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Professor Hari M. Srivastava  
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**Harmonic Index and Zagreb Indices of Vertex-Semitotal  
Graphs**

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**Abstract.** Graph theory is one of the rising areas in mathematics due to its applications in many areas of science. Amongst several study areas in graph theory, spectral graph theory and topological descriptors are in front rows. These descriptors are widely used in QSPR/QSAR studies in mathematical chemistry. Vertex-semitotal graphs are one of the derived graph classes which are useful in calculating several physico-chemical properties of molecular structures by means of molecular graphs modelling the molecules. In this paper, several topological descriptors of vertex-semitotal graphs are calculated. Some new relations on these values are obtained by means of a recently defined graph invariant called omega invariant.

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## 1. Introduction

Several topological graph indices have been defined and studied by many mathematicians and chemists. They are defined as topological graph invariants measuring several physical, chemical, pharmacological, pharmaceutical, biological, etc. properties of graphs which are modelling real life situations. They can be grouped mainly into three classes according to the way they are defined: by vertex degrees, by matrices or by distances. We consider degree based-topological indices of some derived graphs through this paper.

Let  $G = (V, E)$  be a simple graph with  $|V(G)| = n$  vertices and  $|E(G)| = m$  edges, where  $V(G) = \{v_1, v_2, \dots, v_n\}$  and  $E(G) = \{v_i v_j : v_i, v_j \in V(G)\}$ . That is, we do not

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allow loops or multiple edges. For any vertex  $v \in V(G)$ , we denote the degree of  $v$  by  $d_G(v)$  or  $d_v$ .

If  $v_i$  and  $v_j$  are adjacent vertices of  $G$ , and if the edge  $e$  connects them, this situation will be denoted by  $e = v_i v_j$ . In such a case, the vertices  $v_i$  and  $v_j$  are called adjacent vertices and the edge  $e$  is said to be incident to  $v_i$  and  $v_j$ . Adjacency and incidence play a very important role in the spectral graph theory, the sub area of graph theory dealing with linear algebraic study of graphs. The smallest and biggest vertex degrees in a graph will be denoted by  $\delta$  and  $\Delta$ , respectively.

Written with multiplicities, a degree sequence in general is written as

$$D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \dots, \Delta^{(a_\Delta)}\}.$$

Let  $D$  be a set of some non-decreasing non-negative integers. We say that a graph  $G$  is a realization of the set  $D$  if the degree sequence of  $G$  is equal to  $D$ .

**Definition 1.** [7] Let  $D = \{1^{(a_1)}, 2^{(a_2)}, 3^{(a_3)}, \dots, \Delta^{(a_\Delta)}\}$  be a realizable degree sequence and  $G$  be one of its realizations. The  $\Omega(G)$  of  $G$  is defined in terms of the degree sequence as

$$\begin{aligned} \Omega(G) &= a_3 + 2a_4 + 3a_5 + \dots + (\Delta - 2)a_\Delta - a_1 \\ &= \sum_{i=1}^{\Delta} a_i(i - 2). \end{aligned}$$

A vertex-semi-total graph  $T_1(G)$  is constructed from  $G$  by inserting a new vertex for each edge of  $G$  and then by joining every inserted vertex to the end vertices of the corresponding edge, that is, by replacing each edge by a triangle. See Fig. 1. Thus  $|V(T_1)| = |V(G)| + |E(G)| = n + m$  and  $|E(T_1)| = |E(S)| + |E(G)| = 2m + m = 3m$ .

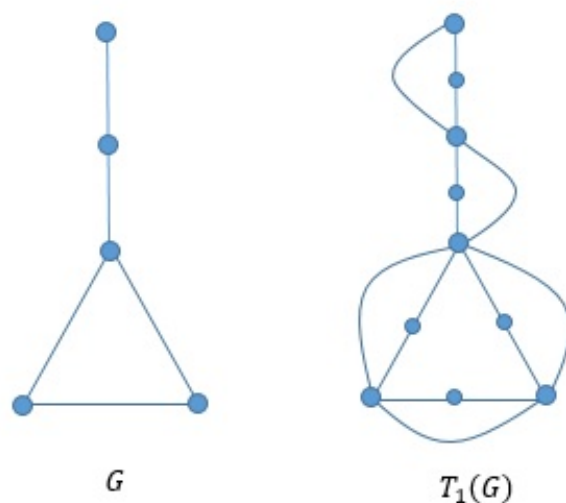
Two of the most important topological graph indices are called the first and second Zagreb indices denoted by  $M_1(G)$  and  $M_2(G)$ , respectively:

$$M_1(G) = \sum_{u \in V(G)} d_G^2(u) \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v). \quad (1)$$

They were first defined in 1972 by Gutman and Trinajstic, [12], and are referred to due to their uses in QSAR and QSPR studies. In [4], some results on the first Zagreb index together with some other indices are given. For some graph operations, these indices are calculated in [5, 14, 17].

The  $F$ -index or forgotten index of a graph  $G$  denoted by  $F(G)$  or  $M_3(G)$  is defined as

$$F(G) = \sum_{u \in V(G)} d_G^3(u). \quad (2)$$



**Figure 1** The vertex-semitotal graph  $T_1(G)$  of  $T_{3,2}$

It was first appeared in the study of structure-dependency of total  $\pi$ -electron energy in 1972, [12]. Recently, this sum was named as the forgotten index or the  $F$ -index by Furtula and Gutman, [10].

The hyper-Zagreb index was defined as a variety of the classical Zagreb indices as

$$HM(G) = \sum_{uv \in E} (d_u + d_v)^2, \quad (3)$$

see e.g. [10].

Inspired by the study of heat of formation for heptanes and octanes, in [9] Furtula et al. proposed an index called Augmented Zagreb index which gives a better prediction power. It is defined by

$$AZI(G) = \sum_{uv \in E(G)} \left( \frac{d_u d_v}{d_u + d_v - 2} \right)^3. \quad (4)$$

The Harmonic index was introduced by Zhong [19] who found that it correlates well with  $\Pi$ -electron energy of benzenoid hydrocarbons and defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}. \quad (5)$$

Ranjini et al., [16], introduced the re-defined Zagreb indices, i.e. the redefined first,

second and third Zagreb indices for a graph  $G$  and these are defined as

$$ReZG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u \cdot d_v}, \quad (6)$$

$$ReZG_2(G) = \sum_{uv \in E(G)} \frac{d_u \cdot d_v}{d_u + d_v}, \quad (7)$$

$$ReZG_3(G) = \sum_{uv \in E(G)} (d_u \cdot d_v)(d_u + d_v). \quad (8)$$

Milicevic et al., [15], reformulated the Zagreb indices in terms of the edge degrees instead of the vertex-degrees as

$$EM_1(G) = \sum_{e=uv \in E(G)} d(e)^2 \quad \text{and} \quad EM_2(G) = \sum_{e, f \in E(G)} d_G(e)d_G(f). \quad (9)$$

Aram and Dehgardi, [1], introduced the concept of reformulated F-index as

$$RF(G) = \sum_{e=uv \in E(G)} d(e)^3. \quad (10)$$

Eliasi et. al. [8] introduced the multiplicative sum Zagreb index of  $G$  which is denoted by  $\prod_1^*(G)$  and defined by

$$\prod_1^*(G) = \prod_{uv \in E(G)} (d_G(u) + d_G(v)). \quad (11)$$

Xu et. al. [18] introduced the total multiplicative sum Zagreb index of a graph  $G$  denoted by  $\prod_1^T(G)$  and defined by

$$\prod_1^T(G) = \prod_{u,v \in V(G)} (d_G(u) + d_G(v)). \quad (12)$$

Topological indices of some derived graphs, as subdivision, total, semitotal, line, par-aline graphs are studied in [2] and [13]. In this paper, we examine some degree-based topological indices of vertex-semitotal graph which also is one of the derived graphs, and find relations between these topological indices.

## 2. Main Results

We first recall some results on the topological indices of the vertex-semitotal graphs:

**Proposition 1.** [11] *Let  $T_1(G)$  be the vertex-semitotal graph of the graph  $G$  of order  $n = n(G)$  and size  $m = m(G)$ . Then*

$$M_1(T_1(G)) = 4M_1(G) + 4m(G).$$

**Theorem 1.** [2] Let  $G$  be a graph of order  $n = n(G)$  and size  $m = m(G)$ . Then

$$M_2(T_1(G)) = 2EM_1(G) + EM_2(G) + 2M_1(G) + M_2(G) + F(G) - 4m(G).$$

**Proposition 2.** [6] Let  $G$  be a graph of order  $n = n(G)$  and size  $m = m(G)$ . Then

$$F(T_1(G)) = 8F(G) + 8m(G).$$

**Theorem 2.** [13] If  $T_1(G)$  is a vertex-semi-total graph of  $G$  of order  $n = n(G)$  and size  $m = m(G)$ . Then

$$EM_1(T_1(G)) = 8(F(G) - M_1(G) + M_2(G)) + 4m(G)$$

and

$$EM_2(T_1(G)) = \frac{1}{3} (14({}^4M_1(G)) + 4EF(G) + 68m(G)) + 4EM_2(G) + 6F(G) - 30M_1(G) + 28M_2(G)$$

where  ${}^\alpha M_1(G) = \sum_{v \in V(G)} d(v)^\alpha$  and  $EF(G)$  is the reformulated forgotten index.

**Theorem 3.** [3] Let  $G$  be a graph of order  $n = n(G)$  and size  $m = m(G)$ . Then

$$\prod_1(T_1(G)) = \prod_1(G) \left[ \prod_1^*(G) \right]^2.$$

and

$$\prod_2(T_1(G)) = \prod_2(G) \prod_2^*(G).$$

Now we will determine some well-known Zagreb indices of vertex-semi-total graph of  $G$ .

**Lemma 1.** Let  $G$  be a connected simple graph of order  $n = n(G)$  and size  $m = m(G)$  and let  $T_1(G)$  be the vertex-semi-total graph of  $G$ . Then,

$$\Omega(T_1(G)) - \Omega(G) = 2m(G).$$

The proof is clear from the definition of  $\Omega$  invariant of  $G$ .

**Theorem 4.** Let  $G$  be a graph with order  $n = n(G)$  and size  $m = m(G)$ . Then the hyper Zagreb index of  $T_1(G)$  is

$$HM(T_1(G)) = 4(2M_1(G) + F(G) + HM(G) + 2m(G)).$$

*Proof.* By Eqn. (3), we have

$$HM(T_1(G)) = \sum_{v_i v_j \in E(T_1(G))} [d_{T_1(G)}(v_i) + d_{T_1(G)}(v_j)]^2$$

$$\begin{aligned}
 &= \sum_{v_i v_j \in E(G)} [d_{T_1(G)}(v_i) + d_{T_1(G)}(v_j)]^2 \\
 &+ \sum_{v_i c_{ij} \in E(T_1(G))} [d_{T_1(G)}(v_i) + 2]^2 \\
 &= 4 \sum_{v_i v_j \in E(G)} (d_G(v_i) + d_G(v_j))^2 + 4 \sum_{v_i \in V(G)} (1 + d_G(v_i))^2 d_G(v_i),
 \end{aligned}$$

and the result follows.

**Theorem 5.** Let  $G$  be a graph with order  $n = n(G)$  and size  $m = m(G)$ . Then augmented Zagreb index of  $T_1(G)$  is

$$AZI(T_1(G)) = 8 \sum_{v_i v_j \in E(G)} \left( \frac{d_G(v_i) d_G(v_j)}{d_G(v_i) + d_G(v_j) - 1} \right)^3 + 16m(G).$$

*Proof.* Using Eqn.(4), we get

$$\begin{aligned}
 AZI(T_1(G)) &= \sum_{v_i v_j \in E(G)} \left( \frac{d_{T_1(G)}(v_i) \cdot d_{T_1(G)}(v_j)}{d_{T_1(G)}(v_i) + d_{T_1(G)}(v_j) - 2} \right)^3 \\
 &+ \sum_{v_i c_{ij} \in E(T_1(G))} \left( \frac{2 \cdot 2d_G(v_i)}{2 + 2d_G(v_i) - 2} \right)^3 d_G(v_i) \\
 &= \sum_{v_i v_j \in E(G)} \left( \frac{2d_G(v_i) \cdot 2d_G(v_j)}{2d_G(v_i) + 2d_G(v_j) - 2} \right)^3 + 8 \sum_{v_i \in V(G)} d_G(v_i),
 \end{aligned}$$

and the result follows.

**Theorem 6.** Let  $G$  be a graph with order  $n = n(G)$  and size  $m = m(G)$ . Re-defined versions of Zagreb indices of  $T_1(G)$  are

- i)*  $ReZG_1(T_1(G)) = \frac{1}{2} (ReZG_1(G) + n(G)) + m(G)$ .
- ii)*  $ReZG_2(T_1(G)) = 2 \left[ ReZG_2(G) + \sum_{u \in V(G)} \frac{d_G^2(u)}{1+d_G(u)} \right]$ .
- iii)*  $ReZG_3(T_1(G)) = ReZG_3(G) + 8(M_1(G) + F(G)) + m(G)$ .

*Proof.* From Eqn. (6), we have

$$\begin{aligned}
 ReZG_1(T_1(G)) &= \sum_{v_i v_j \in E(T_1(G))} \frac{d_{T_1(G)}(v_i) + d_{T_1(G)}(v_j)}{d_{T_1(G)}(v_i) \cdot d_{T_1(G)}(v_j)} \\
 &= \sum_{v_i v_j \in E(G)} \frac{2d_G(v_i) + 2d_G(v_j)}{2d_G(v_i) \cdot 2d_G(v_j)} + \sum_{v_i c_{ij} \in E(T_1(G))} \frac{2 + 2d_G(v_i)}{2 \cdot 2d_G(v_i)} \cdot d_G(v_i)
 \end{aligned}$$

$$= \frac{1}{2} \sum_{v_i v_j \in E(G)} \frac{d_G(v_i) + d_G(v_j)}{d_G(v_i) \cdot d_G(v_j)} + \frac{1}{2} \sum_{v_i \in V(G)} (1 + d_G(v_i)),$$

and the result follows.

Using Eqns.(7) and (8), we get the results for (ii) and (iii) by similar methods.

**Theorem 7.** *Let  $G$  be a graph with order  $n = n(G)$  and size  $m = m(G)$ . Reformulated forgotten index of  $T_1(G)$  is*

$$RF(T_1(G)) = 8 (2M^4(G) + 3ReZG_3(G) - m(G)) - 24 (F(G) + 2M_2(G) - M_1(G)).$$

*Proof.* For vertex-semi total graph  $T_1(G)$  of a graph  $G$ , there are two types of vertices: Firstly, the vertices corresponding to the vertices of  $G$ , secondly, the vertices corresponding to the edges of  $G$ . We will denote them  $v_i$  and  $c_{ij}$ , respectively. Depending on the nature of end vertices, we can divide the edges of  $T_1$  into two types:

- i)  $v_i v_j$ -edge: an edge between two vertices in  $G$ .
- ii)  $v_i c_{ij}$ -edge: an edge between the vertices of  $G$  and the vertices corresponding to the edges of  $G$ .

Using Eqn. (9), we have

$$\begin{aligned} RF(T_1(G)) &= \sum_{e \in E(T_1(G))} (d_e)^3 \\ &= \sum_{e_{v_i v_j} \in E(T_1)} d_{T_1}(e_{v_i v_j})^3 + \sum_{e_{v_i c_{ij}} \in E(T_1)} d_{T_1}(e_{v_i c_{ij}})^3 \\ &= \sum_{v_i v_j \in E(T_1)} [d_{T_1}(v_i) + d_{T_1}(v_j) - 2]^3 + \sum_{v_i c_{ij} \in E(T_1)} [d_{T_1}(v_i) + d_{T_1}(c_{ij}) - 2]^3. \end{aligned}$$

For  $v_i c_{ij}$ -edges in the second term, it is clear that every  $v_i$  vertex of  $T_1(G)$  is connected with  $d_G(v_i)$   $c_{ij}$  vertices, each of degree 2. Therefore, corresponding to every vertex  $v_i$  in  $G$ , there are  $d_G(v_i)$  edges in  $T_1$  each of edge degree  $[2d_G(v_i) + 2 - 2]$ . So,

$$\begin{aligned} RF(T_1(G)) &= \sum_{v_i v_j \in E(G)} [2d_G(v_i) + 2d_G(v_j) - 2]^3 + \sum_{v_i \in V(G)} d_G(v_i)[2d_G(v_i) + 2 - 2]^3 \\ &= 8 \left[ \sum_{v_i v_j \in E(G)} (d_G^3(v_i) + d_G^3(v_j)) + 3 \sum_{v_i v_j \in E(G)} d_G(v_i)d_G(v_j)(d_G(v_i) + d_G(v_j)) \right] \\ &\quad - 6 \sum_{v_i v_j \in E(G)} (2d_G(v_i) + d_G(v_j))^2 + 12 \sum_{v_i v_j \in E(G)} (2d_G(v_i) + d_G(v_j)) \\ &\quad - \sum_{v_i v_j \in E(G)} 8 + 8 \sum_{v_i \in V(G)} d_G^4(v_i) \\ &= 8 [M^4(G) + 3ReZG_3(G) - m(G)] - 24 [F(G) + 2M_2(G) - M_1(G)]. \end{aligned}$$

**Theorem 8.** Let  $G$  be a graph of order  $n = n(G)$  and size  $m = m(G)$ . Multiplicative sum Zagreb index of  $T_1(G)$  is

$$\prod_1^*(T_1(G)) = 4 \prod_1^*(G) \prod_{v_i \in V(G)} (1 + d_G(v_i)).$$

*Proof.*

$$\begin{aligned} \prod_1^*(T_1(G)) &= \prod_{v_i, v_j \in E(T(G))} (d_{T(G)}(v_i) + d_{T(G)}(v_j)) \\ &= \prod_{v_i, v_j \in E(G)} (d_{T(G)}(v_i) + d_{T(G)}(v_j)) \cdot \prod_{v_i, c_{ij} \in E(T(G))} (2 + d_{T(G)}(v_i)) \\ &= \prod_{v_i, v_j \in E(G)} (2d_G(v_i) + 2d_G(v_j)) \cdot 2 \prod_{v_i, c_{ij} \in E(T(G))} (1 + d_G(v_i)) \end{aligned}$$

and the result follows.

**Theorem 9.** Let  $G$  be a graph of order  $n = n(G)$  and size  $m = m(G)$ . Total multiplicative sum Zagreb index of  $T_1(G)$  is

$$\prod^T(T_1(G)) = 2^{m(G)^2+1} \prod^T(G) \prod_{v_i \in V(G)} (1 + d_G(v_i))^{m(G)}.$$

*Proof.* From the definition of  $\prod^T(G)$ , we have

$$\begin{aligned} \prod^T(T_1(G)) &= \prod_{v_i, v_j \in V(T(G))} (d_{T(G)}(v_i) + d_{T(G)}(v_j)) \\ &= \prod_{v_i, v_j \in V(G)} (2d_{(G)}(v_i) + 2d_{(G)}(v_j)) \cdot \prod_{v_i, c_{ij} \in V(T(G))} (2 + 2d_{(G)}(v_i))^{m(G)} \\ &\quad \cdot \prod_{c_{ij}, c_{kt} \in V(S(G))} (2 + d_{(G)}(v_i)) \\ &= 2 \prod^T(G) \cdot 2^m \prod_{v_i \in V(G)} (1 + d_G(v_i))^{m(G)} \cdot 4^{\binom{m(G)}{2}} \end{aligned}$$

and the result follows.

### 3. Conclusions

In this paper, we obtained the formulae for the topological indices, especially the Zagreb indices and harmonic index, of some class of derived graphs called vertex-semi-total graphs. We used for the first time a newly introduced graph invariant called omega invariant to obtain some of the relations. The methods used here can be applied to all topological graph indices and to other derived graphs and graph operations.



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