International Journal of Mathematical Archive-8(8), 2017, 102-108
Available online through www.ijma.info ISSN 2229 – 5046

NEW AUGMENTED ZAGREB INDICES

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(Received On: 08-07-17; Revised & Accepted On: 07-08-17)

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.

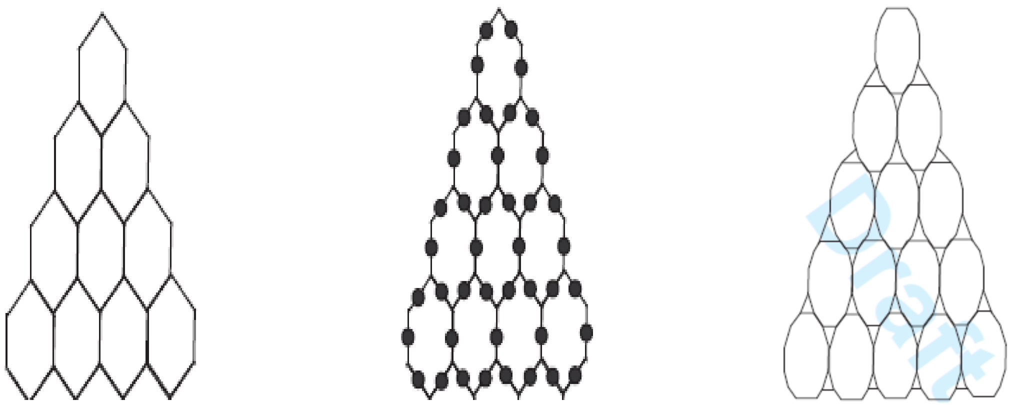
We need the following results.

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

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

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

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

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

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

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

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

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

$S_G(u), S_G(v) \backslash uv \in E(G)$	(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

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

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

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

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

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

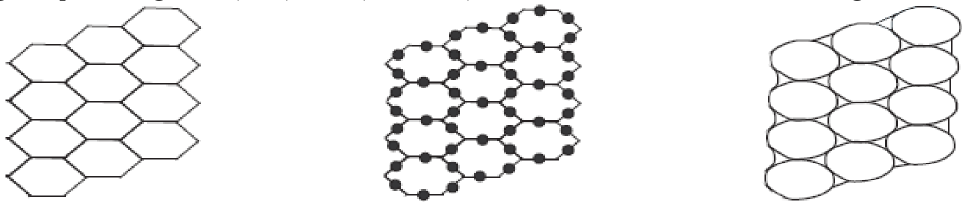
Case-2: Suppose $n = 1$.

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

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

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

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

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

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

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

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

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

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

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

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

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)	9mn–8(m+n)+7

Table-5: Edge partition of G

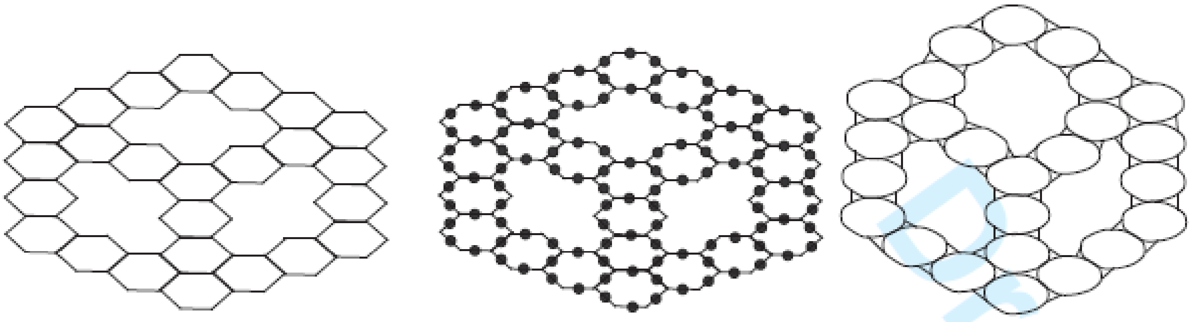
Suppose $n \neq 1$, and $m>1$.

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

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

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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Source of support: Nil, Conflict of interest: None Declared.