### On Gourava Indices of Some Chemical Graphs

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### **Abstract:**

In this paper, we compute Gourava indices of triangular benzenoid  $T_n$ , hexagonal parallelogram nanotube P(m,n), zigzag—edge coronoid fused with starphene nanotube ZCS(k,l,m) by using the line graphs of the subdivision graphs of these chemical structures.

**Keywords:** Gourava indices, Hyper Gourava indices, triangular benzenoid, hexagonal parallelogram nanotube, zigzag–edge coronoid fused with starphene nanotube.

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### 1. INTRODUCTION

Cheminformatics is new subject which is a combination of chemistry, mathematics and information science. last decades, there is a lot of research which is done in A molecular graph or a chemical graph is a graph such that its vertices correspond to the atoms and edges to the bonds. A single number that can be computed from the molecular graph and used to characterize some property of the underlying molecule is said to be a topological index or molecular structure descriptor. Graph theory has provided to theoretical chemists with a variety of useful tools, such as topological indices, topological polynomials and topological matrices. Numerous such descriptors have been considered in Theoretical Chemistry and have found applications in Quantitative Structure Property Relationship /Quantitative Structure Activity Relationship [QSPR/QSAR]research see[2, 13].

In this article, we consider only finite, simple and connected graphs with vertex set V(G) and edge set E(G). 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. We refer to [4] for undefined terms and notations.

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.

The first and second Zagreb indices [3] of a molecular graph G are defined as

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)],$$

$$M_2(G) = \sum_{uv \in E(G)} [d_G(u)d_G(v)].$$

Motivated by the definition of the Zagreb indices and their wide applications, Kulli introduced the first Gourava index of a molecular graph [5] as follows:

The first Gourava index of a graph G is defined as

$$GO_1(G) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v)) + (d_G(u)d_G(v))].$$

The second Gourava index [5] of a molecular graph G is defined as

$$GO_2(G) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v))(d_G(u)d_G(v))].$$

In [6], Kulli introduced the first and second Hyper–Gourava indices of a molecular graph G which are defined as

$$HGO_1(G) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v)) + (d_G(u)d_G(v))]^2,$$

$$HGO_2(G) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v))(d_G(u)d_G(v))]^2.$$

In this paper, we compute *Gourava indices* 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 [1]. The topological indices are widely studied and have numerous applications in chemistry for details refer [1, 7, 8, 9, 10, 11, 12].

The line graph L(G) [4] 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.

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The subdivision graph S(G) [4] 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 to prove our results:

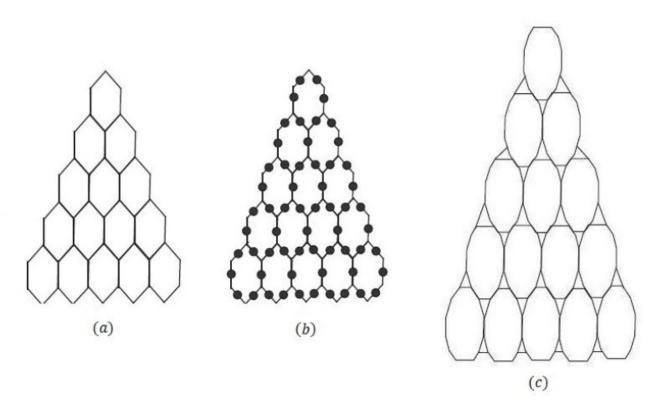
**Lemma 1.1.** [4] Let G be a (p,q) graph. Then L(G) has q vertices and  $\frac{1}{2} \sum_{i=1}^{p} d_G(u_i)^2 - q$  edges.

**Lemma 1.2.** [4] 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, which is the generalization of benzene molecule  $C_6H_6$  in which benzene rings form a triangular shape. The benzene molecule is useful molecule in physics, chemistry and nanosciences and is useful to synthesize aromatic compounds. These graphs consists of a hexagonal cycles arranged in rows and in each row one hexagon increases. 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.



**Figure 1:** (a) Triangular benzenoid  $T_5$ , (b) subdivision graph  $T_5$ , (c) line graph of the subdivision graph of a triangular benzenoid  $T_5$ .

The line graph of the subdivision graph of a triangular benzenoid  $T_n$  is shown in Figure 1 (c). Here G be the line graph of the subdivision graph of a triangular benzenoid  $T_n$ .

The edge partition of G based on degree of each edge is given in Table 1.

We now compute Gourava indices of the line graph of the subdivision graph of a triangular benzenoid.

Table 1: The edge partition of  ${\cal G}$  based on degree of each edge

$d_G(u), d_G(v) : uv \in E(G)$	(2,2)	(2,3)	(3,3)
Number of edges	3(n+3)	6(n-1)	$\frac{3}{2}(3n^2+n-4)$
	$=  E_{22} $	$=  E_{23} $	$=  E_{33} $

**Theorem 2.1.** Let G be the line graph of the subdivision graph of a triangular benzenoid  $T_n$ ,  $n \in N$ . Then first Gourava index is

$$GO_1(G) = 67.5n^2 + 112.5n - 84.$$

*Proof.* Since the graph of a triangular benzenoid  $T_n$  has  $n^2+4n+1$  vertices and  $\frac{3}{2}n(n+3)$  edges by Lemma 1.2 and Lemma 1.1, the line graph of the subdivision graph G is 3n(n+3) vertices and  $\frac{3}{2}(3n^2+7n-2)$  edges. Further, the edge partition of G based on degree of each edge is given in Table 1. To compute  $GO_1(G)$  from definition, we have

$$GO_1(G) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v)) + (d_G(u)d_G(v))]$$

$$= |E_{22}|[(2+2) + (2\cdot 2)] + |E_{23}|[(2+3) + (2\cdot 3)]$$

$$+ |E_{33}|[(3+3) + (3\cdot 3)]$$

$$= 3(n+3)(4+4) + 6(n-1)(5+6)$$

$$+ \frac{3}{2}(3n^2 + n - 4)(6+9)$$

$$= 67.5n^2 + 112.5n - 84.$$

**Theorem 2.2.** For the line graph of the subdivision graph of a triangular benzenoid  $T_n$ ,  $n \in \mathbb{N}$ . The second Gourava indices

$$GO_2(G) = 243n^2 + 309n - 360.$$

*Proof.* The order and size of a triangular benzenoid  $T_n$  is  $n^2+4n+1$  and  $\frac{3}{2}n(n+3)$  and by Lemma 1.2 and Lemma 1.1, the order and size of line graph of the subdivision graph G is 3n(n+3) and  $\frac{3}{5}(3n^2+7n-2)$ .

By making use of Table 1 and from the definition, we have

$$GO_2(G) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v))(d_G(u)d_G(v))]$$

$$= |E_{22}|[(2+2)(2\cdot 2)]$$

$$+ |E_{23}|[(2+3)(2\cdot 3)] + |E_{33}|[(3+3)(3\cdot 3)]$$

$$= 3(n+3)(4\cdot 4) + 6(n-1)(5\cdot 6)$$

$$+ \frac{3}{2}(3n^2 + n - 4)(6\cdot 9)$$

$$= 243n^2 + 309n - 360.$$

**Theorem 2.3.** Let G be the line graph of the subdivision graph of a triangular benzenoid  $T_n$ ,  $n \in N$ . Then first Hyper Gourava index is

$$HGO_1(G) = 1012.5n^2 + 1255.5n - 871.5.$$

*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 1.2 and Lemma 1.1, 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 each edge is given in Table 1.

To compute  $HGO_1(G)$ , we see that

$$\begin{split} HGO_1(G) &= \sum_{uv \in E(G)} [(d_G(u) + d_G(v)) + (d_G(u)d_G(v))]^2 \\ &= |E_{22}|[(2+2) + (2\cdot 2)]^2 + |E_{23}|[(2+3) + (2\cdot 3)]^2 \\ &+ |E_{33}|[(3+3) + (3\cdot 3)]^2 \\ &= 3(n+3)(4+4)^2 + 6(n-1)(5+6)^2 \\ &+ \frac{3}{2}(3n^2 + n - 4)(6+9)^2 \\ &= 1012.5n^2 + 1255.5n - 871.5. \end{split}$$

**Theorem 2.4.** Let G be the line graph of the subdivision graph of a triangular benzenoid  $T_n$ ,  $n \in N$ . Then second Hyper Gourava index is

$$HGO_2(G) = 13122n^2 + 10542n - 20592.$$

*Proof.* The graph of a triangular benzenoid  $T_n$  has  $|V(G)|=n^2+4n+1$  and  $|E(G)|=\frac{3}{2}n(n+3)$ . By Lemma 1.2 and Lemma 1.1, the line graph of the subdivision graph G has |V(G)|=3n(n+3) and  $|E(G)|=\frac{3}{2}(3n^2+7n-2)$ . From Table 1 and from definition, we have

$$HGO_{2}(G) = \sum_{uv \in E(G)} [(d_{G}(u) + d_{G}(v))(d_{G}(u)d_{G}(v))]^{2}$$

$$= |E_{22}|[(2+2)(2\cdot 2)]^{2} + |E_{23}|[(2+3)(2\cdot 3)]^{2}$$

$$+ |E_{33}|[(3+3)(3\cdot 3)]^{2}$$

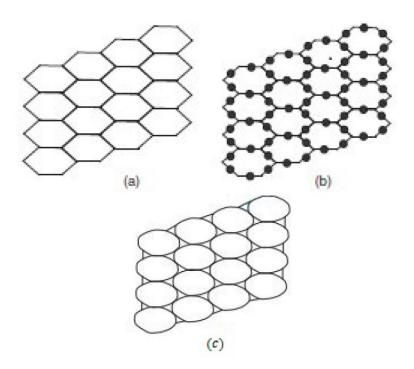
$$= 3(n+3)(4\cdot 4)^{2} + 6(n-1)(5\cdot 6)^{2}$$

$$+ \frac{3}{2}(3n^{2} + n - 4)(6\cdot 9)^{2}$$

$$= 13122n^{2} + 10542n - 20592.$$

# 3. RESULTS FOR HEXAGONAL PARALLELOGRAM P(m,n) FOR ANY $m,n\in N$ NANOTUBES.

In this section, we consider hexagonal parallelogram nanotubes. These nanotubes usually symbolized as P(m,n) consists of a hexagons arranged in a parallelogram fashion. Here P(m,n) for any  $m,n\in N$  in which m is the number of hexagons in a row and n is the number of 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 respectively.



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

The line graph of the subdivision graph of a hexagonal parallelogram P(4,4) is depicted in Figure 2 (c). Here G be the line graph of the subdivision graph of a hexagonal parallelogram P(m,n).

The edge partition of G based on degree of each edge is given in Table 2.

**Table 2:** The edge partition of G based on degree of each edge

$d_G(u), d_G(v) : uv \in E(G)$	(2,2)	(2,3)	(3,3)
Number of edges	2(m+n+4)	4(m+n-2)	9mn - 2m - 2n - 5
	$=  E_{22} $	$=  E_{23} $	$=  E_{33} $

In the following theorem, we compute Gourava indices 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 first Gourava index is

$$GO_1(G) = 135mn + 30(m+n) - 99.$$

*Proof.* The graph of a hexagonal parallelogram P(m,n) has 2(m+n+mn) vertices and 3mn+2m+2n-1 edges. By Lemma 1.2 and Lemma 1.1, 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 each edge is given in Table 2.

To compute  $GO_1(G)$ , we see that

$$GO_1(G) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v)) + (d_G(u)d_G(v))]$$

$$= |E_{22}|[(2+2) + (2\cdot 2)] + |E_{23}|[(2+3) + (2\cdot 3)]$$

$$+ |E_{33}|[(3+3) + (3\cdot 3)]$$

$$= 2(m+n+4)(4+4) + 4(m+n-2)(5+6)$$

$$+ (9mn - 2m - 2n - 5)(6+9)$$

$$= 135mn + 30(m+n) - 99.$$

**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 second Gourava index is

$$GO_2(G) = 486mn + 44(m+n) - 382.$$

*Proof.* The graph of a hexagonal parallelogram P(m,n) has |V(G)|=2(m+n+mn) and |E(G)|=3mn+2m+2n-1. By Lemma 1.2 and Lemma 1.1, the line graph of the subdivision graph G has |V(G)|=2(3mn+2m+2n-1) and |E(G)|=9mn+4m+4n-5. From Table 2 and from definition, we have

$$\begin{split} GO_2(G) &= \sum_{uv \in E(G)} [(d_G(u) + d_G(v))(d_G(u)d_G(v))] \\ &= |E_{22}|[(2+2)(2\cdot 2)] + |E_{23}|[(2+3)(2\cdot 3)] \\ &+ |E_{33}|[(3+3)(3\cdot 3)] \\ &= 2(m+n+4)(4\cdot 4) + 4(m+n-2)(5\cdot 6) \\ &+ (9mn-2m-2n-5)(6\cdot 9) \\ &= 486mn + 44(m+n) - 382. \end{split}$$

**Theorem 3.3.** Let G be the line graph of the subdivision graph of a hexagonal parallelogram P(m,n) for any  $m,n \in N$ . Then first Hyper Gourava index is

$$HGO_1(G) = 2025mn + 162(m+n) - 1581.$$

*Proof.* Since the graph of a hexagonal parallelogram P(m,n) has 2(m+n+mn) vertices and 3mn+2m+2n-1 edges by Lemma 1.2 and Lemma 1.1, the line graph of the subdivision graph has G has 2(3mn+2m+2n-1) vertices and 9mn+4m+4n-5 edges. Further the edge partition of G based on degree of each edge is given in Table 2. To compute  $HGO_1(G)$  from definition, we have

$$HGO_1(G) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v)) + (d_G(u)d_G(v))]^2$$

$$= |E_{22}|[(2+2) + (2\cdot 2)]^2 + |E_{23}|[(2+3) + (2\cdot 3)]^2 + |E_{33}|[(3+3) + (3\cdot 3)]^2$$

$$= 2(m+n+4)(4+4)^2 + 4(m+n-2)(5+6)^2 + (9mn-2m-2n-5)(6+9)^2$$

$$= 2025mn + 162(m+n) - 1581.$$

**Theorem 3.4.** For the line graph of the subdivision graph of a hexagonal parallelogram P(m,n) for any  $m,n \in N$ . The second Hyper Gourava indices

$$HGO_2(G) = 26244mn - 1720(m+n) - 19732.$$

*Proof.* The order and size of a hexagonal parallelogram P(m,n) is 2(m+n+mn) and 3mn+2m+2n-1 and by Lemma 1.2 and Lemma 1.1, the order and size of line graph of the subdivision graph G is 2(3mn+2m+2n-1) and 9mn+4m+4n-5. By making use of Table 2 and from the definition, we have.

$$HGO_{2}(G) = \sum_{uv \in E(G)} [(d_{G}(u) + d_{G}(v))(d_{G}(u)d_{G}(v))]^{2}$$

$$= |E_{22}|[(2+2)(2\cdot 2)]^{2} + |E_{23}|[(2+3)(2\cdot 3)]^{2}$$

$$+ |E_{33}|[(3+3)(3\cdot 3)]^{2}$$

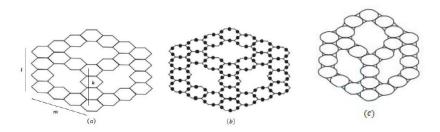
$$= 2(m+n+4)(4\cdot 4)^{2} + 4(m+n-2)(5\cdot 6)^{2}$$

$$+ (9mn-2m-2n-5)(6\cdot 9)^{2}$$

$$= 26244mn - 1720(m+n) - 19732.$$

# 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 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.



**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 the subdivision graph of a hexagonal parallelogram ZCS(4,4,4).

The line graph of the subdivision graph of a zigzag-edge coronoid fused with starphene nanotube ZCS(4,4,4) is depicted in Figure 3 (c). Here G be the line graph of the subdivision graph of a zigzag-edge coronoid fused with starphene nanotube ZCS(k,l,m).

The edge partition of G based on degree of each edge is given in Table 3.

**Table 3:** The edge partition of G based on degree of each edge

$d_G(u), d_G(v) : uv \in E(G)$	(2,2)	(2,3)	(3,3)
Number of edges	6(k+l+m)-30	12(k+l+m) - 84	21(k+l+m)-39
	$=  E_{22} $	$=  E_{23} $	$=  E_{33} $

In the following theorem, we compute Gourava indices of the line graph of the subdivision graph of a zigzag–edge coronoid fused with starphene nanotube ZCS(k,l,m).

**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 first Gourava index is

$$GO_1(G) = 495(k+l+m) - 1749.$$

*Proof.* Since 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 1.2 and Lemma 1.1, 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 each edge is given in Table 3. To compute  $GO_1$  from definition, we have

$$\begin{split} GO_1(G) &= \sum_{uv \in E(G)} [(d_G(u) + d_G(v)) + (d_G(u)d_G(v))] \\ &= |E_{22}|[(2+2) + (2\cdot 2)] + |E_{23}|[(2+3) + (2\cdot 3)] \\ &+ |E_{33}|[(3+3) + (3\cdot 3)] \\ &= (6(k+l+m) - 30)(4+4) \\ &+ (12(k+l+m) - 84)(5+6) \\ &+ (21(k+l+m) - 39)(6+9) \\ &= 495(k+l+m) - 1749. \end{split}$$

**Theorem 4.2.** The second Gourava index is  $GO_2(G) = 1590(k + l + m) - 5106$ , where G is the line graph of the subdivision graph of a zigzag-edge coronoid fused with starphene nanotube ZCS(k, l, m) for every  $k = l = m \ge 4$ .

*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 and from Lemma 1.2 and Lemma 1.1, the line graph of the subdivision graph G has 30(k+l+m)-126 vertices and 39(k+l+m)-153 edges. Making use

of Table 3, we compute  $GO_2(G)$ 

$$\begin{split} GO_2(G) &= \sum_{uv \in E(G)} [(d_G(u) + d_G(v))(d_G(u)d_G(v))] \\ &= |E_{22}|[(2+2)(2\cdot 2)] + |E_{23}|[(2+3)(2\cdot 3)] \\ &+ |E_{33}|[(3+3)(3\cdot 3)] \\ &= (6(k+l+m)-30)(4\cdot 4) \\ &+ (12(k+l+m)-84)(5\cdot 6) \\ &+ (21(k+l+m)-39)(6\cdot 9) \\ &= 1590(k+l+m) - 5106. \end{split}$$

**Theorem 4.3.** 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 first Hyper Gourava index is

 $\Box$ 

$$HGO_1(G) = 6561(k+l+m) - 20859.$$

*Proof.* The order and size of zigzag-edge coronoid fused with starphene nanotube ZCS(k,l,m) is 36k-54 and 15(k+l+m)-63 and by Lemma 1.2 and Lemma 1.1, the order and size of the line graph of the subdivision graph G is (30(k+l+m)-126) and (39(k+l+m)-153). Further, the edge partition of G based on degree of each edge is given in Table 3.

To compute  $HGO_1(G)$  from definition, we have

$$HGO_1(G) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v)) + (d_G(u)d_G(v))]^2$$

$$= |E_{22}|[(2+2) + (2\cdot 2)]^2 + |E_{23}|[(2+3) + (2\cdot 3)]^2$$

$$+ |E_{33}|[(3+3) + (3\cdot 3)]^2$$

$$= (6(k+l+m) - 30)(4+4)^2$$

$$+ (12(k+l+m) - 84)(5+6)^2$$

$$+ (21(k+l+m) - 39)(6+9)^2$$

$$= 6561(k+l+m) - 20859.$$

**Theorem 4.4.** For the line graph of the subdivision graph of a zigzag-edge coronoid fused with starphene nanotube

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ZCS(k,l,m) for every  $k=l=m\geq 4$ . The second Hyper Gourava indices

$$HGO_2(G) = 73572(k+l+m) - 197004.$$

*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 1.2 and Lemma 1.1, 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 each edge is given in Table 3. To compute  $HGO_2$  from definition, we have

$$\begin{split} HGO_2(G) &= \sum_{uv \in E(G)} [(d_G(u) + d_G(v))(d_G(u)d_G(v))]^2 \\ &= |E_{22}|[(2+2)(2\cdot 2)]^2 + |E_{23}|[(2+3)(2\cdot 3)]^2 \\ &+ |E_{33}|[(3+3)(3\cdot 3)]^2 \\ &= (6(k+l+m) - 30)(4\cdot 4)^2 \\ &+ (12(k+l+m) - 84)(5\cdot 6)^2 \\ &+ (21(k+l+m) - 39)(6\cdot 9)^2 \\ &= 73572(k+l+m) - 197004. \end{split}$$

### 5. ACKNOWLEDGEMENT

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