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*Research Article*

# Second Zagreb and Sigma Indices of Semi and Total Transformations of Graphs

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The study of structure-property relations including the transformations of molecules is of utmost importance in correlations with corresponding physicochemical properties. The graph topological indices have been used effectively for such study and, in particular, bond-based indices play a vital role. The bond-additive topological indices of a molecular graph are defined as a sum of edge measures over all edges in which edge measures can be computed based on degrees, closeness, peripherality, and irregularity. In this study, we provide the mathematical characterization of the transformation of a structure that can be accomplished by the novel edge adjacency and incidence relations. We derive the exact expressions of bond type indices such as second Zagreb, sigma indices, and their coindices of total transformation and two types of semitransformations of the molecules which in turn can be used to characterize the topochemical and topostructural properties.

## 1. Introduction

Topological indices are graph invariants that play an important role in chemical and pharmaceutical sciences, since they can be used to predict physicochemical properties of organic compounds in view of successful applications in QSAR and QSPR techniques [1–5]. These indices are mainly classified into distance-based and degree-based. Development of such topological indices is of immense value in quantitative structure-activity relations. The first and second Zagreb indices were the oldest degree-based indices and found significant applications [6, 7]. The Zagreb indices have first appeared in the topological formula for the total $\pi$-energy of conjugated molecules and also useful in the study of anti-inflammatory activities of chemical instances. The generalization of the first Zagreb index is named as general sum-connectivity index [8] and there are many types of generalization and reformulation on the Zagreb indices based on vertex and edge degrees [8–11], in particular, the forgotten index is recently revisited with important applications to drug molecular structures [12, 13].

It was known that most of the molecular structures are not regular and, hence, the quantitative measure based on irregularity is of great importance in mathematical chemistry. In the case of octane isomers, the application of various degree-based irregularity measures for the prediction of physicochemical properties such as boiling point, standard enthalpy of vaporization, acentric factor, enthalpy of vaporization, and entropy was tested and predicted with good accuracy [14]. As a result of which many topological indices of this kind have been discussed and a few of them are Collatz–Sinogowitz, degree variance, discrepancy, Albertson, Bell, and total irregularity and sigma indices [14–17].

The Albertson index is the most commonly used irregularity measures that provide the structural perfection of chemical compounds. For this purpose, the imbalance of an edge is defined as the absolute difference between the degrees of end vertices and the summation is taken over all edges. In this paper, we focus our attention on the recently popular, sigma index, which is defined as the sum of squares of imbalance of every edge. Moreover, there is a nice relationship between second Zagreb, forgotten, and sigma indices which states that the difference between forgotten and sigma indices is twice the second Zagreb index [18] and some properties of the sigma index discussed in [19].

The structure of a molecular graph $G$ can be transformed into another graph $T(G)$ by imposing desired rules based on the original structure of $G$ so that there is a one-to-one correspondence between original graph $G$ and the transformation graph $T(G)$. Such a transformation of graphs and their characterization was attempted by many researchers in chemical graph theory [20–26] because the complex structure of transformation graph can be easily analyzed by the original graph. For instance, the first Zagreb index [21, 25], second Zagreb index [21, 27], forgotten index [20, 28] of transformation graphs, and Zagreb indices of transformation of line graph of subdivision graphs [29] were discussed. In this, we observe that the entire process of the second Zagreb index [27] was wrongly dealt and we will discuss with details in Section 3. Moreover, the forgotten index [20, 28] of transformation of graphs was considered with vertex a-Zagreb and (a, b)-Zagreb indices. In this study, we give the correct expressions for the second Zagreb index of transformation graphs and rewrite for the forgotten index via general sum-connectivity index. Finally, we derive the analytical expressions for the sigma index of two types of semitransformations and a total transformation.

Throughout this paper, we write $G$ to denote a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The number of elements in the vertex set and the edge set, respectively, is denoted by $n$ (order) and $m$ (size). The number of edges incident with a vertex $s \in V(G)$ is called the degree of the vertex $s$, denoted by $d_G(s)$. The neighborhood of a vertex $s$, denoted by $N_G(s)$, is a set of all vertices which are adjacent to $s$. Two edges $e, f \in E(G)$ are said to be adjacent if they share a common vertex and we write as $e \sim f$ and in case they are not adjacent, $e \nsim f$. In the same line of notation, $s \in V(G)$, $f \in E(G)$, and $s \sim f$ mean that $s$ is an end vertex of $f$ while $s \nsim f$ that $s$ is not an end vertex of $f$. The degree of an edge $e = st$, denoted by $d_G(e)$, is the number of edges that are adjacent to $e$, i.e., $d_G(e) = d_G(s) + d_G(t) - 2$. The complement of a graph $G$, represented by $\overline{G}$, is a graph obtained from $G$ with the same vertex set of $G$ such that $s$ is adjacent to $t$ in $\overline{G}$ if and only if $s$ is not adjacent to $t$ in $G$. Hence, the size of $\overline{G}$ is $(1/2)[n^2 - n - 2m]$, and the degree of each vertex $s \in V(\overline{G})$ is $d_{\overline{G}}(s) = n - d_G(s) - 1$.

We close this section by listing down (in Table 1) certain bond-additive topological indices [7–13, 18, 28, 30, 31] and their coindices which are needed for our study.

## 2. Transformation Graphs

The concept of transformation graphs is to construct a new graph from the original graph $G$ based on the structural connectivity. Generally, we can transform the original graph by imposing any combinations of the following:

For $\alpha, \beta, \gamma \in \{+, -\}$, $v_i \in V(G)$, $1 \le i \le n$, and $e_j \in E(G)$, $1 \le j \le m$,

(1) $v_i, v_j \in V(G)$, $v_i$ is adjacent to $v_j$ in $G$ if $\alpha = +$ and $v_i$ is not adjacent to $v_j$ in $G$ if $\alpha = -$

(2) $e_i, e_j \in E(G)$, $e_i$ is adjacent to $e_j$ in $G$ if $\beta = +$ and $e_i$ is not adjacent to $e_j$ in $G$ if $\beta = -$

(3) $v_i \in V(G)$ and $e_j \in E(G)$, $e_j$ is incident to $v_i$ in $G$ if $\gamma = +$ and $e_j$ is not incident to $v_i$ in $G$ if $\gamma = -$

The type-I semitransformation of a graph $G$, denoted by $T_{1\alpha\gamma}(G)$, is a graph with the vertex set $V(G) \cup E(G)$, and for $s, t \in V(T_{1\alpha\gamma}(G))$, $s$ and $t$ are adjacent in $T_{1\alpha\gamma}(G)$ if and only if (#1) and (#3) hold [21]. Following this, it is natural to define another semitransformation, called type-II semitransformation and denoted by $T_{2\beta\gamma}(G)$, whose vertex set is $V(G) \cup E(G)$, and for $s, t \in V(T_{2\beta\gamma}(G))$, $s$ and $t$ are adjacent in $T_{2\beta\gamma}(G)$ if and only if (#2) and (#3) hold. The total transformation graph $T_{\alpha\beta\gamma}(G)$ is a graph with the same vertex set as above $V(G) \cup E(G)$, and for $s, t \in V(T_{\alpha\beta\gamma}(G))$, $s$ and $t$ are adjacent in $T_{\alpha\beta\gamma}(G)$ if and only if (#1), (#2), and (#3) hold [32].

The concept of semitotal point, semitotal line, and total graphs came into the literature earlier [33, 34] and these three graphs are particular cases of our $T_{1\alpha\gamma}(G)$, $T_{2\beta\gamma}(G)$, and $T_{\alpha\beta\gamma}(G)$, i.e., $T_{1++}(G)$ is the semitotal point graph, $T_{2++}(G)$ is the semitotal line graph, and $T_{+++}(G)$ is the total graph. Since there are four distinct 2-permutations of $\{+, -\}$, we can construct totally eight different graphs from two types of semitransformations. For a graph $G$ depicted in Figure 1, the two types of semitransformation graphs are shown in Figure 2. In the same way, there are eight distinct 3-permutations of $\{+, -\}$ and again totally eight graphs can be constructed from the total transformation in which $\overline{T_{---}(G)} \cong T_{+++}(G)$, $\overline{T_{--+}(G)} \cong T_{++-}(G)$, $\overline{T_{-+-}(G)} \cong T_{+-+}(G)$, and $\overline{T_{-++}(G)} \cong T_{+--}(G)$. For the same graph in Figure 1, the eight classes of total transformation graphs are given in Figure 3.

**Lemma 1** (see [21]). *Let G be graph with n and m as its order and size, respectively. Then, the order of* $T_{1\alpha\gamma}(G)$ *is* $(m + n)$, *and the size is*

$$\left|ET_{1\alpha\gamma}(G)\right| = \begin{cases} 3m, & : \alpha = +, \gamma = +, \\ m(n-1), & : \alpha = +, \gamma = -, \\ \dfrac{1}{2}n(n-1) + m, & : \alpha = -, \gamma = +, \\ \dfrac{1}{2}n(n-1) + m(n-3), & : \alpha = -, \gamma = -. \end{cases} \tag{1}$$

Table 1: Bond-additive indices of $G$.

| Item | Index | Coindex |
|---|---|---|
| First Zagreb | $M_1(G) = \sum_{st\in E(G)} [d_G(s) + d_G(t)]$ | $\overline{M_1}(G) = \sum_{st\notin E(G)} [d_G(s) + d_G(t))]$ |
| Second Zagreb | $M_2(G) = \sum_{st\in E(G)} d_G(s) d_G(t)$ | $\overline{M_2}(G) = \sum_{st\notin E(G)} d_G(s) d_G(t)$ |
| Forgotten | $F(G) = \sum_{st\in E(G)} [d_G(s)^2 + d_G(t)^2]$ | $\overline{F}(G) = \sum_{st\notin E(G)} [d_G(s)^2 + d_G(t)^2]$ |
| Sum-connectivity | $\chi_\alpha(G) = \sum_{st\in E(G)} [d_G(s) + d_G(t)]^\alpha$ | $\overline{\chi_\alpha}(G) = \sum_{st\notin E(G)} [d_G(s) + d_G(t)]^\alpha$ |
| Reformulated first Zagreb | $EM_1(G) = \sum_{e,f\in E(G) e\sim f} [d_G(e) + d_G(f)]$ | $\overline{EM_1}(G) = \sum_{e,f\in E(G) e\nsim f} [d_G(e) + d_G(f)]$ |
| Reformulated second Zagreb | $EM_2(G) = \sum_{e,f\in E(G) e\sim f} d_G(e) d_G(f)$ | $\overline{EM_2}(G) = \sum_{e,f\in E(G) e\nsim f} d_G(e) d_G(f)$ |
| Sigma | $\sigma(G) = \sum_{st\in E(G)} [d_G(s) - d_G(t)]^2$ | $\overline{\sigma}(G) = \sum_{st\notin E(G)} [d_G(s) - d_G(t)]^2$ |

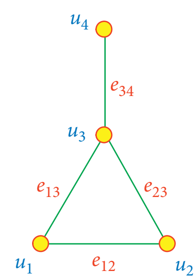



Figure 1: The graph $G$.

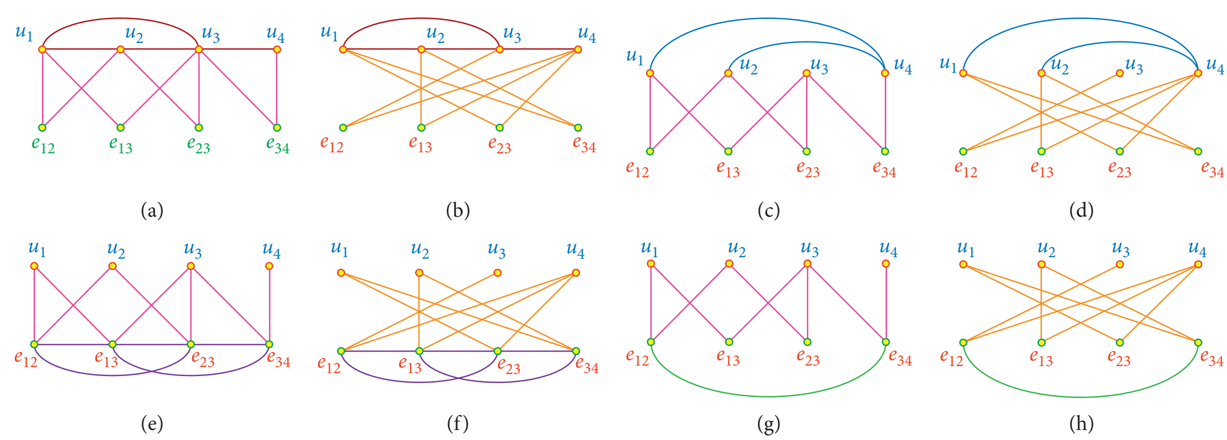


Figure 2: (a) $T_{1++}(G)$; (b) $T_{1+-}(G)$; (c) $T_{1-+}(G)$; (d) $T_{1--}(G)$; (e) $T_{2++}(G)$; (f) $T_{2+-}(G)$; (g) $T_{2-+}(G)$; (h) $T_{2--}(G)$.

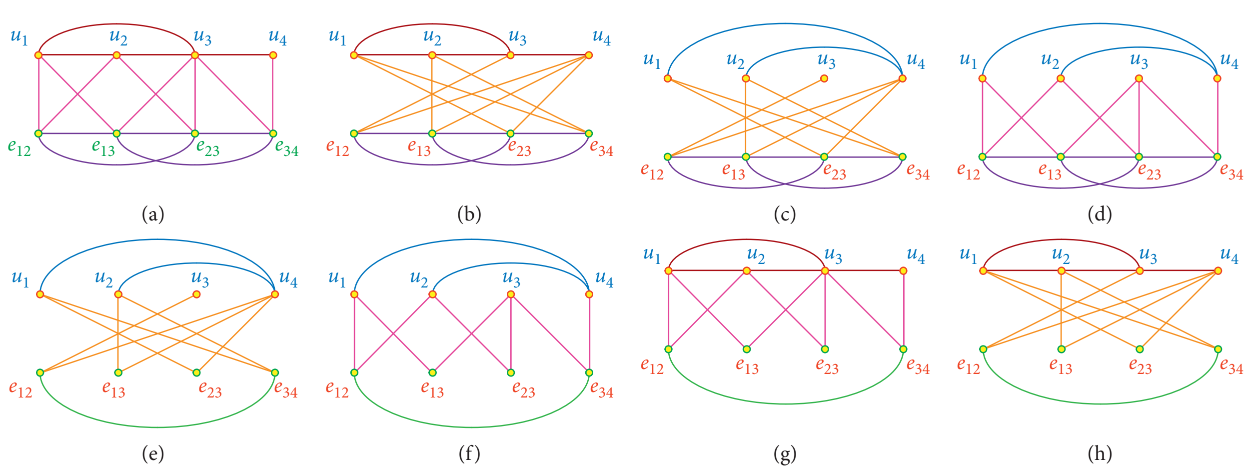


Figure 3: (a) $T_{+++}(G)$; (b) $T_{++-}(G)$; (c) $T_{-+-}(G)$; (d) $T_{-++}(G)$; (e) $T_{---}(G)$; (f) $T_{--+}(G)$; (g) $T_{+-+}(G)$; (h) $T_{+--}(G)$.

**Lemma 2.** *Let G be graph with n and m as its order and size, respectively. Then, the order of $T_{2\beta\gamma}(G)$ is $(m+n)$, and the size is*

$$\left|E\left(T_{2\beta\gamma}(G)\right)\right| = \begin{cases} \frac{1}{2}M_1(G)+m, & :\beta=+,\gamma=+,\\ \frac{1}{2}M_1(G)+mn-3m, & :\beta=+,\gamma=-,\\ \frac{1}{2}\left[m^2+5m-M_1(G)\right], & :\beta=-,\gamma=+,\\ \frac{1}{2}\left[m^2+2mn-3m-M_1(G)\right], & :\beta=-,\gamma=-. \end{cases} \quad (2)$$

**Lemma 3.** *Let G be graph with n and m as its order and size, respectively. Then, the order of $T_{\alpha\beta\gamma}(G)$ is $(m+n)$, and the size is*

$$\left|E\left(T_{\alpha\beta\gamma}(G)\right)\right| = \begin{cases} \frac{1}{2}\left[M_1(G)+4m\right], & :\alpha=+,\beta=+,\gamma=+,\\ \frac{1}{2}\left[M_1(G)+2m(n-2)\right], & :\alpha=+,\beta=+,\gamma=-,\\ \frac{1}{2}\left[m^2+7m-M_1(G)\right], & :\alpha=+,\beta=-,\gamma=+,\\ \frac{1}{2}\left[M_1(G)+n(n-1)\right], & :\alpha=-,\beta=+,\gamma=+,\\ \frac{1}{2}\left[(m+n)^2-5m-n-M_1(G)\right], & :\alpha=-,\beta=-,\gamma=-,\\ \frac{1}{2}\left[m^2+n(n-1)+3m-M_1(G)\right], & :\alpha=-,\beta=-,\gamma=+,\\ \frac{1}{2}\left[M_1(G)+2m(n-4)+n(n-1)\right], & :\alpha=-,\beta=+,\gamma=-,\\ \frac{1}{2}\left[m^2+2mn-m-M_1(G)\right], & :\alpha=+,\beta=-,\gamma=-. \end{cases} \quad (3)$$

We now recall the results pertaining to the first and second Zagreb indices of type-I semitransformation graphs and the first Zagreb index of total transformation graph which are helpful for our study.

**Lemma 4** (see [21, 25]). *Let G be a graph with order n and size m. Then,*

(i) $M_1(T_{1++}(G)) = 4[m+M_1(G)]$
(ii) $M_1(T_{1+-}(G)) = nm^2+m(n-2)^2$
(iii) $M_1(T_{1-+}(G)) = n(n-1)^2+4m$
(iv) $M_1(T_{1--}(G)) = 4M_1(G)+m(n-2)^2+(m+n-1)[n(m+n-1)-8m]$

**Lemma 5** (see [21]). *Let G be a graph with order n and size m. Then,*

(i) $M_2(T_{1++}(G)) = 4M_1(G)+4M_2(G)$
(ii) $M_2(T_{1+-}(G)) = m^3+m^2(n-2)^2$
(iii) $M_2(T_{1-+}(G)) = (1/2)[n(n-1)^3-2m(n-1)^2+8m(n-1)]$

(iv) $M_2(T_{1--}(G)) = (1/2)[4(n-2)M_1(G) - 4(m+n-1)\overline{M_1}(G) + 8\overline{M_2}(G) + (m+n-1)^2(n^2-n-2m) + 2m(m+n-1)(n-2)^2 - 8m^2(n-2)]$

**Lemma 6** (see [25]). *Let G be a graph with order n and size m. Then,*

(i) $M_1(T_{+++}(G)) = 4M_1(G) + 2M_2(G) + F(G)$

(ii) $M_1(T_{++-}(G)) = mn(m+n-8) + 16m + 2(n-4)M_1(G) + 2M_2(G) + F(G)$

(iii) $M_1(T_{+-+}(G)) = m(m+3)^2 - 2(m+1)M_1(G) + 2M_2(G) + F(G)$

(iv) $M_1(T_{-++}(G)) = n(n-1)^2 + 2M_2(G) + F(G)$

(v) $M_1(T_{---}(G)) = (m+n)[(m+n)^2 - 10m - 2n + 1] + 8m - 2(m+n-3)M_1(G) + 2M_2(G) + F(G)$

(vi) $M_1(T_{--+}(G)) = n(n-1)^2 + m(m+3)^2 - (2m+6)M_1(G) + 2M_2(G) + F(G)$

(vii) $M_1(T_{-+-}(G)) = m(m+3)^2 + (m+n)(m+n-1)^2 - 2(m^2+7m)(m+n-1) + 2(n-2)M_1(G) + 2M_2(G) + F(G)$

(viii) $M_1(T_{+--}(G)) = m[(mn+1) + (m+n)(m+n-2)] - 2(m+n-1)M_1(G) + 2M_2(G) + F(G)$

## 3. Main Results

In this section, we derive the analytic expressions for the sigma index and coindex of semi and total transformations of graphs. Bearing the relation $\sigma(G) = F(G) - 2M_2(G)$ in mind, we first study the second Zagreb index and then the forgotten index and finally deduce the results for the sigma index.

*3.1. Second Zagreb Index of Transformation Graphs.* The second Zagreb index of total transformation of graphs was expressed in [27], and by careful inspection, we notice that the entire process is vague and results in incorrect expressions. For instance, it was proved [27] that $M_2(T_{+++}(G)) = 8M_1(G) + 6M_2(G) + F(G)$. Suppose $G = P_n$, a path on $n$ vertices. Then, $T_{+++}(P_n)$ is a graph on $2n-1$ vertices and $4n-5$ edges in which 2 vertices of degrees 2 and 3 each and $2n-5$ vertices of degree 4 while 2 edges with degrees of end vertices $(2,3)$ and $(2,4)$each, and 4 edges with $(3,4)$ and $4n-13$ edges with $(4,4)$. Hence, $M_2(T_{+++}(G)) = 6\times 2 + 8\times 2 + 12\times 4 + 16\times(4n-13) = 64n-132$. However, $M_1(P_n) = 4n-6$, $M_2(P_n) = 4n-8$, and $F(P_n) = 8n-14$, resulting that $8M_1(P_n) + 6M_2(P_n) + F(G) = 64n-110$. Hence, we now compute the correct analytic expressions of the second Zagreb index and coindex of total transformation graphs using reformulated Zagreb indices. Moreover, the type-II semitransformation is newly introduced in this paper, and hence we also obtain the exact expressions for first and second Zagreb indices. The following theorem gives the exact expression for second Zagreb indices of first four transformations in terms of edge version of first and second Zagreb indices of the arbitrary graph.

**Theorem 1.** *Let G be a graph with order n and size m. Then,*

(i) $M_2(T_{+++}(G)) = EM_2(G) + 2EM_1(G) + 8M_2(G) + 2M_1(G) + 2F(G) - 4m$

(ii) $M_2(T_{++-}(G)) = EM_2(G) + (n-2)EM_1(G) + (1/2)[(n-2)^2 + 2m(n-2)]M_1(G) + m^3 + m^2(n-2)(n-4) - m(n-2)^2$

(iii) $M_2(T_{+-+}(G)) = \overline{EM_2}(G) - (m+1)\overline{EM_1}(G) + (1/2)[m(m+1)^3] - (1/2)[(m^2-2m-11)M_1(G)] - 2F(G)$

(iv) $M_2(T_{-++}(G)) = EM_2(G) + 2EM_1(G) + 2nM_1(G) + (1/2)n(n-1)^3 - m[n^2-2n+5]$

*Proof.* The graph $T_{+++}(G)$ has $m+n$ vertices and $(1/2)M_1(G) + 2m$ edges in which $m$ edges are actual edges in $G$ by condition (#1), $(1/2)M_1(G) - m$ edges are produced by condition (#2) called edge adjacency relation edges (line graph edges), and $2m$ edges are edges produced by condition (#3) called incidence relation edges. For any vertex $s \in V(T_{+++}(G))$,

$$d_{T_{+++}(G)}(s) = \begin{cases} 2d_G(s), & \text{if } s \in V(G), \\ d_G(s) + 2, & \text{if } s \in E(G). \end{cases} \quad (4)$$

Therefore,

$$\begin{aligned} M_2(T_{+++}(G)) &= \sum_{st\in E(T_{+++}(G))} d_{T_{+++}(G)}(s) d_{T_{+++}(G)}(t) \\ &= \sum_{st\in E(T_{+++}(G))\cap E(G)} d_{T_{+++}(G)}(s) d_{T_{+++}(G)}(t) + \sum_{st\in E(T_{+++}(G))\cap E(L(G))} d_{T_{+++}(G)}(s) d_{T_{+++}(G)}(t) \\ &\quad + \sum_{st\in E(T_{+++}(G))\smallsetminus[E(G)\cup E(L(G))]} d_{T_{+++}(G)}(s) d_{T_{+++}(G)}(t) \\ &= \sum_{st\in E(G)} 2d_G(s) 2d_G(t) + \sum_{s,t\in E(G) s\sim t} (d_G(s)+2)(d_G(t)+2) \end{aligned}$$

$$\begin{aligned}
&+ \sum_{s\in V(G),t\in E(G)s\sim t} 2d_G(s)\left(d_G(t)+2\right) \\
&= 4M_2(G) + \sum_{s,t\in E(G)s\sim t} d_G(s)d_G(t) \\
&+ \sum_{s,t\in E(G)s\sim t} 2\left[d_G(s)+d_G(t)\right] + 4|E(L(G))| \\
&+ \sum_{s\in V(G)}\sum_{x\in N_G(s)} 2d_G(s)\left[d_G(s)+d_G(x)\right] \\
&= 4M_2(G) + EM_2(G) + 2EM_1(G) + 4|E(L(G))| \\
&+ 2\sum_{s\in V(G)} d_G(s)^3 + 2\sum_{s\in V(G)}\sum_{x\in N_G(s)} d_G(s)d_G(x) \\
&= 4M_2(G) + EM_2(G) + 2EM_1(G) + 4\left(\frac{M_1(G)}{2} - m\right) + 2F(G) + 4M_2(G) \\
&= EM_2(G) + 2EM_1(G) + 8M_2(G) + 2M_1(G) + 2F(G) - 4m.
\end{aligned} \tag{5}$$

This completes the proof of assertion (i). Next, for any vertex $s \in V(T_{++-}(G))$,

$$d_{T_{++-}(G)}(s) = \begin{cases} m, & \text{if } s \in V(G), \\ d_G(s)+n-2, & \text{if } s \in E(G). \end{cases} \tag{6}$$

It can be seen that

$$\begin{aligned}
M_2(T_{++-}(G)) &= \sum_{st\in E(G)} d_G(s)d_G(t) + \sum_{s,t\in E(G)s\sim t} d_G(s)d_G(t) + \sum_{s\in V(G),t\in E(G)s\nsim t} d_G(s)d_G(t) \\
&= \sum_{st\in E(G)} m\cdot m + \sum_{s,t\in E(G)s\sim t} \left(d_G(s)+n-2\right)\left(d_G(t)+n-2\right) + \sum_{s\in V(G),t\in E(G)s\nsim t} m\left(d_G(t)+n-2\right) \\
&= m^3 + EM_2(G) + (n-2)EM_1(G) + (n-2)^2|E(L(G))| \\
&+ \sum_{t\in E(G)}\sum_{s\in V(G)s\nsim t} m\left(d_G(t)+n-2\right) \\
&= m^3 + EM_2(G) + (n-2)EM_1(G) + (n-2)^2\left(\frac{M_1(G)}{2} - m\right) \\
&+ m\sum_{t\in E(G)} (n-2)\left(d_G(t)+n-2\right) \\
&= m^3 + EM_2(G) + (n-2)EM_1(G) + \frac{1}{2}\left[(n-2)^2M_1(G) - 2m(n-2)^2\right] \\
&+ m(n-2)\left(\sum_{t\in E(G)} d_G(t)\right) + m^2(n-2)^2 \\
&= m^3 + EM_2(G) + (n-2)EM_1(G) + \frac{1}{2}\left[(n-2)^2M_1(G) - 2m(n-2)^2\right] \\
&+ m(n-2)\left[M_1(G) - 2m\right] + m^2(n-2)^2 \\
&= EM_2(G) + (n-2)EM_1(G) + \frac{1}{2}\left[(n-2)^2 + 2m(n-2)\right]M_1(G) \\
&+ m^3 + m^2(n-2)(n-4) - m(n-2)^2.
\end{aligned} \tag{7}$$

To complete the proof of assertion (iii), we notice that for any vertex, $s \in V(T_{+-+}(G))$,

$$d_{T_{+-+}(G)}(s) = \begin{cases} 2d_G(s), & \text{if } s \in V(G), \\ m+1-d_G(s), & \text{if } s \in E(G). \end{cases} \quad (8)$$

As before, we can easily write that

$$\begin{aligned} M_2(T_{+-+}(G)) &= \sum_{st\in E(G)} 2d_G(s)2d_G(t) + \sum_{s,t\in E(G)s\nsim t} (m+1-d_G(s))(m+1-d_G(t)) \\ &\quad + \sum_{s\in V(G),t\in E(G)s\sim t} 2d_G(s)(m+1-d_G(t)) \\ &= 4M_2(G) + (m+1)^2\left[\frac{m(m-1)}{2} - |E(L(G))|\right] - (m+1)\overline{EM_1}(G) + \overline{EM_2}(G) \\ &\quad + 2\sum_{s\in V(G)}\sum_{x\in N_G(s)} d_G(s)(m+3-(d_G(s)+td_Gn(x))) \\ &= \overline{EM_2}(G) - (m+1)\overline{EM_1}(G) + 4M_2(G) + \frac{1}{2}\left[m(m+1)^3 - (m+1)^2M_1(G)\right] \\ &\quad + 2(m+3)M_1(G) - 2F(G) - 4M_2(G) \\ &= \overline{EM_2}(G) - (m+1)\overline{EM_1}(G) + \frac{1}{2}\left[m(m+1)^3\right] - \frac{1}{2}\left[\left(m^2-2m-11\right)M_1(G)\right] - 2F(G). \end{aligned} \quad (9)$$

The final assertion follows from the fact that for any vertex $s \in V(T_{-++}(G))$,

$$d_{T_{-++}(G)}(s) = \begin{cases} n-1, & \text{if } s \in V(G), \\ d_G(s)+2, & \text{if } s \in E(G). \end{cases} \quad (10)$$

□

**Theorem 2.** *Let G be a graph with order n and size m. Then,*

*(1)* $M_2(T_{---}(G)) = (1/2)[M_1^2(G) - (3(m+n-1)^2 - 8(2m+n-2))\ M_1(G) + (4m+4n-22)\ M_2(G) + (2m+2n-7)F(G) - 2EM_2(G) - 4EM_1\ (G) + (m+n)(m+n-1)^3 - 12m(m+n-1)^2 + 8m(2m+1)]$

*(2)* $M_2(T_{--+}(G)) = (1/2)[M_1^2(G) - (3m^2+14m+12n-17)M_1(G) + (4m+4n-6)\ M_2(G) + (2m+2n-3)F(G) - 2EM_2(G) - 2(n-2)EM_1\ (G) + m^4 + 7m^3 + 4m^2n + 11m^2 - 2mn^2 + 24mn - 29m + n^4 - 3n^3 + 3n^2 - n]$

*(3)* $M_2(T_{-+-}(G)) = (1/2)\ [M_1^2(G) + (3(m+n-1)^2 - 2(m^2+7m) - 2(m+1)\ (2m+2n-3) + m^2 - 2m - 11)M_1(G) + 2(2m+2n-3)\ \underline{M_2}(G) + (2m+2n+1)F(G) - 2\overline{EM_2}(G) + 2(m+1)\ \overline{EM_1}\ (G) + (m+n)(m+n-1)^3 - 3(m+n-1)^2(m^2+7m) + (m^2+7m)^2 + m(m+3)^2(2m+2n-3) - m(m+1)^3]$

*(4)* $M_2(T_{+--}(G)) = (1/2)[M_1^2(G) + (2n(n-1) - 3\ (m+n-1)^2 - 4n)M_1(G) + 2(2m+2n-3)M_2(G) + (2m+2n-3)F(G) - 2EM_2(G) - 4EM_1(G) + (m+n)\ (m+n-1)^3 - 3n(n-1)(m+n-1)^2 + n^2(n-1)^2 + n(n-1)^2\ (2m+2n-3) - n(n-1)^3 + 2m(n^2-2n+5)]$

*Proof.* It was proved [35] that

$$M_2(\overline{G}) = \frac{1}{2}n(n-1)^3 - 3m(n-1)^2 + 2m^2 + \frac{2n-3}{2}M_1(G) - M_2(G), \quad (11)$$

and known that $\overline{T_{+++}(G)} \cong T_{---}(G)$, $\overline{T_{++-}(G)} \cong T_{--+}(G)$, $\overline{T_{+-+}(G)} \cong T_{-+-}(G)$, and $\overline{T_{+--}(G)} \cong T_{-++}(G)$. By Lemma 6 and Theorem 1, we can easily complete the proof. □

The Zagreb coindices are introduced in [36] with extensive applications in the field of chemical graph theory and widely discussed in [9, 10, 37–39]. Therefore, it will be worth finding the second Zagreb coindices of total transformations.

**Theorem 3.** *Let G be a graph with order n and size m. Then,*

*(1)* $\overline{M_2}\ (T_{+++}(G)) = (1/2)[M_1^2(G) + 8(m-1)\ M_1(G) - 18M_2(G) - 5F(G) - 2EM_2(G) - 4EM_1(G) + 8m(2m+1)]$

*(2)* $\overline{M_2}(T_{++-}\ (G)) = (1/2)[M_1^2\ (G) + (2mn - 4m - n^2 + 2n + 4)M_1(G) - 2M_2(G) - F\ (G) - 2EM_2\ (G) - 2(n-2)EM_1(G) + 2m^2n^2 - 2m^3 - 5m^2n + mn^2 - 8m]$

*(3)* $\overline{M_2}\ (T_{+-+}\ (G)) = (1/2)\ [M_1^2(G) - (m^2+14m+9)\ \overline{M_1}\ (G) - 2M_2(G) + 3F(G) - 2\overline{EM_2}(G) + 2(m+1)\ \overline{EM_1}(G) + 10m^3 + 40m^2 - 10m]$

*(4)* $\overline{M_2}(T_{-++}(G)) = (1/2)[M_1^2(G) + 2n(n-3)\ M_1(G) - 2M_2(G) - F(G) - 2EM_2\ (G) - 4EM_1(G) + 2m(n^2 - 2n+5)]$

(5) $\overline{M_2}(T_{---}(G)) = (1/2)[2EM_2(G) + 4EM_1(G) + (m^2 + n^2 + 2mn - 10m - 10n + 13)M_1(G) - 4(m + n - 5)M_2(G) - 2(m + n - 3)F(G) + 4m^3 + 8m^2n - 8m^2 + 4mn^2 - 8mn - 4m]$

(6) $\overline{M_2}(T_{--+}(G)) = (1/2)[2EM_2(G) + 2(n-2)EM_1(G) + (m^2 - 2n^2 + 10m + 14n - 11)M_1(G) - 4(m + n - 1)M_2(G) - 2(m + n - 1)F(G) - 2m^3 + 2m^2n^2 - 6m^2n - 8m^2 + 8mn^2 - 30mn + 20m]$

(7) $\overline{M_2}(T_{-+-}(G)) = (1/2)[2\overline{EM_2}(G) - 2(m+1)\overline{EM_1}(G) + (2m^2 - n^2 + 2mn + 4m + 6n + 6)M_1(G) - 4(m + n - 1)M_2(G) - 2(m + n + 1)F(G) + m^2n^2 + 7mn^2 - 32mn - 2m^3 - 16m^2 + 26m]$

(8) $\overline{M_2}(T_{+--}(G)) = (1/2)[2EM_2(G) + 4EM_1(G) + (m^2 + 2mn - 2m + n^2 + 2n + 1)M_1(G) - 4(m + n - 1)M_2(G) - 2(m + n - 1)F(G) + m^2n^2 - 2mn^2 - m^2n + 4mn - 10m]$

*Proof.* It was shown in [35] that

$$\overline{M_2}(G) = 2m^2 - \frac{1}{2}M_1(G) - M_2(G), \tag{12}$$

and combining the results of Lemma 6 and Theorem 1, we can finish the proof by simple mathematical calculations. □

The following theorem fills the gap in the literature with respect to the results found in [21, 25].

**Theorem 4.** *Let G be a graph with order n and size m. Then,*

(1) $M_1(T_{2++}(G)) = M_1(G) + F(G) + 2M_2(G)$ [25]

(2) $M_1(T_{2+-}(G)) = 2M_2(G) + F(G) + (2n-7)M_1(G) + mn(m+n) - 4m(m + 2n - 4)$

(3) $M_1(T_{2-+}(G)) = 2M_2(G) + F(G) - (2m+5)M_1(G) + m(m+3)^2$

(4) $M_1(T_{2--}(G)) = 2M_2(G) + F(G) - (2m + 2n - 3)M_1(G) + m^2(n-4) + m(m+n-1)^2$

(5) $\overline{M_1}(T_{2++}(G)) = (m + n - 2)M_1(G) - 2M_2(G) - F(G) + 2mn + 2m(m-1)$ [25]

(6) $\overline{M_1}(T_{2+-}(G)) = (m - n + 6)M_1(G) - 2M_2(G) - F(G) + mn(m+n) - 2m(m+5)$

(7) $\overline{M_1}(T_{2-+}(G)) = (m - n + 6)M_1(G) - 2M_2(G) - F(G) + mn(m+5) - 2m(m+7)$

(8) $\overline{M_1}(T_{2--}(G)) = (m + n - 2)M_1(G) - 2M_2(G) - F(G) + mn(n-3) + 2m(m+1)$

*Proof.* From the construction of type-II semitransformation, it is easily seen that for any vertex $s \in V(T_{2\beta\gamma}(G))$ such that $s \in V(G)$,

$$d_{T_{2\beta\gamma}(G)}(s) = \begin{cases} d_G(s), & : \beta = +, \gamma = +, \\ d_G(s), & : \beta = -, \gamma = +, \\ m - d_G(s), & : \beta = +, \gamma = -, \\ m - d_G(s), & : \beta = -, \gamma = -. \end{cases} \tag{13}$$

In the same way, for any vertex $s \in V(T_{2\beta\gamma}(G))$ such that $s \in E(G)$,

$$d_{T_{2\beta\gamma}(G)}(s) = \begin{cases} d_G(s) + 2, & : \beta = +, \gamma = +, \\ m + 1 - d_G(s), & : \beta = -, \gamma = +, \\ n - 2 + d_G(s), & : \beta = +, \gamma = -, \\ m + n - 3 - d_G(s), & : \beta = -, \gamma = -. \end{cases} \tag{14}$$

The proof follows from routine mathematical simplifications and, in addition, using the relation $\overline{M_1}(G) = 2m(n-1) - M_1(G)$ [35]. □

In [25], the authors have made an attempt to find the second Zagreb index of type-I semitransformation and left the calculations of type-II semitransformation due to its computational complexity. The following theorem gives the exact analytical expressions of the second Zagreb indices for type-II transformations of an arbitrary graph.

**Theorem 5.** *Let G be a graph with order n and size m. Then,*

(1) $M_2(T_{2++}(G)) = EM_2(G) + 2EM_1(G) + 2M_2(G) + 2M_1(G) + F(G) - 4m$

(2) $M_2(T_{2+-}(G)) = EM_2(G) + (n-2)EM_1(G) + 2M_2(G) + (1/2)[n^2 + 2mn - 8m - 2n - 4]M_1(G) + F(G) + m^2(n-4)^2 - m(n-2)^2$

(3) $M_2(T_{2-+}(G)) = \overline{EM_2}(G) - (m+1)\overline{EM_1}(G) - 2M_2(G) - (1/2)(m^2 - 5)M_1(G) - F(G) + (1/2)m(m+1)^3$

(4) $M_2(T_{2--}(G)) = \overline{EM_2}(G) - (m + n - 3)\overline{EM_1}(G) - (1/2)[(m+n-3)^2 + 2mn - 10m - 2n + 2]M_1(G) - 2M_2(G) - F(G) + (1/2)[m(m+1)(m+n-3)^2 + 2m^2(n-4)(m+n-1)]$

(5) $\overline{M_2}(T_{2++}(G)) = (1/2)[M_1^2(G) + (4m-5)M_1(G) - 3F(G) - 2EM_2(G) - 4EM_1(G) - 6M_2(G) + 4m(m+2)]$

(6) $\overline{M_2}(T_{2+-}(G)) = (1/2)[M_1^2(G) + (2mn - n^2 - 4m + 11)M_1(G) - 3F(G) - 2EM_2(G) - 2(n-2)EM_1(G) - 6M_2(G) + mn(2mn - 9m + n) + 8m(m-1)]$

(7) $\overline{M_2}(T_{2-+}(G)) = (1/2)[M_1^2(G) - m(m+8)M_1(G) + 2M_2(G) - 2\overline{EM_2}(G) + 2(m+1)\overline{EM_1}(G) + F(G) + 2m(3m^2 + 8m - 5)]$

(8) $\overline{M_2}(T_{2--}(G)) = (1/2)[M_1^2(G) - (m^2 - n^2 + 8m + 6n - 8)M_1(G) + 2M_2(G) + F(G) - 2\overline{EM_2}(G) + 2(m + n - 3)\overline{EM_1}(G) + mn(mn - m - 2n + 8) + 2m(3m^2 + 2m - 5)]$

*Proof.* The proof of (i)–(iv) is similar to Theorem 1, and for the sake the completeness, we give the proof of (i). The graph $T_{2++}(G)$ has $m + n$ vertices and $(1/2)M_1(G) + m$ edges in which $(1/2)M_1(G) - m$ edges are produced by condition (#2) called edge adjacency relation edges (line graph edges) and $2m$ edges are edges produced by condition (#3) called incidence relation edges. Also, for any vertex, $s \in V(T_{2++}(G))$,

$$d_{T_{2++}(G)}(s) = \begin{cases} d_G(s), & \text{if } s \in V(G), \\ d_G(s) + 2, & \text{if } s \in E(G). \end{cases} \quad (15)$$

Hence,

$$\begin{aligned}
M_2(T_{2++}(G)) &= \sum_{st \in E(T_{2++}(G))} d_{T_{2++}(G)}(s) d_{T_{2++}(G)}(t) \\
&= \sum_{st \in E(T_{2++}(G)) \cap E(L(G))} d_{T_{2++}(G)}(s) d_{T_{2++}(G)}(t) + \sum_{st \in E(T_{2++}(G)) \setminus E(L(G))} d_{T_{2++}(G)}(s) d_{T_{2++}(G)}(t) \\
&= \sum_{s,t \in E(G) s \sim t} (d_G(s) + 2)(d_G(t) + 2) + \sum_{s \in V(G), t \in E(G) s \sim t} d_G(s)[d_G(t) + 2] \\
&= \sum_{s,t \in E(G) s \sim t} d_G(s) d_G(t) + \sum_{s,t \in E(G) s \sim t} 2[d_G(s) + d_G(t)] + 4|E(L(G))| \\
&\quad + \sum_{s \in V(G)} \sum_{x \in N_G(s)} d_G(s)[d_G(s) + d_G(x)] \\
&= \sum_{s,t \in E(G) s \sim t} d_G(s) d_G(t) + \sum_{s,t \in E(G) s \sim t} 2[d_G(s) + d_G(t)] + 4|E(L(G))| + \sum_{s \in V(G)} d_G(s)^3 + \sum_{s \in V(G)} \sum_{x \in N_G(s)} d_G(s) d_G(x) \\
&= \mathrm{EM}_2(G) + 2\mathrm{EM}_1(G) + 4\left(\frac{M_1(G)}{2} - m\right) + F(G) + 2M_2(G) \\
&= \mathrm{EM}_2(G) + 2\mathrm{EM}_1(G) + 2M_2(G) + 2M_1(G) + F(G) - 4m.
\end{aligned} \quad (16)$$

To complete the remaining parts, we apply equation (12) with the help of Theorem 4. □

*3.2. F-Index of Transformation Graphs.* The forgotten index and coindex of type-I semi and total transformations of graphs have been obtained [20, 28] in terms of first Zagreb, second Zagreb, vertex a-Zagreb, and (a, b)-Zagreb indices. In this section, we rewrite vertex a-Zagreb and (a, b)-Zagreb indices in terms of the sum-connectivity index. Before proceeding to this, we shall state a basic lemma.

**Lemma 7** (see [28]). *Let G be a connected graph of order n and size m. Then,*

(i) $F(\overline{G}) = n(n-1)^3 - F(G) - 6m(n-1)^2 + 3(n-1)M_1(G)$

(ii) $\overline{F}(G) = (n-1)M_1(G) - F(G)$

The following theorem is crucial for finding the sigma index of the transformation of an arbitrary graph.

**Theorem 6.** *Let G be a connected graph of order n and size m. Then,*

(1) $F(T_{+++}(G)) = 8F(G) + \chi_3(G)$

(2) $F(T_{++-}(G)) = \chi_3(G) + (3n-12)[F(G) + 2M_2(G)] + 3(n-4)^2 M_1(G) + m(n-4)^3 + m^3 n$

(3) $F(T_{+-+}(G)) = (3m+17)F(G) - \chi_3(G) + m(m+3)^3 - 3(m+3)^2 M_1(G) + 6(m+3)M_2(G)$

(4) $F(T_{-++}(G)) = n(n-1)^3 + \chi_3(G)$

(5) $F(T_{---}(G)) = 6(m+n-1)M_2(G) - (3m^2 - 18m + 6mn - 18n + 3n^2 + 15)M_1(G) + (3m + 3n - 11)F(G) - \chi_3(G) + (m+n)(m+n-1)^3 - 12m(m+n-1)^2$

(6) $F(T_{--+}(G)) = (3m+9)F(G) - \chi_3(G) - (3m^2 + 18m + 27)M_1(G) + (6m+18)M_2(G) + m^4 + 9m^3 + 27m^2 + 27m + n^4 - 3n^3 + 3n^2 - n$

(7) $F(T_{-+-}(G)) = \chi_3(G) + (3n-20)F(G) + (3n^2 - 12n + 12m + 36)M_1(G) + (6n-24)M_2(G) + (m+n)(m+n-1)^3 - m(m+3)^3 - 3(m+n-1)^2(m^2 + 7m) + 3m(m+3)^2(m+n-1)$

(8) $F(T_{+--}(G)) = 3(m+n-1)F(G) + 6(m+n-1)M_2(G) - 3(m+n-1)^2M_1(G) - \chi_3(G) + (m+n)(m+n-1)^3 - n(n-1)^3 - 3mn(n-1)(m+n-1)$

*Proof.* The proof of (i)–(iv) can be derived using the degrees of vertices from the proof of Theorem 1 and the remaining parts from Lemma 7. □

The following theorem is an easy consequence of combining Lemma 7 and Theorem 6, which will be used to compute the analytical expressions of the forgotten coindices of total transformations of an arbitrary graph.

**Theorem 7.** *Let G be a connected graph of order n and size m. Then,*

(1) $\overline{F}(T_{+++}(G)) = 4(m+n-1)M_1(G) + 2(m+n-1)M_2(G) + (m+n-9)F(G) - \chi_3(G)$

(2) $\overline{F}(T_{++-}(G)) = (m-2n+11)F(G) - \chi_3(G) - (n^2 - 2mn + 8m - 14n + 40)M_1(G) + (2m-4n+22)M_2(G) + 2m^2n^2 - 9m^2n + 16m^2 + 3mn^2 - 24mn + 48m$

(3) $\overline{F}(T_{+-+}(G)) = (n-2m-18)F(G) + \chi_3(G) + (m^2 + 18m - 2mn - 2n + 29)M_1(G) + (2n-4m-20)M_2(G) + m^3n - 4m^3 + 6m^2n - 24m^2 + 9mn - 36m$

(4) $\overline{F}(T_{-++}(G)) = (m+n-1)F(G) + 2(m+n-1)M_2(G) - \chi_3(G) + mn^3 - 2mn^2 + mn$

(5) $\overline{F}(T_{---}(G)) = \chi_3(G) - (2m+2n-10)F(G) + (m^2 + n^2 + 2mn - 10m - 10n + 9)M_1(G) - 4(m+n-1)M_2(G) + 4m^3 + 8m^2n - 8m^2 + 4mn^2 - 8mn + 4m$

(6) $\overline{F}(T_{--+}(G)) = \chi_3(G) + (m^2 + 14m - 2mn - 6n + 33)M_1(G) - (4m-2n+20)M_2(G) - (2m-n+10)F(G) + m^3n - 4m^3 + 6m^2n - 24m^2 + mn^3 - 2mn^2 + 10mn - 36$

(7) $\overline{F}(T_{-+-}(G)) = 2(m-2n+11)M_2(G) - \chi_3(G) - (n^2 - 2mn + 16m - 6n + 32)M_1(G) + (m-2n+19)F(G) + 4m^3 + m^2n^2 + 8m^2 + 7mn^2 - 32mn + 52m$

(8) $\overline{F}(T_{+--}(G)) = \chi_3(G) - 4(m+n-1)M_2(G) - 2(m+n-1)F(G) + (m+n-1)^2M_1(G) + m^2n^2 - m^2n$

**Theorem 8** (see [20]). *Let G be a connected graph of order n and size m. Then,*

(1) $F(T_{1++}(G)) = 8F(G) + 8m$

(2) $F(T_{1+-}(G)) = nm^3 + m(n-2)^3$

(3) $F(T_{1-+}(G)) = n(n-1)^3 + 8m$

(4) $F(T_{1--}(G)) = 12(m+n-1)M_1(G) - 8F(G) + n(m+n-1)^3 - 12m(m+n-1)^2 + m(n-2)^3$

(5) $\overline{F}(T_{1++}(G)) = 4m(m+n-1) - 8m + 4(m+n-1)M_1(G) - 8F(G)$

(6) $\overline{F}(T_{1+-}(G)) = (m+n-1)(nm^2 + m(n-2)^2) - nm^3 - m(n-2)^3$

(7) $\overline{F}(T_{1-+}(G)) = (m+n-1)(4m + n(n-1)^2) - n(n-1)^3 - 8m$

(8) $\overline{F}(T_{1--}(G)) = 8F(G) - 8(m+n-1)M_1(G) + m(m+n-1)(n-2)^2 + (m+n-1)^2(n(m+n-1) + 4m) - n(m+n-1)^3 - m(n-2)^3$

**Theorem 9.** *Let G be a connected graph of order n and size m. Then,*

(1) $F(T_{2++}(G)) = F(G) + \chi_3(G)$

(2) $F(T_{2+-}(G)) = m^3(n-6) + m(n-4)^3 + \chi_3(G) + (3n-13)F(G) + 6(n-4)M_2(G) + [3(n-4)^2 + 3m]M_1(G)$

(3) $F(T_{2-+}(G)) = F(G) + m(m+3)^3 - 3(m+3)^2M_1(G) + 3(m+3)[F(G) + 2M_2(G)] - \chi_3(G)$

(4) $F(T_{2--}(G)) = m^3(n-6) + m(m+n-1)^3 + (3m + 3n - 4)F(G) + 6(m+n-1)M_2(G) + [3m - 3(m+n-1)^2]M_1(G) - \chi_3(G)$

(5) $\overline{F}(T_{2++}(G)) = (m+n-1)[M_1(G) + 2M_2(G)] + (m+n-2)F(G) - \chi_3(G)$

(6) $\overline{F}(T_{2+-}(G)) = (2m-4n+22)M_2(G) + (2mn - n^2 + 15n - 10m - 41)M_1(G) + (m-2n+12)F(G) - \chi_3(G) + (m+n-1)(mn(m+n) - 4m(m+2n-4)) - m^3(n-6) - m(n-4)^3$

(7) $\overline{F}(T_{2-+}(G)) = (2n-4m-20)M_2(G) + (n-2m-11)F(G) + (m^2 + 15m - 2mn - 5n + 32)M_1(G) + \chi_3(G) + m(m+3)^2(n-4)$

(8) $\overline{F}(T_{2--}(G)) = \chi_3(G) - 4(m+n-1)M_2(G) + (m^2 + 2mn - 4m - n + n^2)M_1(G) - (2m+2n-3)F(G) + 2m^3 + m^2n^2 - 5m^2n + 4m^2$

*Proof.* The proof of the theorem follows from using the degrees of vertices as given in the proof of Theorem 4 and Lemma 7. □

*3.3. σ-Index of Transformation Graphs.* In this section, we first derive a relation between $\sigma$-index of a graph and its coindex. Following this, we derive another relation between $\sigma$-coindex of a graph and $\sigma$-index of the complement graph. Finally, we list down the $\sigma$-index and coindex of semi and total transformations of graphs from the above subsections. The following theorem gives the relationship between the sigma index and its coindex.

**Theorem 10.** *Let G be any graph with n vertices and m edges. Then,*

$$\sigma(G) + \overline{\sigma}(G) = nM_1(G) - 4m^2. \tag{17}$$

*Proof.* The proof is completed from the definitions of $\sigma$-index and coindex as explained in the following:

$$\begin{aligned}\sigma(G) + \overline{\sigma}(G) &= \sum_{st\in E(G)} [d_G(s) - d_G(t)]^2 + \sum_{st \notin E(G)} [d_G(s) - d_G(t)]^2 \\ &= \sum_{\{s,t\}\subseteq V(G)} [d_G(s) - d_G(t)]^2 \\ &= \sum_{\{s,t\}\subseteq V(G)} \left[d_G(s)^2 + d_G(t)^2 - 2d_G(s)d_G(t)\right] \\ &= \sum_{\{s,t\}\subseteq V(G)} \left[d_G(s)^2 + d_G(t)^2\right] - \sum_{\{s,t\}\subseteq V(G)} 2d_G(s)d_G(t) \\ &= F(G) + \overline{F}(G) - 2M_2(G) - 2\overline{M_2}(G) \\ &= (n-1)M_1(G) - 2M_2(G) - 2\left(2m^2 - M_2(G) - \frac{M_1(G)}{2}\right) \\ &= nM_1(G) - 4m^2.\end{aligned} \tag{18}$$

□

**Corollary 1.** *Let G be any graph with n vertices and m edges. Then,*

$$\overline{\sigma}(G) = nM_1(G) + 2M_2(G) - F(G) - 4m^2. \tag{19}$$

The following theorem establishes interesting result that the sigma index of the complement of a graph and sigma coindex of a graph is one and the same.

**Theorem 11.** *Let G be any graph with n vertices and m edges. Then,*

$$\sigma(\overline{G}) = \overline{\sigma}(G). \tag{20}$$

*Proof.* For any vertex $s \in V(G)$, $d_{\overline{G}}(s) = n - 1 - d_G(s)$, and we have

$$\begin{aligned}\sigma(\overline{G}) &= \sum_{st\in E(\overline{G})} \left[d_{\overline{G}}(s) - d_{\overline{G}}(t)\right]^2 \\ &= \sum_{st \notin E(G)} [(n-1-d_G(s)) - (n-1-d_G(t))]^2 \\ &= \sum_{st \notin E(G)} [d_G(t) - d_G(s)]^2 \\ &= \overline{\sigma}(G).\end{aligned} \tag{21}$$

□

**Corollary 2.** *Let G be any graph with n vertices and m edges. Then,*

$$\overline{\sigma}(\overline{G}) = \sigma(G). \tag{22}$$

The main objective of this section is the following theorem.

**Theorem 12.** *Let G be a connected graph of order n and size m. Then,*

(1) $\sigma(T_{+++}(G)) = 4F(G) + \chi_3(G) - 2EM_2(G) - 4EM_1(G) - 16M_2(G) - 4M_1(G) + 8m$

(2) $\sigma(T_{++-}(G)) = \chi_3(G) + (3n-12)[F(G) + 2M_2(G)] - [(n-2)^2 + 2m(n-2) - 3(n-4))^2]M_1(G) - 2EM_2(G) - 2(n-2)EM_1(G) - 2m^3 - 2m^2(n-2)(n-4) + 2m(n-2)^2 + m(n-4)^3 + m^3n$

(3) $\sigma(T_{+-+}(G)) = 12F(G) - \chi_3(G) + 3(m+3)\chi_2(G) - 2\overline{EM_2}(G) + 2(m+1)\overline{EM_1}(G) + [m^2 - 2m - 11 - 3(m+3)^2]M_1(G) + m(m+3)^3 - m(m+1)^3$

(4) $\sigma(T_{-++}(G)) = \chi_3(G) - 2EM_2(G) - 4EM_1(G) - 4nM_1(G) + 2m(n^2 - 2n + 5)$

(5) $\sigma(T_{---}(G)) = 2EM_2(G) + 4EM_1(G) - M_1^2(G) + 4(n-m+1)M_1(G) + 2(m+n+8)M_2(G) + (m+n-4)F(G) - \chi_3(G) - 8m(2m+1)$

(6) $\sigma(T_{--+}(G)) = 2EM_2(G) + 2(n-2)EM_1(G) - M_1^2(G) - \chi_3(G) + (12n - 4m - 44)M_1(G) + (2m - 4n + 24)M_2(G) + (m - 2n + 12)F(G) + 2m^3 + 16m^2 - 4m^2n + 2mn^2 - 24mn + 56m$

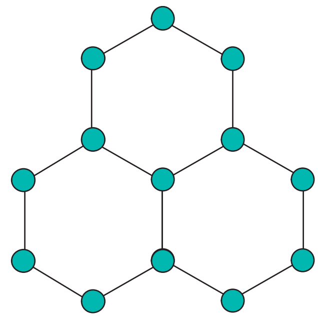


Figure 4: The molecular graph of perhydrophenalene $G$.

Table 2: Second Zagreb and sigma indices of total transformations of perhydrophenalene $G$.

| S. no. | Total transformations of $G$ | Second Zagreb index | Sigma index |
|---|---|---|---|
| 1. | $T_{+++}(G)$ | 1587 | 48 |
| 2. | $T_{++-}(G)$ | 41652 | 342 |
| 3. | $T_{+-+}(G)$ | 16968 | 2334 |
| 4. | $T_{-++}(G)$ | 11331 | 1584 |
| 5. | $T_{---}(G)$ | 155358 | 504 |
| 6. | $T_{--+}(G)$ | 28560 | 534 |
| 7. | $T_{-+-}(G)$ | 86868 | 12582 |
| 8. | $T_{+--}(G)$ | 99894 | 8760 |

Table 3: Second Zagreb and sigma indices for semitransformations of perhydrophenalene $G$.

| S. no. | Semitransformations of $G$ | Second Zagreb index | Sigma index |
|---|---|---|---|
| 1. | $T_{1++}(G)$ | 636 | 288 |
| 2. | $T_{1+-}(G)$ | 30600 | 2640 |
| 3. | $T_{1-+}(G)$ | 9792 | 3000 |
| 4. | $T_{1--}(G)$ | 72372 | 22608 |
| 5. | $T_{2++}(G)$ | 885 | 192 |
| 6. | $T_{2+-}(G)$ | 33069 | 318 |
| 7. | $T_{2-+}(G)$ | 15678 | 3654 |
| 8. | $T_{2--}(G)$ | 217794 | 15120 |

(7) $\sigma(T_{-+-}(G)) = 2\overline{EM_2}(G) - 2(m+1)\overline{EM_1}(G) - M_1^2(G) + \chi_3(G) + (2m^2 + 32m - 2mn + 38 - 2n)M_1(G) + (2n - 4m - 18)M_2(G) + (n - 2m - 21)F(G) + m^3 n - 14m^3 + 6m^2 n - 64m^2 + 9mn - 26m$

(8) $\sigma(T_{+--}(G)) = 2EM_2(G) + 4EM_1(G) - M_1^2(G) - \chi_3(G) - 2n(n-3)M_1(G) + (2m + 2n)M_2(G) + (m + n)F(G) + n^3 m - 4n^2 m + 5nm - 10m$

In sequence to Theorems 3 and 7, we have the following.

**Theorem 13.** *Let G be a connected graph of order n and size m. Then,*

(1) $\overline{\sigma}(T_{+++}(G)) = 2EM_2(G) + 4EM_1(G) + 2(m+n+8)M_2(G) + 4(n-m+1)M_1(G) + (m+n-4)F(G) - \chi_3(G) - M_1^2(G) - 16m^2 - 8m$

(2) $\overline{\sigma}(T_{++-}(G)) = 2EM_2(G) + 2(n-2)EM_1(G) + 2(m - 2n + 12)M_2(G) + 4(3n - m - 11)M_1(G) + (m - 2n + 12)F(G) - \chi_3(G) - M_1^2(G) + 2m^3 - 4m^2 n + 16m^2 + 2mn^2 - 24mn + 56m$

(3) $\overline{\sigma}(T_{+-+}(G)) = 2\overline{EM_2}(G) - 2(m+1)\overline{EM_1}(G) + \chi_3(G) - M_1^2(G) + (2n - 4m - 18)M_2(G) + (2m^2 + 32m - 2mn + 38 - 2n)M_1(G) + (n - 2m - 21)F(G) + m^3 n - 14m^3 + 6m^2 n - 64m^2 + 9mn - 26m$

(4) $\overline{\sigma}(T_{-++}(G)) = 2EM_2(G) + 4EM_1(G) + 2(m+n)M_2(G) - 2n(n-3)M_1(G) + (m+n)F(G) - \chi_3(G) - M_1^2(G) + mn(n-1)^2 - 2m(n^2 - 2n + 5)$

(5) $\overline{\sigma}(T_{---}(G)) = \sigma(T_{+++}(G))$

(6) $\overline{\sigma}(T_{--+}(G)) = \sigma(T_{++-}(G))$

(7) $\overline{\sigma}(T_{-+-}(G)) = \sigma(T_{+-+}(G))$

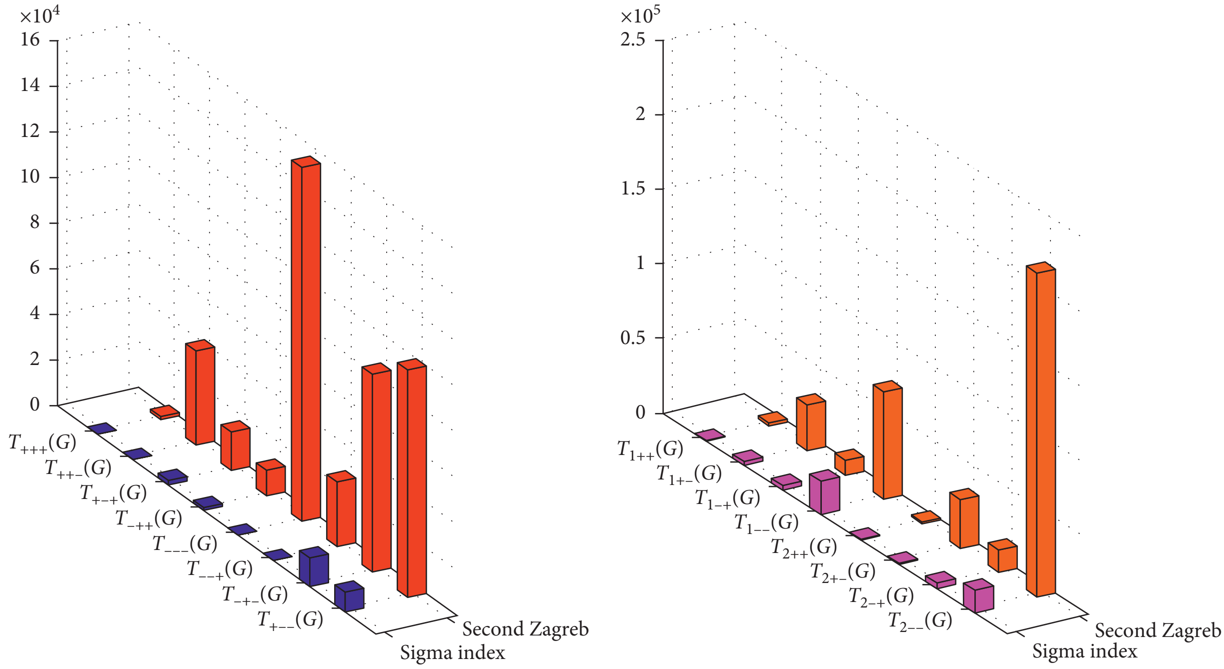
(8) $\overline{\sigma}(T_{+--}(G)) = \sigma(T_{-++}(G))$

The following theorems give the exact expressions of the sigma index of type-I and type-II semitransformations.

**Theorem 14.** *Let G be graph with n and m as its order and size, respectively. Then,*

(1) $\sigma(T_{1++}(G)) = 8F(G) - 8M_1(G) - 8M_2(G) + 8m$

(2) $\sigma(T_{1+-}(G)) = nm^3 + m(n-2)^3 - 2m^3 - 2m^2(n-2)^2$




(a) (b)

Figure 5: (a) Total transformation of the second Zagreb and sigma indices; (b) semitransformation of second the Zagreb and sigma indices.

(3) $\sigma(T_{1-+}(G)) = 2m(n-1)^2 - 8m(n-1) + 8m$

(4) $\sigma(T_{1--}(G)) = 4(m+n-1)\overline{M_1}(G) - 8F(G) + 4(3m+2n-1)M_1(G) - 8\overline{M_2}(G) + m^3n - 8mn^2 - 6m^2n + 17mn - 10m^3 - 4m^2 - 10m$

(5) $\overline{\sigma}(T_{1++}(G)) = 4(m+n+2)M_1(G) + 8M_2(G) - 8F(G) - 4m(8m-n+2)$

(6) $\overline{\sigma}(T_{1+-}(G)) = 2m^2(m-2n+4) + 2mn(n-4) + 8m$

(7) $\overline{\sigma}(T_{1-+}(G)) = mn^3 - 8mn^2 + 21mn - 18m$

(8) $\overline{\sigma}(T_{1--}(G)) = 8F(G) - 4(2m+n-1)M_1(G) - 4(m+n-1)\overline{M_1}(G) + 8\overline{M_2}(G) + 2m^2(m+4n-10) + 2m(4n^2-8n+5)$

**Theorem 15.** *Let G be graph with n and m as its order and size, respectively. Then,*

(1) $\sigma(T_{2++}(G)) = \chi_3(G) - 2EM_2(G) - 4EM_1(G) - 4M_2(G) - 4M_1(G) - F(G) + 8m$

(2) $\sigma(T_{2+-}(G)) = \chi_3(G) + 3(n-5)F(G) + 2(3n-14)M_2(G) + (2n^2 - 2mn + 11m - 22n + 52)M_1(G) - 2EM_2(G) - 2(n-2)EM_1(G) + m^3n + mn^3 - 6m^3 - 2m^2n^2 + 16m^2n - 10mn^2 - 32m^2 + 40mn - 56m$

(3) $\sigma(T_{2-+}(G)) = 2(m+1)\overline{EM_1}(G) - 2\overline{EM_2}(G) - (2m^2 + 18m + 32)M_1(G) + 3(m+4)F(G) + 2(3m+11)M_2(G) - \chi_3(G) + 6m^3 + 24m^2 + 26m$

(4) $\sigma(T_{2--}(G)) = 2(m+n-3)\overline{EM_1}(G) - 2\overline{EM_2}(G) - (2m^2 + 2mn + 2n^2 + 7m + 2n - 8)M_1(G) + (3m+3n-2)F(G) + (6m+6n-2)M_2(G) - \chi_3(G) + 4m^3 + mn^3 - 4mn^2 + 8m^2n + 9mn - 8m^2 - 10m$

(5) $\overline{\sigma}(T_{2++}(G)) = 2EM_2(G) + 4EM_1(G) - (3m-n-4)M_1(G) - M_1^2(G) + (m+n+1)F(G) + 2(m+n+2)M_2(G) - \chi_3(G) - 4m^2 - 8m$

(6) $\overline{\sigma}(T_{2+-}(G)) = 2EM_2(G) + 2(n-2)EM_1(G) - M_1^2(G) - \chi_3(G) + (15n - 6m - 52)M_1(G) + (2m - 4n + 28)M_2(G) + (m - 2n + 15)F(G) + 2m^3 - 4m^2n + 12m^2 + 2mn^2 - 24mn + 56m$

(7) $\overline{\sigma}(T_{2-+}(G)) = 2\overline{EM_2}(G) - 2(m+1)\overline{EM_1}(G) - M_1^2(G) + \chi_3(G) + (2m^2 - 2mn + 23m - 5n + 32)M_1(G) - 2(2m-n+11)M_2(G) - (2m-n+12)F(G) + m^3n - 10m^3 + 6m^2n - 40m^2 + 9mn - 26m$

(8) $\overline{\sigma}(T_{2--}(G)) = 2\overline{EM_2}(G) - 2(m+n-3)\overline{EM_1}(G) + \chi_3(G) - M_1^2(G) + (2m^2 + 2mn + 4m + 5n - 8)M_1(G) - 2(2m+2n-1)M_2(G) - 2(m+n-1)F(G) - 4m^3 - 4m^2n + 2mn^2 - 8mn + 10m$

## 4. Results and Discussion

The various expressions for the Zagreb and sigma topological indices computed here can be extremely useful in the thermodynamic properties such as the heat of formation and entropy for the structure-property predictions of the transformation of molecular materials when combined with total and semitype transformations. Since the enumeration and construction of different structures under given specific constraints have found potential applications in drug discovery via topological indices [40, 41], it can help the chemists by reducing the number of potential drug compounds that need to be experimentally considered. We computed expressions based on the degree measures of the given graph, and hence it can be considered as an efficient technique for vibrational spectroscopic chemical analysis through the vertex partitioning and providing significant simplifications in the vibrational mode analysis. Moreover, sigma indices obtained here offer the regularity perfection of the structure.

The semi and total transformation considered here provide 16 classes of new structures for the given graph based on the edge adjacency and incidence relations. Once we compute the topological indices such as Zagreb, reformulated Zagreb, forgotten, sum-connectivity, and sigma for the base graph and then using the results from Theorems 1–15 , one can readily obtain the Zagreb and sigma indices for the new structures.

We now present the applications of our computed results for perhydrophenalene. The molecular graph of perhydrophenalene $G$ is shown in Figure 4 and has 13 vertices and 15 edges. Moreover, $G$ has 9 vertices of degree 2 and 4 vertices of degree 3. Clearly, the edge partition of $G$ has three classes based on the degree of end vertices, namely, $(2,2)$, $(2,3)$, and $(3,3)$ while the number of edges in the classes, respectively, are 6, 6, and 3.

From the above data, one can easily derive $M_1(G) = 72$, $M_2(G) = 87$, $EM_1(G) = 126$, $EM_2(G) = 195$, $F(G) = 180$, $\overline{EM_1}(G) = 462$, $\overline{EM_2}(G) = 624$, $\overline{M_1}(G) = 288$, $\overline{M_2}(G) = 327$, $\chi_2(G) = 354$, and $\chi_3(G) = 1782$. Then, the calculations of second Zagreb and sigma indices of total and semitransformations of $G$ are obtained from Theorems 1–15 and presented in Tables 2 and 3, respectively. These values are compared graphically and depicted in Figure 5.

In the case of the second Zagreb index of the molecular graph $G$ of perhydrophenalene, we infer that $M_2(T_{+++}(G)) \le M_2(T_{-++}(G)) \le M_2(T_{+-+}(G)) \le M_2(T_{--+}(G)) \le M_2(T_{++-}(G)) \le M_2(T_{-+-}(G)) \le M_2(T_{+--}(G)) \le M_2(T_{---}(G))$ and $M_2(T_{1++}(G)) \le M_2(T_{2++}(G)) \le M_2(T_{1-+}(G)) \le M_2(T_{2-+}(G)) \le M_2(T_{1+-}(G)) \le M_2(T_{2+-}(G)) \le M_2(T_{1--}(G)) \le M_2(T_{2--}(G))$.

On the other side, for the sigma index, we observe that $\sigma(T_{+++}(G)) \le \sigma(T_{++-}(G)) \le \sigma(T_{---}(G)) \le \sigma(T_{--+}(G)) \le \sigma(T_{-++}(G)) \le \sigma(T_{+-+}(G)) \le \sigma(T_{+--}(G)) \le \sigma(T_{-+-}(G))$ and $\sigma(T_{2++}(G)) \le \sigma(T_{1++}(G)) \le \sigma(T_{2+-}(G)) \le \sigma(T_{1+-}(G)) \le \sigma(T_{1-+}(G)) \le \sigma(T_{2-+}(G)) \le \sigma(T_{2--}(G)) \le \sigma(T_{1--}(G))$.

## 5. Conclusion

The topological characterization of graphs and their transformations has been discussed in many research papers, in particular to Zagreb indices. Unfortunately, we have noticed the study on the second Zagreb index in total transformation graphs with some technical failures such as missing out edge degree-based indices and giving incorrect expressions. In this paper, we made a detailed study and derived the exact analytic expressions by incorporating reformulated Zagreb indices. As a byproduct, we have derived the sigma index of transformation graphs effectively using the forgotten index, and in addition, we have considered all possible semitransformations. The locus of this work will be definitely useful in computing other pending topological indices which are not computed for total transformation of graphs.

## Data Availability

The data used to support the findings of this study are included within paper.

## Conflicts of Interest

The authors declare that they have no conflicts of interest.

## Authors' Contributions

M.A., S.P., and M.A.J. conceptualized the study; M.A. and S.P. investigated the study; S.P. and M.A.J. prepared the original draft; M.A. and S.P. reviewed and edited the manuscript; Z.Y., M.A., and J.-B.L. supervised the study; and Z.Y. was responsible for funding acquisition.

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