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Sharp Bounds of Topological Invariants for Acyclic, Unicyclic, Bicyclic and Tricyclic Graphs

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Abstract. This paper investigates the extremal behavior of several degree-based topological invariants, namely the Platt invariant (Pl), the first and second Gourava invariants (GO_1 and GO_2), the hyper-forgotten invariant (HF), and the hyper-first Gourava invariant (HGO_1). Sharp bounds for these invariants are established for acyclic, unicyclic, bicyclic, and tricyclic graphs using several graph transformations. The proposed transformations characterize the monotonic behavior of the invariants and lead to the identification of graph families attaining the first, second, and third extremal values. These results provide a unified transformation-based framework for determining extremal structures and contribute to the study of degree-based topological invariants in chemical graph theory.

AMS (MOS) Subject Classification Codes: 05C92; 05C09; 05C07
Key Words: Distance(in graphs); Chemical invariant; Tree; Graph transformations; Unicyclic graph; Bicyclic graph; Tricyclic graph.

1. Introduction

Let $F = (V(F); E(F))$ be a simple undirected connected *graph* with $V(F)$ and $E(F)$ as a vertex set and edge set respectively. The graph having one vertex is a trivial graph and a graph having two or more than two vertices is a non-trivial graph. The number of vertices in F is *order* of F while the number of edges in F is its *size*. Two vertices $h, g \in V(F)$ are *adjacent* if there is an edge formation *i.e.* $e = hg \in E(F)$ between them. The total number of edges in the shortest $h - g$ path in a graph F is known as *distance* between h and g and is denoted by $d_F(h, g)$. As the number of edges incident on a vertex $h \in V(F)$

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is *degree* of that vertex which is denoted by $d_F(h)$. For *neighbors* of a vertex h we look for vertices adjacent to vertex h. In a graph F, two vertices h and g are *equivalent* if $F - g \simeq F - h$ and $|\mathbb{N}(g)| = |\mathbb{N}(h)|$ having the neighbors of same degree sequence. Consider $\aleph_F(h)$ denote the neighbor set of vertex h in F, and degree of a vertex h in F is denoted as $d_F(h) =| \aleph_F(h) |$. A vertex h is said to be pendent if $d_F(h) = 1$. Path in which one end vertex has degree one and other has degree at least three is known as *pendent path*. A path $h_1, h_2, \ldots, h_n$ with end vertices having degree at least two is known as *internal path*. A path in which there is no repetition of vertex and edge except for the first and last vertex forms a *cycle*. A k length cycle is called a k-cycle. A graph having $n - 1$ vertices with degree one and a single vertex with degree $n - 1$, *i.e.* $n - 1$ vertices are joined with a central vertex is called a *star*. Consider the graphs S_n, P_n and C_n as the star, path and cycle on n vertices, respectively. As simple connected graph F with no cycle forms a *tree* (*i.e.* acyclic graph). The graphs having one cycle are *unicyclic graphs*, similarly, the graphs with two and three cycles are defined as *bicyclic* and *tricyclic graphs* respectively. For our results, we introduced some graph terminologies. For other undefined terms, see the book [4].

Chemical graph theory develops mathematical chemistry which combine graph theory and chemistry and plays a considerable role to study the changes in physical or chemical structures of molecular compounds. Quantitative structure-activity relationship $(QSAR)$ and Quantitative structure-property relationship $(QSPR)$ correspond structural properties which determinate characteristics by using statistical tools. $QSAR$ and $QSPR$ usually use a weighted composition of them to work with structural, experimental or theoretical properties in order to characterize a specific property. The idea of $QSPR/QSAR$ is to transform searches for chemical compounds with considerable properties using chemical experience into mathematically estimated and computed form.

In 1947, Wiener [12] proposed the well-known graph invariant *Wiener invariant*, he used it for classifying properties of the Paraffin . The Wiener invariant is sum of all the distances between every pairs of the vertices of a graph under consideration. After that many of the graph invariants are introduced. The most important invariants are *Zagreb invariants* that are introduced more than thirty years ago by Gutman and Trinajstić and are defined as

$$M_1(F) = \sum_{h \in V(F)} [d_F(h)]^2$$

and

$$M_2(F) = \sum_{hg \in E(F)} d_F(h) d_F(g)$$

In 2007, Yan *et al.* [13] discussed monotonicity on the second Zagreb invariant of unicyclic graphs with vertices n and pendent vertices k and concluded that U_{n}^{n} $\underline{3}$ and C_n have the maxima and minima of the second Zagreb invariant among all of the unicyclic graphs with vertices n, respectively.

Ji *et al.* [6], gave some graph transformations that results in increase or decrease of first reformulated Zagreb index. These transformations involved swapping of edges, conversion of pendent path to internal path and internal path to pendent vertices. By using these graph operations, the sharp bounds of the first reformulated Zagreb index were determined among all tricyclic graphs and found the corresponding extremal graphs. In 2017, Gao *et al.* [3]

studied the *hyper-Zagreb invariant* which is defined as

$$HM(F) = \sum_{hg \in E(F)} [d_F(h) + d_F(g)]^2$$

The authors discussed the sharp bounds of the HM invariant under the study of several graph transformations and determined the extremals of trees, unicyclic, and bicyclic graphs. In 2018, Malik *et al.* [11] found the extremal graphs for the F-index among the classes of connected prism like graphs. In 2018, Belavadi *et al.* [1] analysed the concept of degree of an edge gh in social networks which is defined as number of edges incident on vertices g and h other than itself. Further, in defined classes of graphs, Platt number which is defined as

$$\mathcal{F}(F) = \sum_{i}^{m} [D(e_i)]$$

and their total graphs were examined, linked bounds were proposed on connected graphs and an algorithm was presented to find the Platt number of any connected graph. In 2018, Mahadevi *et al.* [10] obtained Platt number for several classes of graphs interpreting molec-ular compounds and several general results were examined. In 2020, Kulli [9] wrote a book on molecular graphs and outlined the mathematical properties of several graph invariants and provided an exhaustive bibliography. In 2020, Chu *et al.* [2] examined the mono-tonicity of the hyper-Zagreb invariant while using same graph transformations that results in increase or decrease of the hyper Zagreb invariant. These graph transformations were very helpful in determining the extremal graphs for the hyper-Zagreb invariant among tri-cyclic graphs. Additionally, the sharp bounds of hyper-Zagreb invariant for these graphs are determined. In 2023, Imtiaz *et al.* [5] found the upper bound of $GO_1(F)$ for trees with given diameter, number of vertices and edges, and pendent nodes by using some graph transformations and discussed the extremals and also presented an ordering of the trees having Gourava invariant with decreasing order. In 2025, Kanwal and Sarwar [8] determined the lower bounds for trees with fixed degree and fixed pendent vertices using certain topological indices. In 2025, Kanwal *et al.* [7] determined sharp bounds for the Forgotten index within the class of tricyclic graphs and identify the extremal graphs achieving these bounds.

In this paper we determined the extremal values of the invariants $TIs(F) = Pl(F)$, $GO_1(F)$, $GO_2(F)$, $HF(F)$, $HGO_1(F)$ which are defined as

$$Pl(F) = \sum_{hg \in E(F)} [d_F(h) + d_F(g) - 2]$$

$$GO_1(F) = \sum_{hg \in E(F)} [d_F(h) + d_F(g) + d_F(h)d_F(g)]$$

$$GO_2(F) = \sum_{hg \in E(F)} [d_F(h) + d_F(g)][d_F(h)d_F(g)]$$

$$HF(F) = \sum_{hg \in E(F)} [d_F(h)^2 + d_F(g)^2]^2$$

$$HGO_1(F) = \sum_{hg \in E(F)} [d_F(h) + d_F(g) + d_F(h)d_F(g)]^2$$

In graph theory, the considered invariants can aid in the identification of graphs that maximize or minimize specified characteristics such as connectedness or robustness. This may include identifying extremal graphs that meet specific restrictions, which is critical for network design applications. Although extremal results for Zagreb invariants have been extensively studied, analogous results for the Platt, Gourava, hyper-forgotten, and hyper-first Gourava invariants remain limited, particularly for graphs containing cycles. Unlike the existing Zagreb-index literature, this work develops a unified graph transformation approach to establish sharp bounds and characterize extremal graphs for these invariants over acyclic, unicyclic, bicyclic, and tricyclic graph classes. In addition, the proposed transformations identify not only the extremal graphs but also the graph families attaining the second and third extremal values, which has not been systematically addressed in the existing literature. In section 2, some edge transformations are presented that preserve the monotonicity of graph invariants. In section 3, the results from these transformations are stated. In section 4, the extremals of the families under consideration with (maximum or minimum) topological invariants are determined.

2. Graph transformations

In the following section, several graph transformations that were presented by Gao *et al.* [3] are mentioned which will help in proving our results.

1^{st} ***Transformation***: Let a non-trivial connected graph F having fixed vertex r in it provided, $d_F(r) \geq 3$. For attaining a graph D from F, attach two paths: $P_1 = rg_1g_2\dots g_e$ and $P_2 = rh_1h_2\dots h_f$ having length e and f respectively. If $D = E(F) - rh_1 + g_eh_1$, we attain D from F by 1^{st} Transformation, as represented in Figure 1.

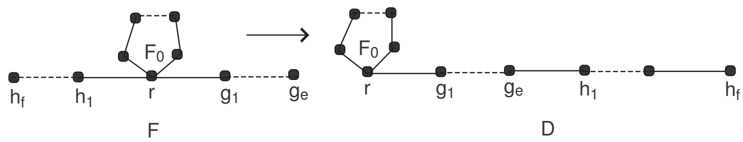

Figure 1. 1^{st} Transformation

2^{nd} ***Transformation***: Let F be a connected graph having an edge rh with $d_F(r) \geq 2$. Suppose that the neighbors of vertex h are $r, g_1, g_2, \dots, g_t$, while $g_1, g_2, \dots, g_t$ are pendent vertices where $t \geq 1$. If $D = E(F) - \{hg_1, hg_2, \dots, hg_t\} + \{rg_1, rg_2, \dots, rg_t\}$, we attain D from F by 2^{nd} Transformation, as represented in Figure 2.

3^{rd} ***Transformation***: F being a non-trivial connected graph with $h, r \in V(F)$ where

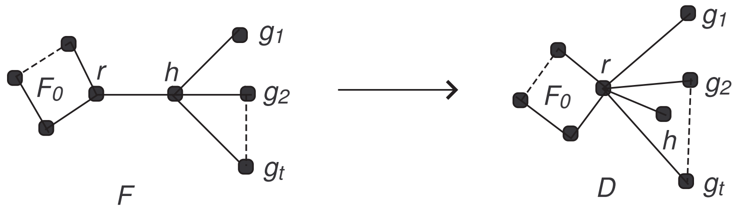

FIGURE 2. 2^{nd} Transformation

we can let $d_{F_1}(h) = \alpha \geq 1$ and $d_{F_2}(r) = \beta \geq 1$. Suppose for connecting vertices h and r, there is a non-trivial path of F: $P_e = (h =)h_1h_2 \ldots h_e(= r)$ where $e \geq 2$. If $D = E(F) - \{h_1h_2, h_2h_3, \ldots, h_{e-1}h_e\} + \{gh_1, gh_2, \ldots, gh_{e-1}\}$, where $h + r = g$ obtained by merging h and g, we attain D from F by 3^{rd} Transformation, as represented in Figure 3.

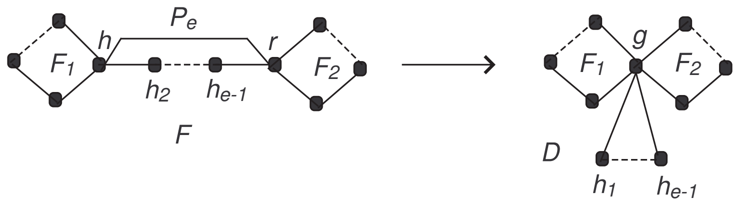

FIGURE 3. 3^{rd} Transformation

4^{th} ***Transformation***: Let a non-trivial acyclic subgraph F_0 of F with $|F_0| = t \geq 1$, attached at h_1 in graph F; let two neighbors of vertex h_1, h and g being different from those in F_0; also $d(h) = \alpha \geq 1$ and $d(g) = \beta \geq 1$. If $D = E(F) - (F_0 - h_1) + \{h_1h_2 + h_2h_3 + \ldots + h_tg\}$, we attain D from F by 4^{th} Transformation, as represented in Figure 4.

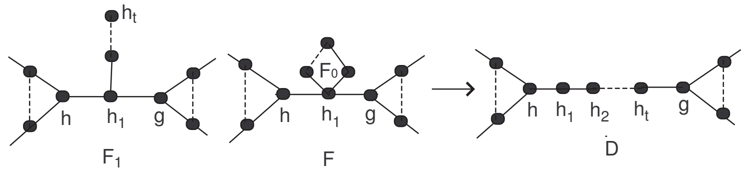

FIGURE 4. 4^{th} Transformation

5^{th} ***Transformation***: Let F_0 be a non-trivial connected graph with equivalent vertices h

and g in F_0 such that $d_{F_0}(h) = d_{F_0}(g) = \alpha \geq 1$. Let by attaching S_{e+1} and S_{f+1} at the vertices h and g of F_0, respectively, we present a graph F where $e \geq f \geq 1$. By deleting pendent vertices connected at g and connecting them at vertex h, we attain a graph D as represented in Figure 5.

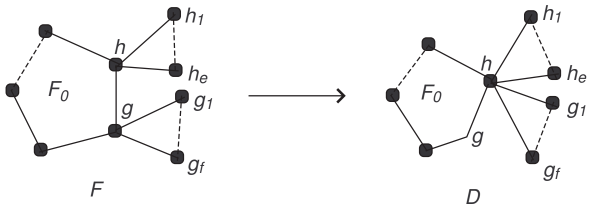

FIGURE 5. 5^{th} Transformation

3. RESULTS

In this section the above mentioned graph transformations are used to prove some results for TIs. As a result of these transformations, degree of some vertex is increased or decreased and we are not considering all edges incident to that vertex. Since we are ignoring some edges and if the degree of vertex is increased in transformed graph so that the difference $TI(F) - TI(D)$ will be greater, however if the degree of vertex is decreased in transformed graph then the difference $TI(D) - TI(F)$ will be greater.

Lemma 3.1. 1^{st} *Transformation strictly decreases TIs for a graph F* i.e *for D attained from F through 1^{st} Transformation as depicted in Figure 1, we have*

$$TIs(D) < TIs(F)$$

Proof. In this Transformation, there is decrease in degree of r by 1 while increase in degree of g_e by 1 and the degree of every other neighbor remains unchanged. For $TI = HGO_1$,

$$\begin{aligned}
&HGO_1(F) - HGO_1(D) > [d_F(r) + d_F(h_1) + d_F(r)d_F(h_1)]^2 + [d_F(r) + d_F(g_1) \\
&+ d_F(r)d_F(g_1)]^2 + [d_F(g_e) + d_F(g_{e-1}) + d_F(g_e)d_F(g_{e-1})]^2 - [(d_F(r) - 1) \\
&+ d_D(g_1) + (d_F(r) - 1)d_D(g_1)]^2 - [d_D(g_e) + d_D(g_{e-1}) + d_D(g_e)d_D(g_{e-1})]^2 \\
&- [d_D(g_e) + d_D(h_1) + d_D(g_e)d_D(h_1)]^2 \\
&= [d_F(r) + 2 + 2d_F(r)]^2 + [d_F(r) + 2 + 2d_F(r)]^2 + [1 + 2 + 2]^2 \\
&- [d_F(r) - 1 + 2 + 2d_F(r) - 2]^2 - [2 + 2 + 4]^2 - [2 + 2 + 4]^2 \\
&= 3d_F(r)(3d_F(r) + 10) > 0\,;\; d_F(r) \geq 0
\end{aligned}$$

Likewise, for $TI = HF$,

$$\begin{aligned}
&HF(F) - HF(D) > [d_F(r)^2 + d_F(h_1)^2]^2 + [d_F(r)^2 + d_F(g_1)^2]^2 \\
&+ [d_F(g_e)^2 + d_F(g_{e-1})^2]^2 - [(d_F(r) - 1)^2 + d_D(g_1)^2]^2 \\
&- [d_D(g_e)^2 + d_D(g_{e-1})^2]^2 - [d_D(g_e)^2 + d_D(h_1)^2]^2 \\
&= [d_F(r)^2 + 4]^2 + [d_F(r)^2 + 4]^2 + [1 + 4]^2 - [(d_F(r) - 1)^2 + 4]^2 \\
&- [4 + 4]^2 - [4 + 4]^2 \\
&= d_F(r)^4 + 4d_F(r)^3 + 2d_F(r)^2 + 20d_F(r) - 96 > 0\,;\ d_F(r) \geq 3
\end{aligned}$$

Similarly for $TI = Pl$,

$$Pl(F) - Pl(D) > d_F(r) - 2 > 0\,;\, d_F(r) \geq 3$$

Similarly for $TI = GO_1$,

$$GO_1(F) - GO_1(D) > 3d_F(r) - 6 > 0\,;\ d_F(r) \geq 3$$

Similarly for $TI = GO_2$,

$$GO_2(F) - GO_2(D) > 2d_F(r)^2 + 8d_F(r) - 24 > 0\,;\ d_F(r) \geq 3$$

□

Lemma 3.2. *2^{nd} Transformation strictly increases the TIs for graph F i.e for D attained from F through 2^{nd} Transformation as depicted in Figure 2, we have*

$$TIs(F) < TIs(D)$$

Proof. Clearly, there is increase in degree of r but $d(h) + d(r)$ remains unchanged. Hence, for $TI = HGO_1$,

$$\begin{aligned}
&HGO_1(D) - HGO_1(F) > [d_D(r) + d_D(h) + d_D(r)d_D(h)]^2 + \sum_{i=1}^{t}[d_D(r) + d_D(g_i) \\
&+ d_D(r)d_D(g_i)]^2 + \sum_{\alpha_i \in N_{F_0}(r)}[d_{\alpha_i} + d_D(r) + d_{\alpha_i}d_D(r)]^2 - \sum_{\alpha_i \in N_{F_0}(r)}[d_{\alpha_i} + d_F(r) \\
&+ d_{\alpha_i}d_F(r)]^2 - [d_F(r) + d_F(h) + d_F(r)d_F(h)]^2 - \sum_{i=1}^{t}[d_F(h) + d_F(g_i) \\
&+ d_F(h)d_F(g_i)]^2 \\
&= [x + t + 1 + 1 + x + t + 1]^2 + t[x + t + 1 + 1 + x + t + 1]^2 \\
&+ \sum_{\alpha_i \in N_{F_0}(r)}[d_{\alpha_i} + x + t + 1 + d_{\alpha_i}(x + t + 1)]^2 - \sum_{\alpha_i \in N_{F_0}(r)}[d_{\alpha_i} + x + 1 \\
&+ d_{\alpha_i}(x + 1)]^2 - [x + 1 + t + 1 + (x + 1)(t + 1)]^2 - t[t + 1 + 1 + t + 1]^2 \\
&= \sum_{\alpha_i \in N_{F_0}(r)}[t^2d_{\alpha_i}^2 + 4td_{\alpha_i}^2 + 2xtd_{\alpha_i}^2 + 2t^2d_{\alpha_i} + 6td_{\alpha_i} + 4xtd_{\alpha_i} + t^2 + 2xt + 2t] \\
&+ 4xt^2 + 6xt - x^2t^2 \geq xt[8t + 18 + 8x - xt]\ \text{for} d_{\alpha_i} \geq 1; \sum d_{\alpha_i} \geq x
\end{aligned}$$

For $t \geq 1$

$$= x(7x + 26) > 0$$

Similarly for $TI = HF$,

$$HF(D) - HF(F) > [d_D(r)^2 + d_D(h)^2]^2 + \sum_{i=1}^{t}[d_D(r)^2 + d_D(g_i)^2]^2$$
$$- [d_F(r)^2 + d_F(h)^2]^2 - \sum_{i=1}^{t}[d_F(h)^2 + d_F(g_i)^2]^2$$
$$= (t+1)[(d_F(r) + t)^2 + 1]^2 - [d_F(r)^2 + (t+1)^2]^2 - t[(t+1)^2 + 1]^2$$
$$= 4t^4(d_F(r) - 1) + 4t^2(d_F(r)^3 - 3) + t(d_F(r)^4 - 7) + 2td_F(r)^2$$
$$(2d_F(r) - 1) + 2t^3(3d_F(r)^2 - 5) + 4t^2 d_F(r)(2 + d_F(r)) + 4td_F(r) > 0;$$
$$d_F(r) \geq 2, t \geq 1$$

For $TI = Pl$,

$$Pl(D) - Pl(F) > t(d_F(r) - 1) > 0\,;\ d_F(r) \geq 2, t \geq 1$$

For $TI = GO_1$,

$$GO_1(D) - GO_1(F) > t(d_F(r) - 1) > 0\,;\ d_F(r) \geq 2, t \geq 1$$

For $TI = GO_2$,

$$GO_2(D) - GO_2(F) > [d_F(r) - 1][t^2 + t] > 0\,;\ d_F(r) \geq 2, t \geq 1$$

□

Lemma 3.3. *For D attained from F through 3^{rd} Transformation as depicted in Figure 3, we have*

$$TIs(F) < TIs(D)$$

Proof. Let $d_{F_1}(h) = \alpha \geq 1$ and $d_{F_2}(r) = \beta \geq 1$, while by merging h and r, we attain g with $d_D(g) = \alpha + \beta + e - 1$, where $e \geq 2$. Here for $TI = HGO_1$,

$$
\begin{aligned}
&HGO_1(D) - HGO_1(F) > \sum_{i=1}^{e-1}[d_D(g) + d_D(h_i) + d_D(g)d_D(h_i)]^2 \\
&+ \sum_{\alpha_i \in N_{F_1}(g)} [d_{\alpha_i} + d_D(g) + d_{\alpha_i} d_D(g)]^2 + \sum_{\beta_j \in N_{F_2}(g)} [d_{\beta_j} + d_D(g) + d_{\beta_j} d_D(g)]^2 \\
&- \sum_{\alpha_i \in N_{F_1}(h)} [d_{\alpha_i} + d_F(h) + d_{\alpha_i} d_F(h)]^2 - \sum_{\beta_j \in N_{F_2}(r)} [d_{\beta_j} + d_F(r) + d_{\beta_j} d_F(r)]^2 \\
&- [d_F(h) + d_F(h_2) + d_F(h)d_F(h_2)]^2 - [d_F(h_{e-1}) + d_F(r) + d_F(h_{e-1})d_F(r)]^2 \\
&- \sum_{k=3}^{e-2}[d_F(h_k) + d_F(h_{k-1}) + d_F(h_k)d_F(h_{k-1})]^2 \\
&= (e-1)[x + y + e - 1 + 1 + x + y + e - 1]^2 + \sum_{\alpha_i \in N_{F_1}(g)} [d_{\alpha_i} + x + y + e - 1 \\
&+ d_{\alpha_i}(x + y + e - 1)]^2 + \sum_{\beta_j \in N_{F_2}(g)} [d_{\beta_j} + x + y + e - 1 + d_{\beta_j}(x + y + e - 1)]^2 \\
&- \sum_{\alpha_i \in N_{F_1}(h)} [d_{\alpha_i} + x + 1 + d_{\alpha_i}(x+1)]^2 - \sum_{\beta_j \in N_{F_2}(r)} [d_{\beta_j} + y + 1 + d_{\beta_j}(y+1)]^2 \\
&- [x + 1 + 2 + 2x + 2]^2 - [y + 1 + 2 + 2y + 2]^2 - (e-3)(2+2+4)^2
\end{aligned}
$$

For $d_{\alpha_i}, d_{\beta_j} \geq 1; \sum d_{\alpha_i} \geq x \geq 1, \sum d_{\beta_j} \geq y \geq 1$; where $i = 1, \ldots, x$ and $j = 1, \ldots, y$.

$$
\begin{aligned}
&\geq x^2(6e - 17 + 3y) + y^2(6e - 17 + 3x) + x(12e^2 - 14e - 26) + y(12e^2 - 14e - 26) \\
&+ 12xy(e-1) + 4e^3 - 8e^2 - 59e + 141 + \sum_{\alpha_i \in N_{F_1}(g)} [d^2_{\alpha_i}\{y^2 + 2xy + 2(ey - 2) \\
&+ 2x(e-2)\} + d_{\alpha_i}\{4(xy-1) + 2y(y-1) + 4x(e-2) + 2ey + 2e(y-1)\}] \\
&+ \sum_{\beta_j \in N_{F_2}(g)} [d^2_{\beta_j}\{x^2 + 2xy + 2(ex-2) + 2y(e-2)\} + d_{\beta_j}\{4(xy-1) \\
&+ 2x(x-1) + 4y(e-2) + 2ex + 2e(x-1)\}] > 0; e \geq 3
\end{aligned}
$$

For $f(e) = 4e^3 - 8e^2 - 59e + 141 \Rightarrow f(e)$ is increasing $\forall\, e \geq 3$.
Here, we have a particular case of $e = 2$, where the above final expression will become

$$
\begin{aligned}
&= x^2(6y - 5) + y^2(6x - 5) + 6x(y-1) + 6y(x-1) + 23 \\
&+ \sum_{\alpha_i \in N_{F_1}(g)} [d^2_{\alpha_i}\{4(y-1)\} + d_{\alpha_i}\{4(xy-1) + 2y(y-1) + 4(y-1) + 4y\}] \\
&+ \sum_{\beta_j \in N_{F_2}(g)} [d^2_{\beta_j}\{4(x-1)\} + d_{\beta_j}\{4(xy-1) + 2x(x-1) + 4(x-1) + 4x\}] > 0
\end{aligned}
$$

Similarly,

$$HF(D) - HF(F) > \sum_{i=1}^{e-1}[d_D(g)^2 + d_F(h_i)^2]^2 - [d_F(h)^2 + d_F(h_2)^2]^2$$
$$- [d_F(r)^2 + d_F(h_{e-1})^2]^2 - \sum_{k=3}^{e-2}[d_F(h_k)^2 + d_F(h_{k-1})^2]^2$$
$$= (e-1)[(x+y+e-1)^2+1]^2 - [(x+1)^2+4]^2 - [(y+1)^2+4]^2$$
$$- (e-3)(64)$$
$$= (e-1)(4x^3y + 4xy^3 + 6x^2y^2) + (e-2)(x^4 + y^4 + 4x^3e + 4y^3e$$
$$+ 12ex^2y + 12exy^2) + (e-3)(6x^2e^2 + 12xye^2 + 6y^2e^2) + (e-4)$$
$$(4xe^3 + 4ye^3) + (e-5)e^4 + 4e^2(3e-4) + (7e-6)(4ex+4ey) + (10e-11)$$
$$(2x^2+2y^2) + (xy-1)(12x+12y) + (5e-4)8xy - 52e + 138$$

The above expression is clearly positive for $e \geq 5$. Here, we will present verification for positivity of above final expression for $g = 2, 3, 4$.
Verification for $g = 2$,

$$= 2x(2x^2y + 2y^3 - 3x) + 6y^2(x^2-1) + 12x(y^2-1) + 12y(x^2-1) + 18 > 0$$

Verification for $g = 3$,

$$= x^4 + y^4 + 8x^3y + 8xy^3 + 12x^3 + 12y^3 + 38x^2 + 38y^2 + 12x^2y^2 + 48x^2y + 48xy^2$$
$$+ 60x + 60y + 88xy > 0$$

Verification for $g = 4$,

$$= 2x^4 + 2y^4 + 32x^3 + 32y^3 + 12x^3y + 12xy^3 + 154x^2 + 154y^2 + 108x^2y + 108xy^2$$
$$+ 18x^2y^2 + 340x + 340y + 320xy + 186 > 0$$

Similarly for $TI = Pl$ we have two cases

(i) $e = 2$,

$$Pl(D) - Pl(F) \geq 0$$

(ii) $e \geq 3$,

$$Pl(D) - Pl(F) > (e-2)(\alpha + \beta + e - 3) > 0\,;\ e \geq 3, \alpha, \beta \geq 1$$

Similarly for $TI = GO_1$,

$$GO_1(D) - GO_1(F) > [\sum_{\eta_i \in N_{F_1}(g)} d_{\eta_i} + 3e - 7]\beta + [\sum_{\mu_j \in N_{F_2}(g)} d_{\mu_j} + 3e - 7]\alpha$$
$$+ \sum_{\eta_i \in N_{F_1}(g)} d_{\eta_i}(e-2) + \sum_{\mu_j \in N_{F_2}(g)} d_{\mu_j}(e-2) + 2\alpha\beta + (e-3)(2e-5) > 0;$$
$$d_{\mu_j} \geq 1, d_{\eta_i} \geq 1$$

For $TI = GO_2$,

$$GO_2(D) - GO_2(F) > [\sum_{\eta_i \in N_{F_1}(g)} d_{\eta_i} + e - 3]\beta^2 + [\sum_{\mu_j \in N_{F_2}(g)} d_{\mu_j} + e - 3]\alpha^2$$
$$+ [2e^2 - 3e - 7 + \sum_{\mu_j \in N_{F_2}(g)} d^2_{\mu_j}]\alpha + [2e^2 - 3e - 7 + \sum_{\eta_i \in N_{F_1}(g)} d^2_{\eta_i}]\beta$$
$$+ \sum_{\eta_i \in N_{F_1}(g)} [2\alpha d_{\eta_i}(e-2) + 2\beta d_{\eta_i}(e-1) + e d_{\eta_i}(e-2) + d^2_{\eta_i}(e-2) + 2\alpha\beta d_{\eta_i}]$$
$$+ \sum_{\mu_j \in N_{F_2}(g)} [2\alpha d_{\mu_j}(e-1) + 2\beta d_{\mu_j}(e-2) + d^2_{\mu_j}(e-2) + 2\alpha\beta d_{\mu_j}$$
$$+ e d_{\mu_j}(e-2)] + 2\alpha\beta(e-1) + e^3 - 2e^2 - 15e + 36 > 0;\ d_{\mu_j} \geq 1, d_{\eta_i} \geq 1$$

where $i = 1, \ldots, \alpha$ and $j = 1, \ldots, \beta$. □

Lemma 3.4. *For D attained from F through 4^{th} Transformation as depicted in Figure 4, we have*

$$TIs(D) < TIs(F)$$

Proof. We know that $TIs(F) \geq TIs(F_1)$ by Transformation 2. So, we will prove the following:

$$TIs(F_1) \geq TIs(D)$$

Hence for $TI = HGO_1$,

$$HGO_1(F_1) - HGO_1(D) = [d_{F_1}(h) + d_{F_1}(h_1) + d_{F_1}(h)d_{F_1}(h_1)]^2 + [d_{F_1}(h_1)$$
$$+ d_{F_1}(g) + d_{F_1}(h_1)d_{F_1}(g)]^2 + [d_{F_1}(h_1) + d_{F_1}(h_2) + d_{F_1}(h_1)d_{F_1}(h_2)]^2$$
$$+ [d_{F_1}(h_{t-1}) + d_{F_1}(h_t) + d_{F_1}(h_{t-1})d_{F_1}(h_t)]^2 - [d_D(h) + d_D(h_1)$$
$$+ d_D(h)d_D(h_1)]^2 - [d_D(h_1) + d_D(h_2) + d_D(h_1)d_D(h_2)]^2 - [d_D(h_{t-1})$$
$$+ d_D(h_t) + d_D(h_{t-1})d_D(h_t)]^2 - [d_D(h_t) + d_D(g) + d_D(h_t)d_D(g)]^2$$
$$= [\alpha + 3 + 3\alpha]^2 + [3 + \beta + 3\beta]^2 + [3 + 2 + 6]^2 + [2 + 1 + 2]^2 - [\alpha + 2 + 2\alpha]^2$$
$$- [2 + 2 + 4]^2 - [2 + 2 + 4]^2 - [2 + \beta + 2\beta]^2$$
$$= 7\alpha^2 + 7\beta^2 + 12\alpha + 12\beta + 28 > 0;\ \alpha, \beta \geq 1$$

Similarly for $TI = HF$,

$$HF(F_1) - HF(D) = [d_{F_1}(h)^2 + d_{F_1}(h_1)^2]^2 + [d_{F_1}(h_1)^2 + d_{F_1}(g)^2]^2$$
$$+ [d_{F_1}(h_1)^2 + d_{F_1}(h_2)^2]^2 + [d_{F_1}(h_{t-1})^2 + d_{F_1}(h_t)^2]^2$$
$$- [d_D(h)^2 + d_D(h_1)^2]^2 - [d_D(h_1)^2 + d_D(h_2)^2]^2 - [d_D(h_{t-1})^2 + d_D(h_t)^2]^2$$
$$- [d_D(h_t)^2 + d_D(g)^2]^2$$
$$= [\alpha^2 + 9]^2 + [9 + \beta^2]^2 + [9 + 4]^2 + [4 + 1]^2 - [\alpha^2 + 4]^2 - [4 + 4]^2$$
$$- [4 + 4]^2 - [4 + \beta^2]^2$$
$$= 10\alpha^2 + 10\beta^2 + 196 > 0;\ \alpha, \beta \geq 1$$

For $TI = Pl$,

$$Pl(F_1) - Pl(D) = 2 > 0$$

For $TI = GO_1$,

$$GO_1(F_1) - GO_1(D) = \alpha + \beta + 2 > 0\,;\ \alpha, \beta \geq 1$$

For $TI = GO_2$,

$$GO_2(F_1) - GO_2(D) = \alpha^2 + \beta^2 + 5\alpha + 5\beta + 4 > 0\,;\ \alpha, \beta \geq 1$$

□

Lemma 3.5. *For D attained from F through 5^{th} Transformation as depicted in Figure 5, we have*

$$TIs(F) < TIs(D)$$

Proof. We have for $TI = HGO_1$,

$$\begin{aligned}
HGO_1(D) - HGO_1(F) &> \sum_{i=1}^{e}[d_D(h) + d_D(h_i) + d_D(h)d_D(h_i)]^2 + \sum_{j=1}^{f}[d_D(h) \\
&+ d_D(g_j) + d_D(h)d_D(g_j)]^2 - \sum_{i=1}^{e}[d_F(h) + d_D(h_i) + d_F(h)d_D(h_i)]^2 \\
&- \sum_{j=1}^{f}[d_F(g) + d_D(g_j) + d_F(g)d_D(g_j)]^2 \\
&= e[x+e+f+1+x+e+f]^2 + f[x+e+f+1+x+e+f]^2 \\
&- e[x+e+1+x+e]^2 - f[x+f+1+x+f]^2 \\
&= e(2x+2e+1+2f)^2 + f(2x+2e+1+2f)^2 - e(2x+2e+1)^2 \\
&- f(2x+2f+1)^2 > 0\,;\ e \geq f \geq 1
\end{aligned}$$

Similarly For $TI = HF$,

$$\begin{aligned}
HF(D) - HF(F) &> \sum_{i=1}^{e}[d_D(h)^2 + d_D(h_i)^2]^2 + \sum_{j=1}^{f}[d_D(h)^2 \\
&+ d_D(g_j)^2]^2 - \sum_{i=1}^{e}[d_F(h)^2 + d_F(h_i)^2]^2 - \sum_{j=1}^{f}[d_F(g)^2 + d_F(g_j)^2]^2 \\
&= e[(x+e+f)^2+1]^2 + f[(x+e+f)^2+1]^2 \\
&- e[(x+e)^2+1]^2 - f[(x+f)^2+1]^2 \\
&= e[(x+e+f)^2+1]^2 - e[(x+e)^2+1]^2 \\
&+ f[(x+e+f)^2+1]^2 - f[(x+f)^2+1]^2 > 0\,;\ e \geq f \geq 1
\end{aligned}$$

For $TI = Pl$,

$$Pl(D) - Pl(F) > 2ef > 0\,;\ e \geq f \geq 1$$

For $TI = GO_1$,

$$GO_1(D) - GO_1(F) > 3ef > 0\,;\, e \geq f \geq 1$$

For $TI = GO_2$,

$$GO_2(D) - GO_2(F) > 2ef\alpha + 2e^2f + 2ef^2 + 2ef > 0\,;\, e \geq f \geq 1$$

□

4. EXTREMALS WITH RESPECT TO TIs

In the following section, we characterized extremal graphs amid acyclic, unicyclic, bicyclic and tricyclic graphs with respect to TIs. We define several terminologies which might be used in this section.

Set of all of the bicyclic graphs having number of vertices n is denoted by B_n. Considering graphs, we have three special classes defined as; first, connect two cycles C_l and C_t to a path P_r and we have $P_n^{l,r,t}$ graph of order $n = l + r + t - 2$. Second consists of only two cycles C_s and C_t of order $n = s + t - 1$ having a common vertex and denoted by $C_n(s,t)$. However, to attain the third one, fuse pendent vertices of two triples from three paths P_k, P_l and P_m with two vertices and is denoted by $C_n(k,l,m)$ having order $n = k + l + m - 4$, where $2 \leq k \leq l \leq m$.

If a bicyclic graph F consisting at least one of the three graphs $P_n^{l,r,t}$, $C_n(s,t)$ and $C_n(k,l,m)$ as its subgraph then it is called a brace of F. Setting B_n^1, B_n^2 and B_n^3 as such bicyclic graphs having $P_n^{l,r,t}$, $C_n(s,t)$ and $C_n(k,l,m)$ as their brace, respectively. Now, partitioned subsets of B_n are B_n^1, B_n^2 and B_n^3.

Some graphs which will be used in achieving the extremal graphs are drawn in the following Figure 7. The whole procedure is shown in figure 6. Now we have the following results.

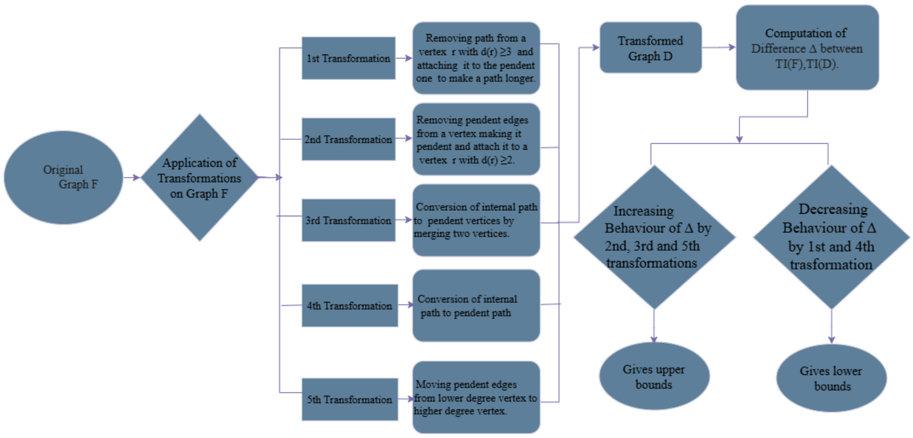

FIGURE 6. Flowchart for finding extremals using transformations

Theorem 4.1. *For a tree F having n number of vertices.*

$$TIs(P_n) \leq TIs(F) \leq TIs(S_n)$$

Proof. By repeated applications of Lemmas 3.1 and 3.2, we get the sharp bounds of TIs for a tree. For the upper bound, by increasing value of TIs using Lemma 3.2, we attain a star S_n. Similarly for the lower bound, by decreasing value of TIs using Lemma 3.1, we attain a path P_n.
By Calculations, we have

$$TI(S_n) = \begin{cases} (n-1)(n-2), \text{TI=Pl}, \\ (2n-1)(n-1), \text{TI=}GO_1, \\ n(n-1)^2, \text{TI=}GO_2, \\ (2n-1)^2(n-1), \text{TI=}HGO_1, \\ (n-1)(n^2-2n+2)^2, \text{TI=HF}. \end{cases} \quad , TI(P_n) = \begin{cases} 2n-4, \text{TI=Pl}, \\ 8n-14, \text{TI=}GO_1, \\ 16n-36, \text{TI=}GO_2, \\ 64n-142, \text{TI=}HGO_1, \\ 64n-142, \text{TI=HF}. \end{cases}$$

□

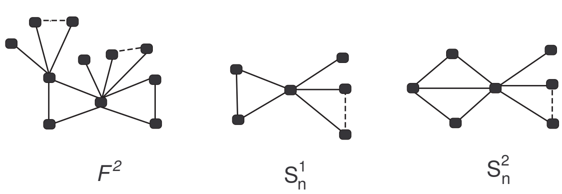

FIGURE 7. Certain unicyclic and bicyclic graphs

Theorem 4.2. *For a unicyclic graph F with n number of vertices.*

$$TIs(C_n) \leq TIs(F) \leq TIs(S_n^1)$$

Proof. For a unicyclic graph F with vertex disjoint attached to vertices of C_k, by Lemma 3.2, we have C_k with pendent vertices attached to vertices of C_k and then by repeated applications of 3^{rd} transformation, we attain cycle of length 3 attached to its three vertices. Since by Lemma 3.3,3.5 TIs of resulting graph is greatest *i.e* we attain a maximum graph S_n^1, as shown in Figure 7. By using Lemmas 3.1 and 3.4, we attain the minima C_n. By calculations we get the bounds as follows:

$$TI(S_n^1) = \begin{cases} n^2-3n+6, \text{TI=Pl}, \\ 2n^2-n+9, \text{TI=}GO_1, \\ n^3+3n+12, \text{TI=}GO_2, \\ 4n^3+2n^2+n+63, \text{TI=}HGO_1, \\ n^5-5n^4+12n^3-4n^2-12n+102, \text{TI=HF}. \end{cases}$$

$$TI(C_n) = \begin{cases} 2n, \text{TI=Pl}, \\ 8n, \text{TI=}GO_1, \\ 16n, \text{TI=}GO_2, \\ 64n, \text{TI=}HGO_1, \\ 64n, \text{TI=HF}. \end{cases}$$

□

Theorem 4.3. *For a bicyclic graph F with n number of vertices.*

$$TIs(\{P_n^{l,r,t} : l \geq 3\} \cup \{C_n(k, l, m) : l \geq 3\}) \leq TIs(F) \leq TIs(S_n^2)$$

Proof. For bicyclic graphs, the lower bound can be easily attained from Lemma 3.1, 3.2 and 3.4.
Clearly, equality holds in case $F \in \{P_n^{l,r,t} : l \geq 3\} \cup \{C_n(k, l, m) : l \geq 3\}$.
So,

$$TI(\{P_n^{l,r,t} : l \geq 3\} \cup \{C_n(k, l, m) : l \geq 3\}) = \begin{cases} 2n + 8, \text{TI=Pl}, \\ 8n + 26, \text{TI=}GO_1, \\ 16n + 100, \text{TI=}GO_2, \\ 64n + 406, \text{TI=}HGO_1, \\ 64n + 694, \text{TI=HF}. \end{cases}$$

,

$$TI(C_n(s, t)) = \begin{cases} 2n + 10, \text{TI=Pl}, \\ 8n + 32, \text{TI=}GO_1, \\ 16n + 144, \text{TI=}GO_2, \\ 64n + 592, \text{TI=}HGO_1, \\ 64n + 1408, \text{TI=HF}. \end{cases}$$

Now, for upper bound of bicyclic graphs with respect to TI. By calculations, we get

$$TI(S_n^2) = \begin{cases} n^2 - 3n + 12, \text{TI=Pl}, \\ 2n^2 + n + 23, \text{TI=}GO_1, \\ n^3 + 2n^2 + 7n + 50, \text{TI=}GO_2, \\ 4n^3 + 14n^2 - 3n + 241, \text{TI=}HGO_1, \\ n^5 - 5n^4 + 12n^3 + 12n^2 - 44n + 472, \text{TI=HF}. \end{cases}$$

So, we demonstrate that if $F \ncong S_n^2$, then

$$TI(F) < TI(S_n^2)$$

$Possibility\,1$ (Brace of F is $K_4 - e$). By Lemma 3.2 and 3.5, we can attain a unique bicyclic graph F^1 which has every TI greater than F (see Figure 7). We have

$$TI(F^1) < TI(S_n^2)$$

$Possibility\,2$ (Brace of F is not $K_4 - e$). By using Lemma 3.3, there may exists a bicyclic graph having brace $K_4 - e$ which has greater values of TI than F. So concluding two possibilities.

$Possibility$ 2.1 (Brace of F is $C_n(3, 2, m)$). By Lemma 3.3, this possibility is converted to $Possibility$ 1.
$Possibility$ 2.2 (Brace of F is not $C_n(3, 2, m)$). We have F^2, a new bicyclic graph by Lemma 3.2, 3.3 and 3.5 in Figure 7, which has greater values of TI than F. We can easily attain

$$TI(F^2) < TI(S_n^2)$$

□

Now consider the family of connected graphs with three cycles *i.e* of size $n + 2$, order n and is represented by χ_n. The class of all possible braces of tricyclic graph is denoted by χ_n^0, χ_n^1 and χ_n^2, where a brace is a graph obtained by removing all its pendent vertices. χ_n^0 denote the class of all possible braces of a graph as shown in Figure 8, χ_n^1 denote the class of braces of tricyclic graph without pendent vertices and having cycle of length atleast 4 and χ_n^2 denote the class of braces having pendent vertices and with cycle of length atleast 3 as shown in Figure 9 and 10 respectively.

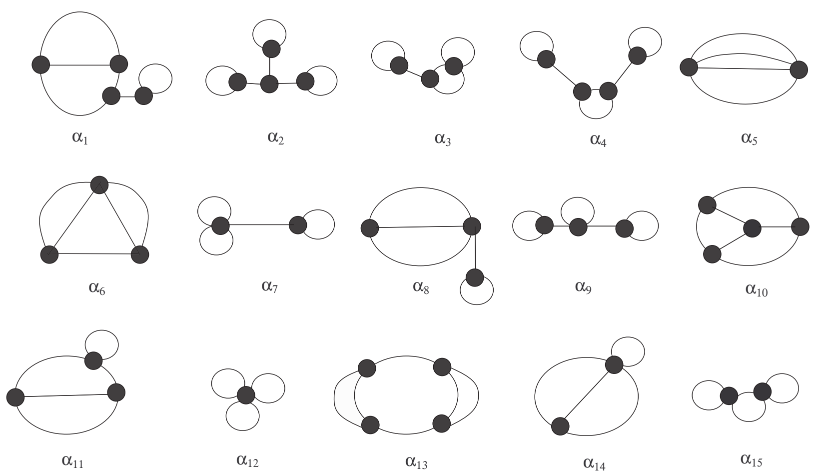

FIGURE 8. All possible braces α_j of tricyclic graphs in χ_n^0

Theorem 4.4. *Let F be any tricyclic graph having n vertices; $n \geq 4$, with*

$$TI(F) \leq \begin{cases} 2n + 16; \ \textit{TI=Pl} \\ 8n + 52; \ \textit{TI=}GO_1 \\ 16n + 200; \ \textit{TI=}GO_2 \\ 64n + 812; \ \textit{TI=}HGO_1 \\ 64n + 1388; \ \textit{TI=HF} \end{cases}$$

then equality holds if and only if $F \in \chi_n^1$.

Proof. Let F be a tricyclic graph with braces α_j as depicted in Figure 8. By applying 4^{th} Transformation α_j can be one of σ_j having internal path of length atleast 4 and consequently by using Lemma 3.4, $TI(\sigma_j) \leq TI(F)$. Evidently, by direct computations,

$$TI(\alpha_j) = \begin{cases} 2n + 16; \text{ TI=Pl} \\ 8n + 52; \text{ TI=}GO_1 \\ 16n + 200; \text{ TI=}GO_2 \\ 64n + 812; \text{ TI=}HGO_1 \\ 64n + 1388; \text{ TI=HF} \end{cases}$$

for $j = 1, 2, 3, 4, 5$.
As a result the proof is complete. □

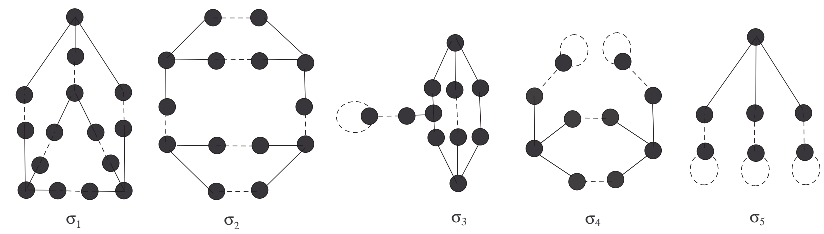

FIGURE 9. Tricyclic graph σ_j (with cycle of length atleast 4) in χ_n^1

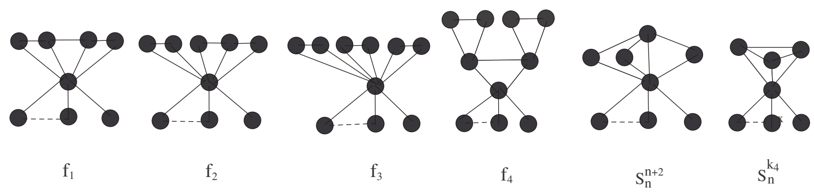

FIGURE 10. Tricyclic graph f_j with pendent vertices in χ_n^2

Theorem 4.5. *Let F be any tricyclic graph having n order with $n \geq 4$, then*

$$TI(F) \leq \begin{cases} n^2 - 3n + 20; \; TI = Pl \\ 2n^2 + 3n + 46; \; TI = GO_1 \\ n^3 + 4n^2 + 13n + 144; \; TI = GO_2 \\ 4n^3 + 28n^2 - 7n + 674; \; TI = HGO_1 \\ n^5 - 5n^4 + 12n^3 + 32n^2 - 96n + 1256; \; TI = HF \end{cases}$$

For $TI = Pl$, equality holds if and only if $F \cong S_n^{k_4}$ or S_n^{n+2}. For $TI = GO_1$, GO_2, HGO_1 and HF, equality holds if and only if $F \cong S_n^{k_4}$

Proof. Let F be a tricyclic graph with brace one of α_j, by repeated applications of 2^{nd}, 3^{rd} and 5^{th} Transformations we will have braces with pendent vertices and then one of the six graphs can be extracted from these braces as depicted in Figure 10. Furthermore, for any tricyclic graph F there exists $f_j \in \chi_n^2$ for $j \leq 6$ such that $TI(F) \leq TI(f_j)$ where, $TI = Pl, GO_1, GO_2, HGO_1, HF$, by Lemma 3.3 and Lemma 3.5. Clearly,

$$\begin{aligned}
&Pl(f_1) = n^2 - 3n + 18, \;\; GO_1(f_1) = 2n^2 + 3n + 38 \\
&Pl(f_2) = n^2 - 3n + 16, \;\; GO_1(f_2) = 2n^2 + 3n + 31 \\
&Pl(f_3) = n^2 - 3n + 14, \;\; GO_1(f_3) = 2n^2 + 3n + 25 \\
&Pl(f_4) = n^2 - 11n + 62, \;\; GO_1(f_4) = 2n^2 - 13n + 117 \\
&Pl(S_n^{n+2}) = n^2 - 3n + 20, \;\; GO_1(S_n^{n+2}) = 2n^2 + 3n + 43 \\
&Pl(S_n^{k_4}) = n^2 - 3n + 20, \;\; GO_1(S_n^{k_4}) = 2n^2 + 3n + 46 \\
&GO_2(f_1) = n^3 + 4n^2 + 11n + 98, \; HGO_1(f_1) = 4n^3 + 26n^2 - 7n + 466 \\
&GO_2(f_2) = n^3 + 4n^2 + 9n + 62, \; HGO_1(f_2) = 4n^3 + 24n^2 - 7n + 305 \\
&GO_2(f_3) = n^3 + 4n^2 + 7n + 36, \; HGO_1(f_3) = 4n^3 + 22n^2 - 7n + 191 \\
&GO_2(f_4) = n^3 - 8n^2 + 35n + 252, \; HGO_1(f_4) = 4n^3 - 14n^2 - 87n + 1803 \\
&GO_2(S_n^{n+2}) = n^3 + 4n^2 + 13n + 126, \; HGO_1(S_n^{n+2}) = 4n^3 + 28n^2 - 7n + 587 \\
&GO_2(S_n^{k_4}) = n^3 + 4n^2 + 13n + 144, \; HGO_1(S_n^{k_4}) = 4n^3 + 28n^2 - 7n + 674 \\
&HF(f_1) = n^5 - 5n^4 + 12n^3 + 28n^2 - 76n + 892 \\
&HF(f_2) = n^5 - 5n^4 + 12n^3 + 24n^2 - 68n + 578 \\
&HF(f_3) = n^5 - 5n^4 + 12n^3 + 20n^2 - 60n + 314 \\
&HF(f_4) = n^5 - 25n^4 + 252n^3 - 1220n^2 + 2676n + 1382 \\
&HF(S_n^{n+2}) = n^5 - 5n^4 + 12n^3 + 32n^2 - 84n + 1544 \\
&HF(S_n^{k_4}) = n^5 - 5n^4 + 24n^3 + 32n^2 - 96n + 1256
\end{aligned}$$

As a result, the proof is complete. $\square$

5. Conclusion

This study derives sharp bounds for the Platt, Gourava, and hyper-forgotten invariants in acyclic, unicyclic, bicyclic, and tricyclic graphs using vertex-path transformations, with extremal structures identified through systematic combinatorial analysis. In this work, we have observed the behavior of Pl, GO_1, GO_2, HGO_1 and HF under these graph transformations for acyclic, unicyclic, bicyclic and tricyclic graphs of order n. We observed that in 2^{nd} transformation when we converted vertex of internal path to pendent vertex then as a result, all the invariants increased, similarly, 3^{rd} and 5^{th} transformations increased the invariants under consideration which gave us upper bound, but in 4^{th} transformation when we converted pendent path to internal path, as a result invariants decreased, which gave us lower bound and in 1^{st} transformation, we increased the length of the path which resulted in lower bound. Further, extreme values of these chemical invariants are determined. The derived sharp bounds and extremal graphs provide a systematic framework for analyzing the behavior of degree-based topological invariants under graph transformations. These results contribute to extremal graph theory and offer potential applications in chemical graph theory for modeling and analyzing molecular structures. This approach can be extended to other degree-based invariants, such as the Sombor and reduced Sombor invariants, as well as to broader graph classes, including cacti, block graphs, and other cyclic graph families.

CREDIT AUTHORSHIP CONTRIBUTION'S STATEMENT

Conceptualization, Salma Kanwal; methodology, Maria Fazal and Hadiqa Fatima; software, Maria Fazal and Hadiqa Fatima; validation, Salma Kanwal, Maria Fazal and Hadiqa Fatima; investigation, Salma Kanwal; writing-original draft, Maria Fazal and Hadiqa Fatima; writing-review and editing, Salma Kanwal, Maria Fazal and Hadiqa Fatima; visualization, Salma Kanwal, Maria Fazal and Hadiqa Fatima; funding acquisition, Salma Kanwal, Maria Fazal and Hadiqa Fatima. All authors have read and agreed to the published version of the manuscript.

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