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Article

A Unified Approach for Extremal General Exponential Multiplicative Zagreb Indices

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Abstract: The study of the maximum and minimal characteristics of graphs is the focus of the significant field of mathematics known as extreme graph theory. Finding the biggest or smallest graphs that meet specified criteria is the main goal of this discipline. There are several applications of extremal graph theory in various fields, including computer science, physics, and chemistry. Some of the important applications include: Computer networking, social networking, chemistry and physics as well. Recently, in 2021 exponential multiplicative Zagreb indices were introduced. In generalization, we introduce the generalized form of exponential multiplicative Zagreb indices for $\alpha \in \mathbb{R}^+ \setminus \{1\}$. Furthermore, to see the behaviour of generalized first and second exponential Zagreb indices for $\alpha \in \mathbb{R}^+ \setminus \{1\}$, we used a transformation method. In term of the two newly developed generalized exponential multiplicative Zagreb indices, we will investigate the extremal bicyclic, uni-cyclic and trees graphs. Four graph transformations are used and some bounds are presented in terms of generalized exponential multiplicative Zagreb indices.

Keywords: extremal graphs; first and second generalized exponential multiplicative Zagreb indices; unified approach; graph transformations

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1. Introduction

Let G be a simple and connected graph and $V(G)$ and $E(G)$ be the vertex set and the edge set of G, respectively. The number of elements of $V(G)$ and $E(G)$ is known as the order and size of G. The number of edges which are incident to vertex v in G is called the degree of the vertex v and it is denoted by $d_G(v)$. The set of adjacent vertices of a vertex v in G is known as the neighborhood of the vertex v in G and it is denoted by $N_G(v)$. If $d_G(v) = 1$, then v is called a pendant vertex. Consider Q as a subset of $V(G)$, such that $G - Q$ is a new graph constructed by deleting the vertices of Q from $V(G)$ in G together with their incident edges. C_n, S_n, and P_n characterize the star, cycle, and path graphs of order n, respectively. If every vertex on a path is of degree two or more, then it is known as an internal path, otherwise it is known as a pendant path. When $n+1$, n, $n-1$ are the size of a graph of order n, respectively, they are called bicyclic, unicyclic, and tree graphs [1–5]. The study of the maximum and minimal characteristics of graphs is the focus of the significant field of mathematics known as extreme graph theory. Finding the largest or smallest graphs that meet specified criteria is the main goal of this discipline. There are several applications of extremal graph theory in various fields, including computer science, physics, and chemistry. Some of the important applications include: Extremal graph theory has several uses in computer science, particularly in the creation and evaluation of algorithms. One well-known problem in extremal graph theory is the maximum clique problem, which asks for the largest complete subgraph in a graph. Social Networks: Extremal graph theory may be used to examine the structure of social networks. Social networks can be modeled as graphs. For instance, research on graph density and the maximum number of edges in a graph might shed light on how social networks are connected [6–8]. In chemistry: Extremal graph theory is used to comprehend the structure of molecules. Molecular graphs can be modeled as graphs. A graph's maximum number of edges, for instance, can be used to forecast a molecule's stability [9–11]. In physics: Extremal graph theory may be used to examine the structure of physical systems that are commonly represented using graphs. For instance, it is possible to forecast the critical temperature of a physical system using the maximum number of edges in a graph [12–14].

As a result, extremal graph theory is a crucial branch of mathematics with several applications. Insights into the structure of complex systems may be gained via the study of maximum and minimum features of graphs, which can then be used to create and analyse algorithms, forecast the stability of molecules, and comprehend the interconnection of social networks.

A mathematical tool used for the modeling of biological, toxicological, pharmacologic, physicochemical, and some relevant properties of chemical compounds, this tool is formally known as a topological index or molecular structure descriptor, which is formally a branch of theoretical chemistry [15]. There exist several types of descriptors, but the main medium is a degree or distance of vertices or edges. After the introduction of the Zagreb index, many other versions of the Zagreb index were introduced, such as the multiplicative version of the Zagreb index which was introduced by [16,17]. The multiplicative Zagreb indices are defined as

$$\prod_1(G) = \prod_{v\in V(G)} d_G^2(v).$$

$$\prod_2(G) = \prod_{vu\in E(G)} [d_G(v) \times d_G(u)] = \prod_{z\in V(G)} \left[d_G(z)^{d_G(z)}\right].$$

It is becoming a trend to introduce new variants of the existing notions. For topological graph indices, the situation is no different. Recently, the exponential multiplicative Zagreb indices were introduced by [18], in 2021.

$$E\prod_1(G) = \prod_{v\in V(G)} e^{\left[d_G^2(v)\right]}.$$

$$E\prod_2(G) = \prod_{vu\in E(G)} \left[e^{[d_G(v)\times d_G(u)]}\right] = \prod_{z\in V(G)} \left[e^{\left[d_G(z)^{d_G(z)}\right]}\right]. \tag{1}$$

In [19], some exact formulations and bounds were presented in terms of topological indices, particularly the first Zagreb index, few inequalities for Zagreb index were computed in [20], some other results on the topological indices were found in [21–23]. Neighborhood first Zagreb index was introduced and its some properties were discussed in [24]. Steric effects in drug design by topological indices was discussed in [25]. The completed survey on Zagreb Indexes 30 years after its introduction was compiled by [20,26]. For more results on the Zagreb index, see [27–29]. A handbook of this mathematical tool can be found in [30], upper bounds of Zagreb indices in [31], and a discussion on the general Zagreb index in terms of unicyclic graphs is detailed in [32]. For some computational work of topological indices, see [33–37].

2. Contribution and Main Results

We introduce the generalization of exponential multiplicative Zagreb indices for $\alpha \in \mathbb{R}^+ \setminus \{1\}$, and formulated as:

$$E\prod_1^{\alpha}(G) = \prod_{v \in V(G)} e^{\left[d_G^{\alpha}(v)\right]} = \prod_{v \in V(G)} e^{[d_G(v)]^{\alpha}}.$$

$$E\prod_2^{\alpha}(G) = \prod_{vu \in E(G)} \left[e^{[d_G(v) \times d_G(u)]^{\alpha}}\right] = \prod_{z \in V(G)} \left[e^{\left[d_G(z)^{\alpha d_G(z)}\right]}\right], \tag{2}$$

where $E\prod_1^{\alpha}(G)$ is a generalized first exponential multiplicative Zagreb index. The $E\prod_2^{\alpha}(G)$ is a generalized second exponential multiplicative Zagreb index, and $d_G(z)$ is the degree of the vertex. For more detailed information on Zagreb indices and multiplicative Zagreb indices [38–41].

2.1. Main Results

In this section, we will investigate the first and second exponential multiplicative Zagreb indices which increase or decrease under some lemmas and graph transformations. After this, we will acquire our main proofs by using graph transformations.

Lemma 1. *For $\chi \geq 2$, and $\alpha > 1$ $f(\chi) = (\chi+1)^{\alpha(\chi+1)} - (\chi)^{\alpha(\chi)} - 4^{\alpha} + 1^{\alpha}$. The $f(\chi)$ is increasing function.*

Proof. Since, $f'(x) = \alpha(\chi+1)^{\alpha(\chi+1)}[1+\ln(\chi+1)] - \alpha(\chi)^{\alpha(\chi)}[1+\ln(\chi)] > 0$, result is hold. □

Transformation 2. *Suppose λ^* to be a simple and finite connected graph and $\eta = k_1k_2, \ldots, k_{t-1}k_t$ and $\zeta = l_1l_2, \ldots, l_{s-1}l_s$ be the two paths of length t and s, respectively. Assumed that u to be a vertex in λ^*, then λ_1^* and λ_2^* are two graphs obtain from λ^* such that $\lambda_1^* = \lambda^* + \{uk_1, k_1k_2, \ldots, k_{t-1}k_t\} + \{ul_1, l_1l_2, \ldots, l_{s-1}l_s\}$, and $\lambda_2^* = \lambda^* + \{uk_1, \ldots, k_{t-1}k_t\} + \{k_tl_1, \ldots, l_{s-1}l_s\}$, respectively. The graphs λ_1^* and λ_2^* are shown in Figure 1.*

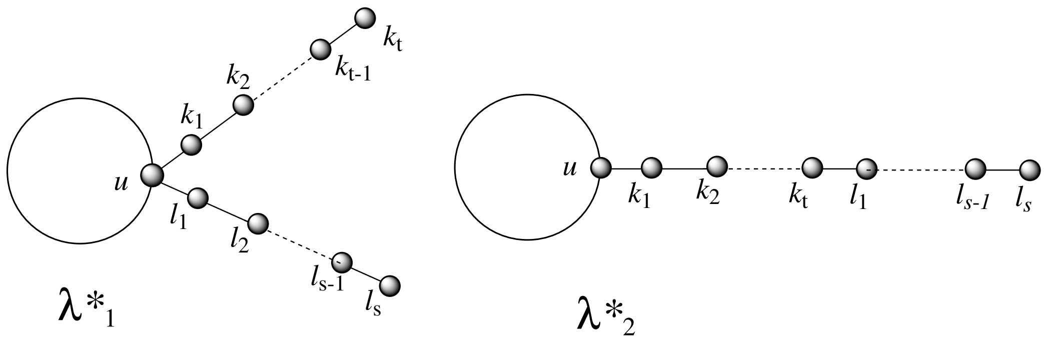


Figure 1. Depiction of transformation 2.

Lemma 3. *Consider that the two graphs λ_1^* and λ_2^* are defined in the above transformation. For $\alpha > 1$, we have*

$$(i) \qquad E\Pi_1^{\alpha}(\lambda_1^*) > E\Pi_1^{\alpha}(\lambda_2^*)$$
$$(ii) \qquad E\Pi_2^{\alpha}(\lambda_1^*) > E\Pi_2^{\alpha}(\lambda_2^*)$$

Proof. Let $d_{\lambda^*}(u) = p \geq 1$. Consider that $d_{\lambda_1^*}(u) = p+2$ and $d_{\lambda_2^*}(u) = p+1$. Then, from the formulation of the first general exponential multiplicative Zagreb indices, we have

$$\frac{E\Pi_1^\alpha(\lambda_2^*)}{E\Pi_1^\alpha(\lambda_1^*)} = \frac{e^{(p+1)^\alpha} e^{2^\alpha}}{e^{(p+2)^\alpha} e^{1^\alpha}} < 1.$$

Let $f(\chi) = (\chi)^{(\alpha)} - (\chi+1)^{(\alpha)} + 2^\alpha - 1$, and $f'(\chi) = \alpha(\chi)^{\alpha-1} - \alpha(\chi+1)^{\alpha-1} < 0$. Thus, $f(\chi)$ is a decreasing function, when $\chi \geq 2$ and $\alpha > 1$. Hence, (i) is true. Similarly, by using the formulation of the second general exponential multiplicative Zagreb indices and apply by Lemma 3, we have

$$\frac{E\Pi_2^\alpha(\lambda_1^*)}{E\Pi_2^\alpha(\lambda_2^*)} = \frac{e^{(p+2)^{\alpha(p+2)}} e^{1^\alpha}}{e^{(p+1)^{\alpha(p+1)}} e^{4^\alpha}} > 1$$

Hence, (ii) is true. □

Transformation 4. *Assuming K^* to be a non-trivial and connected graph, consider that vu and uv_j are the edges of the graph K^*, For $1 \leq j \leq d$, such that $d_{K^*}(v) \geq 2$ and $d_{K^*}(v_j) = 1$ for each j. We get a new graph ${K^*}_1$ from K^* by removing the edges uv_j and adding the edges vv_d for $1 \leq j \leq d$. The construction of ${K^*}_1$ from graph K^* is shown in Figure 2.*

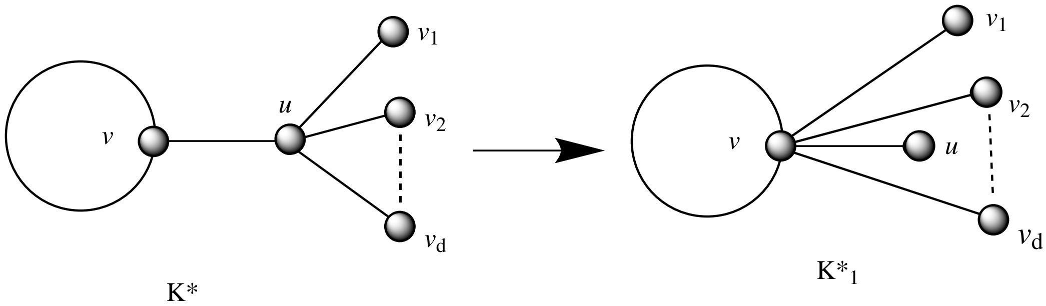


Figure 2. Depiction of transformation 4.

Lemma 5. *Consider K^* and ${K^*}_1$ tp be two graphs described in the transformation 4. We have*

$$\begin{array}{ll} (i) & E\Pi_1^\alpha(K^*) < E\Pi_1^\alpha(K_1^*) \\ (ii) & E\Pi_2^\alpha(K_1^*) > E\Pi_2^\alpha(K^*). \end{array}$$

Proof. Consider that the $d_{k^*}(v) = w+1 \geq 2$, then $d_{K_1^*}(v) = w+d+1$, where $w, d \geq 1$. By applying the formulation of first general exponential multiplicative Zagreb index. For $\alpha > 1$, we have

$$\frac{E\Pi_1^\alpha(K^*)}{E\Pi_1^\alpha(K_1^*)} = \frac{e^{(w+1)^\alpha} e^{(d+1)^\alpha}}{e^{(w+d+1)^\alpha} e^{1^\alpha}} < 1.$$

Let $f(\kappa, \xi) = (\kappa)^\alpha + (\xi)^\alpha - (\kappa+\xi-1)^\alpha - 1^\alpha$, and $f_\kappa(\kappa, \xi) = \alpha(\kappa)^{\alpha-1} - \alpha(\kappa+\xi-1)^{\alpha-1} < 0$, and also $f_\xi(\kappa, \xi) = \alpha(\xi)^{\alpha-1} - \alpha(\kappa+\xi-1)^{\alpha-1} < 0$. Thus, $f(\kappa, \xi)$ is a decreasing function, when $\{\kappa \geq 2, \xi \geq 2, \alpha > 1\}$. Implying that, $E\Pi_1^\alpha(K^*) < E\Pi_1^\alpha(K_1^*)$.

Now, according to the second general exponential multiplicative Zagreb index, also noted that $w, l \geq 1$. Then, we have

$$\frac{E\Pi_2^\alpha(K^*)}{E\Pi_2^\alpha(K_1^*)} = \frac{e^{(w+1)^{\alpha(w+1)}} e^{(d+1)^{\alpha(d+1)}}}{e^{(w+d+1)^{\alpha(w+d+1)}} e^{1^\alpha}} < 1.$$

Let $f(\kappa, \xi) = (\kappa+1)^{\alpha(\kappa+1)} + (\xi+1)^{\alpha(\xi+1)} - (\kappa+\xi+1)^{\alpha(\kappa+\xi+1)} - 1^\alpha$, and $f_\kappa(\kappa, \xi) = \alpha(\kappa+1)^{\alpha(\kappa+1)}[\ln(\kappa+1)+1] - \alpha(\kappa+\xi+1)^{\alpha(\kappa+\xi+1)}[\ln(\kappa+\xi+1)+1] < 0$. Moreover, $f_\xi(\kappa, \xi) =$

$\alpha(\xi+1)^{\alpha(\xi+1)}[\ln(\xi+1)+1] - \alpha(\kappa+\xi+1)^{\alpha(\kappa+\xi+1)}[\ln(\kappa+\xi+1)+1] < 0$. Thus $f(\kappa,\xi)$ is decreasing function, when $\{\kappa \geq 1, \xi \geq 1, \alpha > 1\}$. Implying that, $E\Pi_2^{\alpha}(K_1^*) > E\Pi_2^{\alpha}(K^*)$, this completes the proof. □

Transformation 6. *Let K_1 be a non-trivial and connected graph where w_1, w_2 are two vertices of K_1. Suppose that w_1y_i, w_2l_j, such that $1 \leq i \leq t$ and $1 \leq j \leq s$ are the edges of K_1 and $d_{K_1}(y_i)$= 1 = $d_{K_1}(l_J)$. Now we have derived two new graphs K_2 and K_3 from K_1, respectively. Such that $K_2 = K_1 - w_2l_j + w_1l_j$ for $1 \leq j \leq s$, $K_3 = K_1 - w_1y_i + w_2y_i$ for $1 \leq i \leq t$. The graphs K_2 and K_3 are shown in Figure 3.*

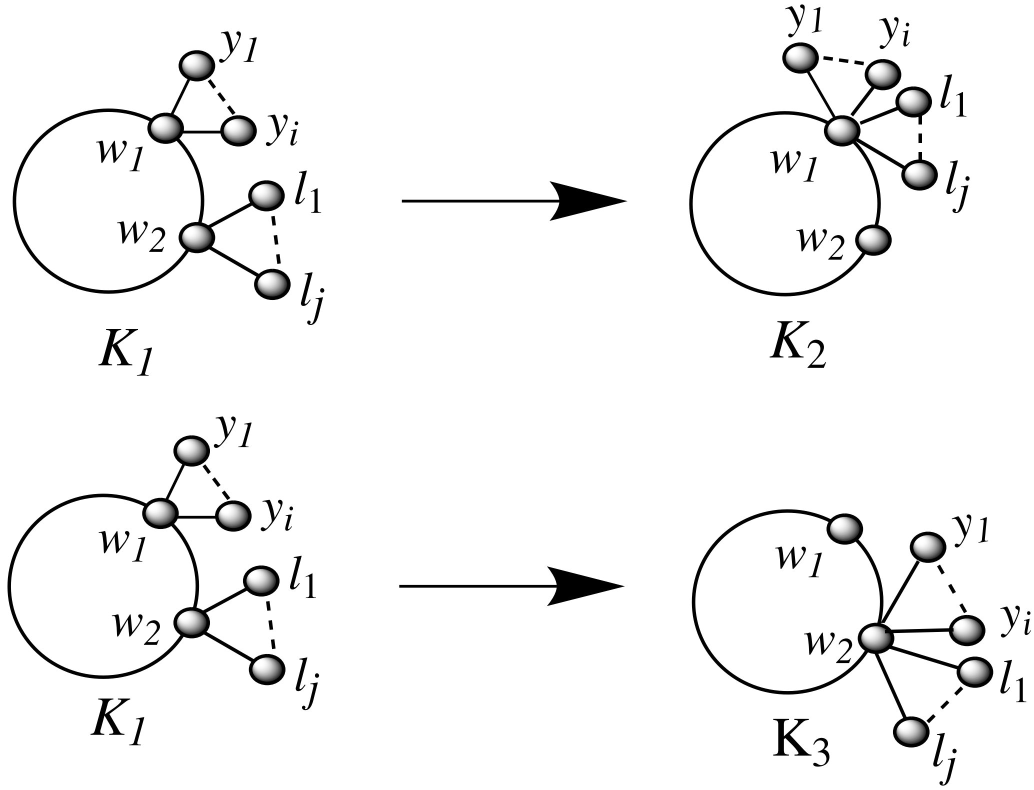


Figure 3. Depiction of transformation 6.

Lemma 7. *Consider three graphs are K_1, K_2 and K_3, as shown in Transformation 6. We have*

$$\begin{aligned}
(i). &\quad \text{either } E\Pi_1^{\alpha}(K_1) < E\Pi_1^{\alpha}(K_2) \\
&\quad \text{or } E\Pi_1^{\alpha}(K_1) < E\Pi_1^{\alpha}(K_3), \\
(ii). &\quad \text{either } E\Pi_2^{\alpha}(K_1) < E\Pi_2^{\alpha}(K_2) \\
&\quad \text{or } E\Pi_2^{\alpha}(K_1) < E\Pi_2^{\alpha}(K_3).
\end{aligned}$$

Proof. Assume that the degrees of vertices w_1 and w_2 are $d_{K_1}(w_1) = p + t$ and $d_{K_1}(w_2) = q + s$. Then, we have

$$\begin{aligned}
\frac{E\Pi_1^{\alpha}(K_1)}{E\Pi_1^{\alpha}(K_2)} =& \frac{e^{(p+t)^{\alpha}} e^{(q+s)^{\alpha}}}{e^{(p+t+s)^{\alpha}} e^{(q)^{\alpha}}}, \\
=& e^{(p+t)^{\alpha}+(q+s)^{\alpha}-(p+t+s)^{\alpha}-(q)^{\alpha}},
\end{aligned}$$

Note that, $p > t$, $q \geq 1$, $s \geq 1$, $q > p$, and $\alpha > 1$. Then, $E\Pi_1^{\alpha}(K_1) < E\Pi_1^{\alpha}(K_2)$. Similarly,

$$
\begin{aligned}
\frac{E\Pi_1^{\alpha}(K_1)}{E\Pi_1^{\alpha}(K_3)} =& \frac{e^{(q+s)^{\alpha}}e^{(p+t)^{\alpha}}}{e^{(q+t+s)^{\alpha}}e^{(p)^{\alpha}}}, \\
=& e^{(p+t)^{\alpha}+(q+s)^{\alpha}-(t+q+s)^{\alpha}-(p)^{\alpha}} < 1, if\ t > p
\end{aligned}
$$

In the following, we will prove (ii). Assume that $f(z) = (z)^{\alpha z}$, and $h(z) = \ln(f(z)) - \ln(f(r)) - \ln(f(z-r+1))$, where $z > r > 1$. Then, $h'(z) = \alpha\left[\ln\left(\frac{z}{z-r+1}\right)\right] > 0$, since $\alpha > 1$. Hence $h(z)$ is an increasing function, for $z > 0$. Moreover, $h'(r) < h(z)$, that is equal to $f(z) > f(r)f(z-r+1)$. Suppose that, $g_1 = \frac{E\Pi_2^{\alpha}(K_1)}{E\Pi_2^{\alpha}(K_2)}$, and

$$
\begin{aligned}
\frac{E\Pi_2^{\alpha}(K_1)}{E\Pi_2^{\alpha}(K_2)} =& \frac{e^{(p+t)^{\alpha(p+t)}}e^{(q+s)^{\alpha(q+s)}}}{e^{(p+t+s)^{\alpha(p+t+s)}}e^{(q)^{q}}}, \\
g_1 =& \frac{e^{(p+t)^{\alpha(p+t)}}e^{(q+s)^{\alpha(q+s)}}}{e^{(p+t+s)^{\alpha(p+t+s)}}e^{(q)^{\alpha q}}} \leq 1, \\
e^{(p+q)^{\alpha(p+q)}}e^{(t+s)^{\alpha(t+s)}} \leq& e^{(p+q+s)^{\alpha(p+q+s)}+(t)^{\alpha t}}.
\end{aligned} \tag{3}
$$

Now $g_2 = \frac{E\Pi_2^{\alpha}(K_1)}{E\Pi_2^{\alpha}(K_3)}$, and

$$
\begin{aligned}
\frac{E\Pi_2^{\alpha}(K_1)}{E\Pi_2^{\alpha}(K_3)} =& \frac{e^{(p+q)^{\alpha(p+q)}}e^{(t+s)^{\alpha(t+s)}}}{e^{(t+q+s)^{\alpha(t+q+s)}}e^{(p)^{\alpha p}}}, \\
g_2 =& \frac{e^{(p+q)^{\alpha(p+q)}}e^{(t+s)^{\alpha(t+s)}}}{e^{(t+q+s)^{\alpha(t+q+s)}}e^{(p)^{\alpha p}}} \leq 1.
\end{aligned}
$$

From Equation (3), we will get

$$
\begin{aligned}
g_2 \leq& e^{(p+q+s)^{\alpha(p+q+s)}+(t)^{\alpha(t)}-(t+q+s)^{\alpha(t+q+s)}-(p)^{\alpha(p)}}, \\
g_2 <& e^{(p+q+s)^{\alpha(p+q+s)}+(t)^{\alpha(t)}-(t+q+s)^{\alpha(t+q+s)}-(p)^{\alpha(p)}} < 1.
\end{aligned}
$$

Which implies that $E\Pi_2^{\alpha}(K_1) < E\Pi_2^{\alpha}(K_2) or$
$E\Pi_2^{\alpha}(K_1) < E\Pi_2^{\alpha}(K_3)$. □

Transformation 8. *Consider that a leaves path $Q = y_1y_2, \ldots, y_{q-1}y_q$ is attached to y_1 in graph H_1 and u_1 and u_2 are two neighbors of y_1 except of y_2. We obtain a new graph $H_2 = H_1 - y_1u_2 + y_qu_2$, from graph H_1. Moreover, the depiction shown in the Figure 4*

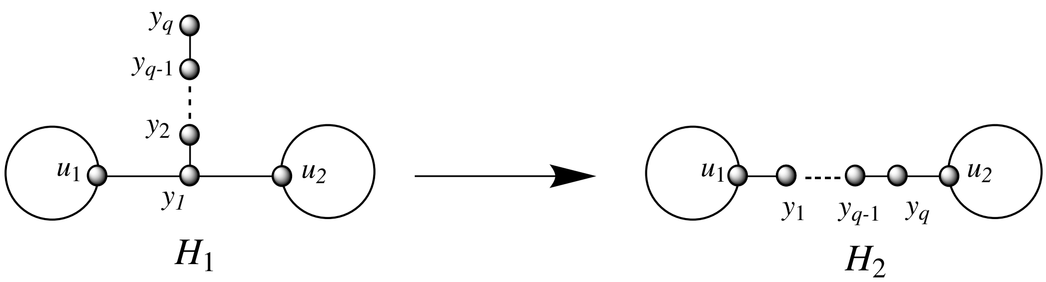


Figure 4. Depiction of transformation 8.

Lemma 9. *Let H_1 and H_2 be two graphs, which are described in the transformation 8. Then, for Π_1^α, also $\alpha > 1$ we have*

$$(i). \qquad E\Pi_1^\alpha(H_1) > E\Pi_1^\alpha(H_2),$$
$$(ii). \qquad E\Pi_2^\alpha(H_1) > E\Pi_2^\alpha(H_2).$$

Proof. By using the formulation of first and second exponential multiplicative Zagreb indices, we have

$$\frac{E\Pi_1^\alpha(H_1)}{E\Pi_1^\alpha(H_2)} = \frac{e^{(3)^\alpha}e^{(1)^\alpha}}{e^{(2)^\alpha}e^{(2)^\alpha}} > 1.$$

$$\frac{E\Pi_2^\alpha(H_1)}{E\Pi_2^\alpha(H_2)} = \frac{e^{(3)^{3\alpha}}e^{(1)^{1\alpha}}}{e^{(2)^{2\alpha}}e^{(2)^{2\alpha}}} > 1$$

both inequalities are true. Hence complete the proof of Lemma 9. □

2.2. Extremal Trees and Unicyclic Graphs with Respect to First and Second Exponential Multiplicative Zagreb Indices

In this part of paper, we present the extremal trees, unicylic graphs by using the above discussed transformations, for the first and second general exponential multiplicative Zagreb indices, for $\alpha > 1$.

Theorem 10. *Let T be a tree with order $n \geq 5$. Then, for $\alpha > 1$ we have*

$$(i). \qquad E\Pi_1^\alpha(P_n) < E\Pi_1^\alpha(T) < E\Pi_1^\alpha(S_n),$$
$$(ii). \qquad E\Pi_2^\alpha(S_n) > E\Pi_2^\alpha(T) > E\Pi_2^\alpha(P_n).$$

Proof. Suppose that two trees T and T^* have an order n and k, respectively. When T^* hooked up with a vertex of T. By using the transformation 2, we create a path graph P_{k+1} from T^*, during this process Lemma 3 affirms that $E\Pi_1^\alpha$ and $E\Pi_2^\alpha$ are minimal for the path graph. Now, by repeating the Transformation 4, we affixed a tree to a vertex T^*, and we obtain a new graph T_{k+1}. By using the Transformation 4 and Lemma 5, provided that the first and second exponential multiplicative Zagreb indices increase, the Star graph gives the maximal $E\Pi_1^\alpha$ and $E\Pi_2^\alpha$.

Hence this proof is completed. □

Let C_n^q be a unicyclic graph is obtaining by affixing $(n-q)$ leaves to one vertex of C_q.

Theorem 11. *Let G be an unicyclic graphs with order n and girth $l \geq 3$. Then for $E\Pi_1^\alpha$ and $E\Pi_2^\alpha$, we have*

$$(i). \qquad E\Pi_1^\alpha(C_n^q) \leq E\Pi_1^\alpha(C_n^3),$$
$$(ii). \qquad E\Pi_2^\alpha(C_n^q) \leq E\Pi_2^\alpha(C_n^3).$$

it is hold when $G = C_n^3$.

Proof. Consider that H is a unicyclic graph with order and girth n and q. By repeating the Transformation 4 and 6, the graph is converted into a unicyclic graph so that every pendant vertices are neighbors to one vertex of H. Lemma 5 and 7 implies that during this process of applying the Transformation 4 and 6, $E\Pi_1^\alpha$ and $E\Pi_2^\alpha$ increases.

Now, we will prove (i) and (ii). We need to compare the $E\Pi_1^\alpha$ and $E\Pi_2^\alpha$ of (C_n^q) and (C_n^3).

$$\frac{E\Pi_1^\alpha(C_n^q)}{E\Pi_1^\alpha(C_n^3)} = \frac{e^{(n-q+2)^{(\alpha)}+n-q+2^{\alpha(q-1)}}}{e^{(n-3)1^{(\alpha)}+(n-1)^\alpha+4^\alpha}} < 1.$$

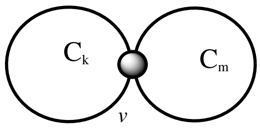
Since, $f(\xi) = (n-\xi+2)^\alpha + 2^{\alpha(\xi-1)} + 3 - \xi - (n-1)^\alpha - 4^\alpha$ is an increasing function, as $f'(\xi) = -\alpha(n-\xi+2)^{\alpha-1} + \alpha(\xi-1)2^{\alpha(xi-1)}log2 - 1 > 0$, when $n-1 > \xi > 3$.

$$\begin{aligned}\frac{E\Pi_1^\alpha(C_n^{n-1})}{E\Pi_1^\alpha(C_n^3)} =& \frac{e^{(3)^{(\alpha)}+1^\alpha+2^{\alpha(n-2)}}}{e^{(n-3)1^{(\alpha)}+(n-1)^\alpha+4^\alpha}} > 1.\\ \frac{E\Pi_2(C_n^q)}{E\Pi_2(C_n^3)} =& \frac{e^{(n-q+2)^{\alpha(n-q+2)}+2^{\alpha(q-1)}}}{e^{(n-1)^{\alpha(n-1)}+4^\alpha+4^\alpha}},\\ =& e^{(n-q+2)^{\alpha(n-q+2)}-(n-1)^{\alpha(n-1)}+2^{\alpha(q-1)}-16^\alpha} < 1.\end{aligned}$$

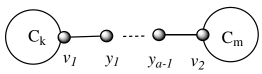
Let $f(y) = (n-y+2)^{\alpha(n-y+2)} - (n-1)^{\alpha(n-1)} - 16^\alpha + 2^{\alpha(y-1)}$, for $y \geq 3$. Then, $f'(y) = \alpha(n-y+2)^{\alpha(n-y+2)}[-\ln(n-y+2) - 1] + \alpha 2^{\alpha(y-1)}.\ln 2 < 0$. So, it is a decreasing function. Hence, both (i) and (ii) are true. The proof is completed. □

2.3. Extremal Bicyclic Graphs with Respect to First and Second Exponential Multiplicative Zagreb Indices

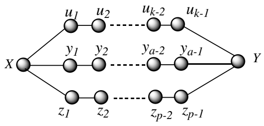
In this section, we will present the extremal bicyclic graphs for the first and second exponential multiplicative Zagreb indices. Let $B(n)$ is the bicyclic graph of order n and the types of the $B(n)$ graphs listed below in the Figure 5d.



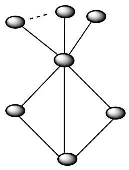
(a) $C_{k,m}$



(b) $C_{k,d,m}$



(c) $C_{k,m}^d$



(d) B_k^*

Figure 5. Bicyclic graphs.

$$\begin{aligned}E\Pi_1^\alpha(B_k^*) =& e^{2(2)^\alpha+3^\alpha+(n-1)^\alpha+(n-4)1^\alpha},\\ E\Pi_2^\alpha(B_k^*) =& e^{(n-4)} + (27)^\alpha + (n-1)^{\alpha(n-1)} + 2(4)^\alpha.\end{aligned}$$

Transformation 12. *Let $R = ut_1, \ldots, t_c v$ be an internal path of G_1 and $d_{G_1}(u), d_{G_1}(v) \geq 2$. We obtained a new graph $G_2 = G_1 - \{t_2t_3, \ldots, t_{c-1}tc\} + \{t_1t_3, t_1t_4, \ldots, t_1t_c\}$, from G_1 which is shown in Figure 6.*

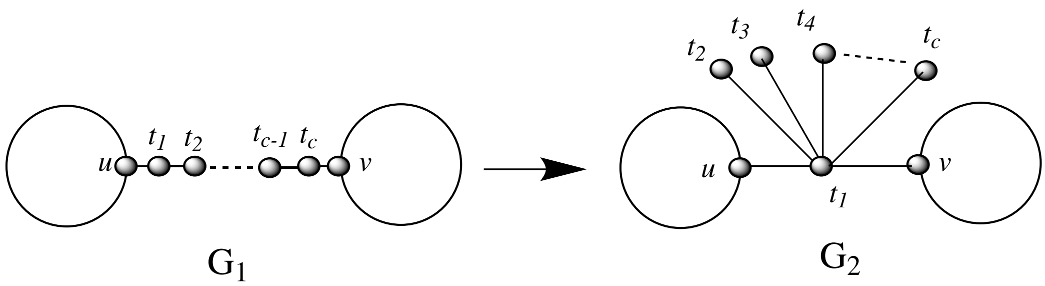


Figure 6. Depiction of Transformation 12.

Lemma 13. *consider that the two graphs G_1 and G_2 show in Transformation 12. Then, for $\alpha > 1$ we have*

$$(i). \qquad E\Pi_1^{\alpha}(G_1) < E\Pi_1^{\alpha}(G_2),$$
$$(ii). \qquad E\Pi_1(G_1) < E\Pi_1(G_2).$$

Proof. From Lemmas 5 and 9, both inequalities are true. Hence complete the proof. □

Theorem 14. *Let G be a bicyclic graph of order $n \geq 4$. For $\alpha > 1$, we have to define,*

$$(i). \qquad E\Pi_1^{\alpha}(G) < E\Pi_1^{\alpha}(B_k^*),$$
$$(ii). \qquad E\Pi_2^{\alpha}(G) < E\Pi_2^{\alpha}(B_k^*).$$

Proof. It is true for $n = 4, 5$. Now, we will discuss for $n \geq 6$.
(i) : Let K^* be a bicyclic graph having larger $E\Pi_1^{\alpha}$ and $E\Pi_2^{\alpha}$. Suppose that B_k is the main subgraph of K^*. Then B_k is either types (a), (b) or (c). By repeating the Transformation 4 and 6. We can get a new graph K^*, such that some leaves, which are neighbors to one vertex of subgraph B_k.

Claim: The maximum length of any cycle in K^* is 4. Contrarily, assume that the length of cycle in K^* is 5. If the main subgraph of B_k is one of the type (a) or (b), then applying the Transformation 12 and Lemma 13, we can obtain a bicyclic graph with greater $E\Pi_1^{\alpha}$ and $E\Pi_2^{\alpha}$. Which is a contradiction.

Now, we assume that graph K^* is a type of (c), $B_k = C_{q,m}^d$ with $1 \leq d \leq min\{q, m\}$ and $q + m > 5$ such that q or m is not less than 3, K^* contains an intrinsic path of length at least 2 in B_k. Using the 5 and 13, we derive a new bicyclic graph K^{**} from graph K^* which shows $E\Pi_1^{\alpha}(K^{**}) > E\Pi_1^{\alpha}(K^*)$, and also $E\Pi_2^{\alpha}(K^{**}) > E\Pi_2^{\alpha}(K^*)$. Which is contradicting.

Now, from claim 1, the length of any cycle in B_k is 3 or 4. Clearly, this shows that $B_k \in \left\{C_{3,3}, C_{3,d,3}, C_{2,2}^d\right\}$. We assert that, if d is one in $B_k = C_{3,d,3}$ then is one of type b, otherwise Lemmas 5 and 9, confirmed that we can get a new, n-order bicyclic graph having the larger $E\Pi_1^{\alpha}$ and $E\Pi_2^{\alpha}$.

We construct new bicyclic graphs from $C_{3,3}$, $C_{3,d,3}$ **and** $C_{2,2}^d$.
(i)—$C_{3,3}^*$ derived from $C_{3,3}$ by affixing $(n-5)$ leaves to a degree two vertex.
(ii)—$C_{3,3}^{**}$ derived from $C_{3,3}$ by affixing n-5 leaves to a degree three vertex .
(iii)—$C_{3,1,3}^*$ derived from $C_{3,1,3}$ by affixing n-6 leaves to a degree two vertex.
(iv)—$C_{3,1,3}^{**}$ produced from $C_{3,1,3}$ by affixing n-6 leaves to a degree three vertex.
(v)—$C_{2,2}^{1*}$ derived from $C_{2,2}^1$ by affixing n-4 leaves to a degree two vertex.
The values of the above discussed graphs for the $E\Pi_1^{\alpha}$. Then, for $\alpha > 1$, we have

$$
\begin{aligned}
E\Pi_1^{\alpha}(C_{3,3}^{*}) &= e^{3(2)^{\alpha}}.e^{2(3)^{\alpha}}.e^{(n-3)^{\alpha}}.e^{(n-5)}, \\
E\Pi_1^{\alpha}(C_{3,3}^{*}) &= e^{(n-3)^{\alpha}+3(2)^{\alpha}+2(3)^{\alpha}+(n-5)}. \\
E\Pi_1^{\alpha}(C_{3,3}^{**}) &= e^{4(2)^{\alpha}}.e^{(3)^{\alpha}}.e^{(n-2)^{\alpha}}.e^{(n-5)}, \\
E\Pi_1^{\alpha}(C_{3,3}^{**}) &= e^{(n-2)^{\alpha}+4(2)^{\alpha}+(3)^{\alpha}+(n-5)}. \\
E\Pi_1^{\alpha}(C_{3,1,3}^{*}) &= e^{3(2)^{\alpha}}.e^{2(3)^{\alpha}}.e^{(n-4)^{\alpha}}.e^{(n-6)}, \\
E\Pi_1^{\alpha}(C_{3,1,3}^{*}) &= e^{(n-4)^{\alpha}+3(2)^{\alpha}+2(3)^{\alpha}+(n-6)}. \\
E\Pi_1^{\alpha}(C_{3,1,3}^{**}) &= e^{4(2)^{\alpha}}.e^{(3)^{\alpha}}.e^{(n-3)^{\alpha}}.e^{(n-6)}, \\
E\Pi_1^{\alpha}(C_{3,1,3}^{**}) &= e^{(n-3)^{\alpha}+4(2)^{\alpha}+(3)^{\alpha}+(n-6)}. \\
E\Pi_1^{\alpha}(C_{2,2}^{1*}) &= e^{3(2)^{\alpha}}.e^{2(3)^{\alpha}}.e^{(n-2)^{\alpha}}.e^{(n-4)}, \\
E\Pi_1^{\alpha}(C_{2,2}^{1*}) &= e^{(n-2)^{(\alpha)}+3(2)^{\alpha}+2(3)^{\alpha}+(n-4)}.
\end{aligned}
$$

In the following, the value of bicyclic graphs with respect to the second general exponential multiplicative Zagreb index.

$$
\begin{aligned}
E\Pi_2^{\alpha}(C_{3,3}^{*}) &= e^{3(2)^{2\alpha}}.e^{2(3)^{3\alpha}}.e^{(n-3)^{\alpha(n-3)}}.e^{(n-5)}, \\
E\Pi_2^{\alpha}(C_{3,3}^{*}) &= e^{(n-3)^{\alpha(n-3)}+3(4)^{\alpha}+2(27)^{\alpha}+(n-5)}. \\
E\Pi_2^{\alpha}(C_{3,3}^{**}) &= e^{4(2)^{2\alpha}}.e^{(3)^{3\alpha}}.e^{(n-2)^{\alpha(n-2)}}.e^{(n-5)}, \\
E\Pi_2^{\alpha}(C_{3,3}^{**}) &= e^{(n-2)^{\alpha(n-2)}+4(4)^{\alpha}+(27)^{\alpha}+(n-5)}. \\
E\Pi_2^{\alpha}(C_{3,1,3}^{*}) &= e^{3(2)^{2\alpha}}.e^{2(3)^{3\alpha}}.e^{(n-4)^{\alpha(n-4)}}.e^{(n-6)}, \\
E\Pi_2^{\alpha}(C_{3,1,3}^{*}) &= e^{(n-4)^{(\alpha n-4)}+3(4)^{\alpha}+2(27)^{\alpha}+(n-6)}. \\
E\Pi_2^{\alpha}(C_{3,1,3}^{**}) &= e^{4(2)^{2\alpha}}.e^{(3)^{3\alpha}}.e^{(n-3)^{\alpha(n-3)}}.e^{(n-6)}, \\
E\Pi_2^{\alpha}(C_{3,1,3}^{**}) &= e^{(n-3)^{\alpha(n-3)}+4(4)^{\alpha}+27^{\alpha}+(n-6)}. \\
E\Pi_2^{\alpha}(C_{2,2}^{1*}) &= e^{3(2)^{2\alpha}}.e^{2(3)^{3\alpha}}.e^{(n-2)^{\alpha(n-2)}}.e^{(n-4)}, \\
E\Pi_2^{\alpha}(C_{2,2}^{1*}) &= e^{(n-2)^{\alpha(n-2)}+3(4)^{\alpha}+2(27)^{\alpha}+(n-4)}.
\end{aligned}
$$

Below are the comparisons between the B_k^* and the above discussed type of bicyclic graphs for Π_1^{α} and Π_2^{α}. For $\alpha > 1$, we have

$$
\begin{aligned}
\frac{E\Pi_1^{\alpha}(B_k^*)}{E\Pi_1^{\alpha}(c_{3,3}^{*})} &= \frac{e^{(n-1)^{\alpha}+2(2)^{\alpha}+3^{\alpha}+n-4}}{e^{(n-3)^{\alpha}+3(2)^{\alpha}+2(3)^{\alpha}+n-5}}, \\
&= e^{(n-1)^{\alpha}-(n-3)^{\alpha}-2^{\alpha}-3^{\alpha}+1} > 1. \\
\frac{E\Pi_1^{\alpha}(B_k^*)}{E\Pi_1^{\alpha}(c_{3,3}^{**})} &= \frac{e^{(n-1)^{\alpha}+2(2)^{\alpha}+3^{\alpha}+n-4}}{e^{(n-2)^{(\alpha)}+4(2)^{\alpha}+(3)^{\alpha}+n-5}} > 1. \\
\frac{E\Pi_1^{\alpha}(B_k^*)}{E\Pi_1^{\alpha}(c_{3,1,3}^{*})} &= \frac{e^{(n-1)^{\alpha}+2(2)^{\alpha}+3^{\alpha}+n-4}}{e^{(n-4)^{(\alpha)}+3(2)^{\alpha}+2(3)^{\alpha}+n-6}} > 1. \\
\frac{E\Pi_1^{\alpha}(B_k^*)}{E\Pi_1^{\alpha}(c_{3,1,3}^{**})} &= \frac{e^{(n-1)^{\alpha}+2(2)^{\alpha}+3^{\alpha}+n-4}}{e^{(n-3)^{(\alpha)}+4(2)^{\alpha}+(3)^{\alpha}+n-6}} > 1. \\
\frac{E\Pi_1^{\alpha}(B_k^*)}{E\Pi_1^{\alpha}(c_{2,2}^{1*})} &= \frac{e^{(n-1)^{\alpha}+2(2)^{\alpha}+3^{\alpha}+n-4}}{e^{(n-2)^{(\alpha)}+3(2)^{\alpha}+2(3)^{\alpha}+n-4}} > 1.
\end{aligned}
$$

Below are the comparisons between the B_k^* and newly constructed graphs with respect to the second exponential multiplicative Zagreb index.

Let

$$\begin{aligned} f(y) = &\ (y-3)^{\alpha(y-3)} + 3(4)^{\alpha} + 2(27)^{\alpha} \\ &+ y - 5 - (y-1)^{\alpha(y-1)} - 2(4)^{\alpha} - 27^{\alpha} - y + 4 \end{aligned}$$

is a decreasing function, since $y \geq 6$, as

$$\begin{aligned} f'(y) = & \\ & \alpha\Big[(y-3)^{\alpha(y-3)}[\ln(y-3)+1] \\ & -(y-1)^{\alpha(y-1)}[\ln(y-1)+1]\Big] < 0. \end{aligned}$$

$$\begin{aligned}
\frac{E\Pi_2^{\alpha}(C_{3,3}^{*})}{E\Pi_2^{\alpha}(B_k^{*})} &= \frac{e^{(n-3)^{\alpha(n-3)}+3(4)^{\alpha}+2(27)^{\alpha}+(n-5)}}{e^{(n-1)^{\alpha(n-1)}+2(4)^{\alpha}+(27)^{\alpha}+(n-4)}} < 1, \\
\frac{E\Pi_2^{\alpha}(C_{3,3}^{**})}{E\Pi_2^{\alpha}(B_k^{*})} &= \frac{e^{(n-2)^{\alpha(n-2)}+4(4)^{\alpha}+27^{\alpha}+(n-5)}}{e^{(n-1)^{\alpha(n-1)}+2(4)^{\alpha}+(27)^{\alpha}+(n-4)}} < 1. \\
\frac{E\Pi_2^{\alpha}(C_{3,1,3}^{*})}{E\Pi_2^{\alpha}(B_k^{*})} &= \frac{e^{(n-4)^{\alpha(n-4)}+3(4)^{\alpha}+2(27)^{\alpha}+(n-6)}}{e^{(n-1)^{\alpha(n-1)}+2(4)^{\alpha}+(27)^{\alpha}+(n-4)}} < 1. \\
\frac{E\Pi_2^{\alpha}(C_{3,1,3}^{**})}{E\Pi_2^{\alpha}(B_k^{*})} &= \frac{e^{(n-3)^{\alpha(n-3)}+4(4)^{\alpha}+27^{\alpha}+(n-6)}}{e^{(n-1)^{\alpha(n-1)}+2(4)^{\alpha}+(27)^{\alpha}+(n-4)}} < 1. \\
\frac{E\Pi_2^{\alpha}(C_{2,2}^{1*})}{E\Pi_2^{\alpha}(B_k^{*})} &= \frac{e^{(n-2)^{\alpha(n-2)}+3(4)^{\alpha}+2(27)^{\alpha}+(n-4)}}{e^{(n-1)^{\alpha(n-1)}+2(4)^{\alpha}+(27)^{\alpha}+(n-4)}} < 1.
\end{aligned}$$

Hence, proof is completed. □

3. Applications of Generalized Exponential Multiplicative Zagreb Indices

A set of graph theory indices known as the Zagreb indices measures a molecular graph's complexity or topological characteristics. They were first introduced in 1978 by Matula and Balaban, and they have a number of uses in mathematical chemistry and chemical graph theory.

The general Zagreb index is defined as the sum of the degrees of all vertices in a graph raised to a certain power. For a graph with vertices $\{v_1, v_2, \ldots, v_n\}$ and degrees $d_1, d_2, \ldots, d_n$, the general Zagreb index of order k, is given by:

$$\begin{aligned} \prod_1(G) &= \prod_{v \in V(G)} d_G^2(v). \\ \prod_2(G) &= \prod_{vu \in E(G)} [d_G(v) \times d_G(u)] = \prod_{z \in V(G)} \Big[d_G(z)^{d_G(z)}\Big], \end{aligned}$$

where the summation is taken over all vertices in the graph.

The exponential multiplicative Zagreb indices are a modification of the general Zagreb indices where instead of summing the degrees raised to a power, the product of the degrees raised to a power is considered. The exponential multiplicative Zagreb indices are defined as:

$$E\prod_1(G) = \prod_{v\in V(G)} e^{\left[d_G^2(v)\right]},$$

$$E\prod_2(G) = \prod_{vu\in E(G)} \left[e^{\left[d_G(v)\times d_G(u)\right]}\right] = \prod_{z\in V(G)} \left[e^{\left[d_G(z)^{d_G(z)}\right]}\right].$$

where the product is taken over all vertices in the graph.

As an alternate method of describing the structural characteristics of molecular networks, the exponential multiplicative Zagreb indices are presented. In order to anticipate diverse chemical properties, such as boiling temperatures, octanol-water partition coefficients, and molecular bioactivity, they have been included into mathematical models.

These indices are very helpful in quantitative structure-activity relationship (QSAR) research, which aim to determine a connection between the structural characteristics of molecules and their biological activities or characteristics. The exponential multiplicative Zagreb indices capture the interaction between the degrees of various graph vertices by taking into account the product of the degrees raised to a power.

It is important to keep in mind that there are more Zagreb index variations, such as the first and second Zagreb indices, which are particular instances of the basic Zagreb index. In chemical graph theory, these indices each have a unique significance and use.

Multiplicative general exponential Chemical graph theory employs topological indices called Zagreb indices to measure the molecular structure of chemical substances. They are developed from the Zagreb indices, a concept from graph theory that stores information about a molecular graph's vertex degrees.

It has been discovered that the generic exponential multiplicative Zagreb indices can be used to forecast a variety of chemical compound attributes, including boiling points, melting points, toxicity, and biological activity. These indices capture crucial molecular structural traits including branching, connection, and symmetry that might affect a molecule's chemical behaviour and characteristics.

The application and utility of any topological index, including the standard exponential multiplicative Zagreb indices, are dependent on the particular property or behaviour being investigated and the dataset being analysed. For different kinds of molecules or features, various topological indices might be more or less pertinent. To achieve a thorough understanding of chemical processes, the use of generic exponential multiplicative Zagreb indices should be taken into account alongside other molecular descriptors and experimental data.

4. Conclusions

Exponential multiplicative Zagreb indices were recently introduced in 2021. For $\alpha \in \mathbb{R}^+ \setminus \{1\}$, we proposed the generalized form of the exponential multiplicative Zagreb indices. Additionally, we employed a transformation method to observe the behavior of generalized first and second exponential Zagreb indices for $\alpha \in \mathbb{R}^+ \setminus \{1\}$. We looked into the extremal bicyclic, unicyclic, and tree graphs in terms of the two recently discovered generalized exponential multiplicative Zagreb indices. A few constraints are shown using extended exponential multiplicative Zagreb indices and four different graph transformations. The Formula is given in Equation (2), is the generalization version of Equation (1). For comparison, by putting the value of $\alpha = 1$, then it becomes Equation (1), it is very clear that Equation (2) will give more generalized result than Equation (1).

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