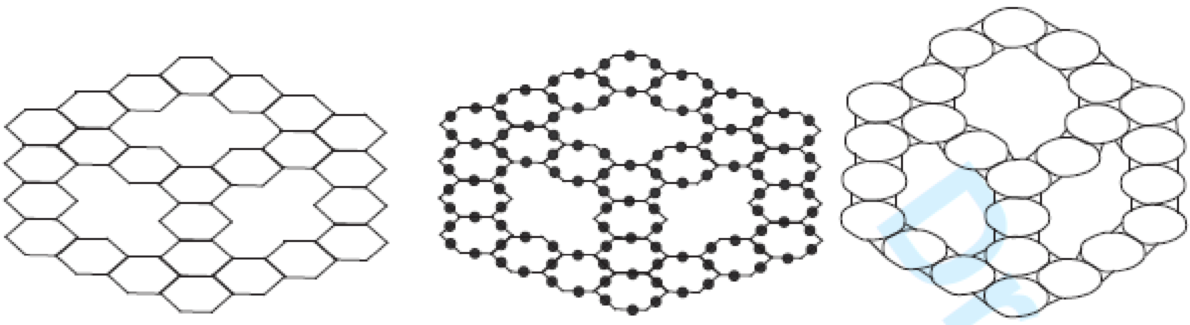
Suppose $n \neq 1$, and $m>1$.

To compute $S(G)$, we see that

$$S(G)=\sum_{uv\in E(G)}\left(\frac{S_G(u)S_G(v)}{S_G(u)+S_G(v)-2}\right)^3$$
$$=8\left(\frac{4\times4}{4+4-2}\right)^3+8\left(\frac{4\times5}{4+5-2}\right)^3+2(m+n-4)\left(\frac{5\times5}{5+5-2}\right)^3+4(m+n-2)\left(\frac{5\times8}{5+8-2}\right)^3$$
$$+2(m+n-2)\left(\frac{8\times8}{8+8-2}\right)^3+4(m+n-2)\left(\frac{8\times9}{8+9-2}\right)^3+\left(9mn-8(m+n)+7\right)\left(\frac{9\times9}{9+9-2}\right)^3$$
$$=9\left(\frac{81}{16}\right)^3 mn+\left[2\left(\frac{25}{8}\right)^3+4\left(\frac{40}{11}\right)^3+2\left(\frac{32}{7}\right)^3+4\left(\frac{72}{15}\right)^3-8\left(\frac{81}{16}\right)^3\right](m+n)$$
$$+8\left(\frac{8}{3}\right)^3+8\left(\frac{20}{7}\right)^3-8\left(\frac{25}{8}\right)^3-8\left(\frac{40}{11}\right)^3-4\left(\frac{32}{7}\right)^3-8\left(\frac{72}{15}\right)^3+7\left(\frac{81}{16}\right)^3.$$

## 4. RESULTS FOR ZIGZAG-EDGE CORONOID FUSED WITH STARPHENE NANOTUBES *ZCS(k, l, m)*

In this section, we consider the system which is a composite benzenoid obtained by a zigzag-edge coronoid *ZC(k, l, m)* with a starphene *St(k, l, m)*. This system is called a zigzag-edge coronoid fused with starphene nanotubes, denoted by *ZCS(k, l, m)*, see Figure 3(a). We see that a zigzag edge coronoid fused with starphene nanotube *ZCS(k,l,m)* has $36k - 54$ vertices and $15(k+l+m) - 63$ edges.



(a) (b) (c)

**Figure-3:** (a) Zigzag-edge coronoid fused with starphene nanotube *ZCS*(4, 4, 4), (b) Subdivision graph of *ZCS* (4, 4, 4), (c) Line graph of subdivision graph of *ZCS*(4, 4, 4)

The line graph of the subdivision graph of zigzag-edge coronoid fused with starphene nanotube *ZCS*(4, 4, 4) is shown in Figure 3(c).

In the following theorem, we compute augmented Zagreb index of the line graph of the subdivision graph of a zigzag coronoid fused with starphene nanotube.

**Theorem 4.1:** Let *G* be the line graph of the subdivision graph of a zigzag-edge coronoid fused with starphene nanotube *ZCS(k, l, m)* for every $k = l = m \geq 4$. Then

$$AZI(G) = 383.203125\,(k + l + m) - 1356.234375.$$

**Proof:** The graph of a zigzag edge coronoid fused with starphene nanotube *ZCS(k.l,m)* has $36k - 54$ vertices and $15(k + l + m) - 63$ edges. By Lemma 2 and Lemma 1, the line graph of the subdivision graph *G* has $30(k+l+m) - 126$ vertices and $39(k+l+m) - 153$ edges. Further, the edge partition of *G* based on degree of end vertices of each edge is given in Table 6.

| $d_G(u), d_G(v) \backslash e = uv \in E(G)$ | (2, 2) | (2, 3) | (3,3) |
|---|---|---|---|
| Number of edges | $6(k+l+m) - 30$ | $12(k+l+m) - 84$ | $21(k+l+m) - 39$ |

**Table-6:** Edge partition of *G*

To compute *AZI(G)*, we see that

$$AZI(G) = \sum_{uv \in E(G)} \left( \frac{d_G(u) d_G(v)}{d_G(u) + d_G(v) - 2} \right)^3$$

$$= \left[6(k+l+m) - 30\right]\left(\frac{2\times 2}{2+2-2}\right)^3 + \left[12(k+l+m) - 84\right]\left(\frac{2\times 3}{2+3-2}\right)^3 + \left[21(k+l+m) - 39\right]\left(\frac{3\times 3}{3+3-2}\right)^3$$

$$= 383.203125\,(k+l+m) - 1356.234375.$$

In the next theorem, we compute Sankruti index of the line graph of the subdivision graph of *ZCS(k, l, m)*.

**Theorem 4.2:** Let *G* be the line graph of the subdivision graph of a zigzag-edge coronoid fused with starphene nanotube *ZCS*(*k, l, m*) for every $k=l=m \geq 4$. Then

$$S(G) = \left[6\left(\frac{25}{8}\right)^3 + 12\left(\frac{40}{11}\right)^3 + 6\left(\frac{32}{7}\right)^3 + 12\left(\frac{72}{15}\right)^3 + 3\left(\frac{81}{16}\right)^3\right](k+l+m)$$

$$+6\left(\frac{8}{3}\right)^3 + 12\left(\frac{20}{7}\right)^3 - 8\left(\frac{25}{8}\right)^3 - 84\left(\frac{40}{11}\right)^3 - 54\left(\frac{32}{7}\right)^3 - 60\left(\frac{72}{15}\right)^3 + 75\left(\frac{81}{16}\right)^3.$$

**Proof:** The edge partition based on the degree sum of neighbor vertices of each edge of *G* is obtained, as given in Table 7.

| $S_G(u), S_G(v) \setminus uv\in E(G)$ | (4,4) | (4,5) | (5,5) | (5, 8) | (8, 8) | (8, 9) | (9,9) |
|---|---|---|---|---|---|---|---|
| Number of edges | 6 | 12 | $6(k+l+m-8)$ | $12(k+l+m-7)$ | $6(k+l+m-9)$ | $12(k+l+m-5)$ | $3(k+l+m+25)$ |

**Table-7:** Edge partition of $G$

To compute $S(G)$, we see that

$$S(G)=\sum_{uv\in E(G)}\left(\frac{S_G(u)S_G(v)}{S_G(u)+S_G(v)-2}\right)^3$$

$$=6\left(\frac{4\times 4}{4+4-2}\right)^3+12\left(\frac{4\times 5}{4+5-2}\right)^3+6(k+l+m-8)\left(\frac{5\times 5}{5+5-2}\right)^3+12(k+l+m-7)\left(\frac{5\times 8}{5+8-2}\right)^3$$

$$+6(k+l+m-9)\left(\frac{8\times 8}{8+8-2}\right)^3+12(k+l+m-5)\left(\frac{8\times 9}{8+9-2}\right)^3+3(k+l+m+25)\left(\frac{9\times 9}{9+9-2}\right)^3$$

$$=\left[6\left(\frac{25}{8}\right)^3+12\left(\frac{40}{11}\right)^3+6\left(\frac{32}{7}\right)^3+12\left(\frac{72}{15}\right)^3+3\left(\frac{81}{16}\right)^3\right](k+l+m)$$

$$+6\left(\frac{8}{3}\right)^3+12\left(\frac{20}{7}\right)^3-8\left(\frac{25}{8}\right)^3-84\left(\frac{40}{11}\right)^3-54\left(\frac{32}{7}\right)^3-60\left(\frac{72}{15}\right)^3+75\left(\frac{81}{16}\right)^3.$$

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