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Retraction

Retracted: On Second Gourava Invariant for *q*-Apex Trees

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This article has been retracted by Hindawi, as publisher, following an investigation undertaken by the publisher [1]. This investigation has uncovered evidence of systematic manipulation of the publication and peer-review process. We cannot, therefore, vouch for the reliability or integrity of this article.

Please note that this notice is intended solely to alert readers that the peer-review process of this article has been compromised.

Wiley and Hindawi regret that the usual quality checks did not identify these issues before publication and have since put additional measures in place to safeguard research integrity.

We wish to credit our Research Integrity and Research Publishing teams and anonymous and named external researchers and research integrity experts for contributing to this investigation.

The corresponding author, as the representative of all authors, has been given the opportunity to register their agreement or disagreement to this retraction. We have kept a record of any response received.

References

[1] Y. Wang, S. Kanwal, M. Liaqat, A. Aslam, and U. Bashir, "On Second Gourava Invariant for *q*-Apex Trees," *Journal of Chemistry*, vol. 2022, Article ID 7513770, 7 pages, 2022.

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Research Article

On Second Gourava Invariant for q-Apex Trees

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Let G be a simple connected graph. The second Gourava index of graph G is defined as $GO_2(G) = \sum_{\theta\vartheta\in E(G)} (d(\theta) + d(\vartheta))d(\theta)d(\vartheta)$ where $d(\theta)$ denotes the degree of vertex θ. If removal of a vertex of G forms a tree, then G is called an apex tree. Let $L \subset V(G)$ with $|L| = q$. If removal of L from $V(G)$ forms a tree and any other subset of $V(G)$ whose cardinality is less than $|L|$ does not form a tree, then G is known as q-apex tree. In this paper, we have calculated upper bound for 2$^{\text{nd}}$ Gourava index with respect to q-apex trees.

1. Introduction

Topological index is basic tool in chemical modeling. In molecular graph, atoms are considered as vertices and chemical bonds as edges. Short graph is a combination of vertices and edges. First topological index was Wiener index introduced by Wiener in 1947 to compare the boiling points of few alkane isomers. He observed that this index is highly correlated with the boiling point of alkanes. Later study on QSAR manifested that this index is also helpful to correlate with other quantities like density, critical point, and surface tension. The mathematical formula of this index is

$$W(G) = \sum_{\{\theta,\vartheta\}} d_G(\theta, \vartheta), \tag{1}$$

where $d_G(\theta, \vartheta)$ denotes the distance between the vertices θ and ϑ in G. The detailed study about this invariant is given in [1]. Among degree-based topological indices, the most studied indices are first Zagreb index and second Zagreb index [2]. The first Zagreb index is defined as the sum of square of degrees of all the vertices of a graph, where in second Zagreb index, we take the sum of product of degrees of all those vertices of graph which are linked by an edge. For more information about these chemical invariants, see [3]. The first and second Gourava indices were presented by Kulli in 2017 [4]. These indices are defined as

$$GO_1(G) = \sum_{\theta\vartheta\in E(G)} [d(\theta) + d(\vartheta) + d(\theta)d(\vartheta)], \tag{2}$$

$$GO_2(G) = \sum_{\theta\vartheta\in E(G)} [d(\theta) + d(\vartheta)](d(\theta)d(\vartheta)). \tag{3}$$

A topological index is a numerical number associated with a molecular graph which has significant applications in chemical graph theory, because it is used as a molecular descriptor to investigate physical as well as chemical properties of chemical structure. Therefore, it is a powerful technique in avoiding high cost and long-term laboratory experiments. There are more than 3,000 topological invariants registered till now. Most of these indices have their applications in chemical graph theory. In these molecular descriptors, Gourava and hyper-Gourava invariants are used to find out the physical and chemical properties (such as entropy, acentric factor, and DHAVP) of octane isomers. The first and second Gourava invariants are highly correlated with entropy and acentric factors, respectively.

All graphs considered in our study are simple and connected. Let G be a simple graph with vertex set V and edge set E. For a graph G, the degree of a vertex θ is defined as the number of edges attached to it. The smallest degree of a vertex in G is denoted by $\delta(G)$. The vertex in a graph whose degree is one is known as pendent vertex. The neighborhood of a vertex θ is the set containing all nodes attached with θ, denoted by $N(\theta)$. There are two types of neighborhood, open neighborhood and closed neighborhood. If $N(\theta)$ includes all the other nodes except θ, then it is called open neighborhood but if it includes the node θ, then it is called closed neighborhood. Closed neighborhood of θ is defined as $N[\theta] = N(\theta) \cup \theta$. If we remove one vertex (say) θ from G , then the resulting graph is denoted by $G - \theta$. If we remove subset (say) $X' \subset V$ of vertex set of graph G, then the obtained graph is denoted by $G - X'$. In molecular graph theory, an acyclic connected graph having order λ is known as tree and is denoted by T^*_λ. A tree with order λ is said to be star if central node has degree $\lambda - 1$ while all other nodes are pendent. In other way, a complete bipartite graph $\kappa_{1,\lambda-1}$ is called a star of order λ. Let G_1 and G_2 be two vertex disjoint graphs then their join is denoted by $G_1 + G_2$ having vertex set as a union of their vertex sets, and the edge set contains all the edges of G_1 and G_2 and all those edges obtained by linking each node of G_1 with each node of G_2.

Ali et al. [5] investigated second and third modified Zagreb invariants for T-sum graph operation. Using the obtained results, they computed the second and third modified Zagreb of certain well-known chemical structures like alkanes. Cao et al. [6] give an exact formulas for the upper bounds of modified first Zagreb connection index and second Zagreb connection index for several binary graph operations like corona, Cartesian, and lexicographic product. Using the obtained closed formulas, they computed these invariants for several well-known graphs. In [7], the Gourava index for several graph operations is presented.

In molecular graph theory, apex graphs play a significant role, which can be elucidated as if removal of single vertex or subset of vertex set from a graph G yields a planar graph, then the graph G is known as apex graph [8]. Embedding of apex graphs having face width three are characterized in [9]. By using the same idea, one can explain the apex and q-apex trees. If we remove a vertex from G and the resulting graph is a tree, then that G is called an apex tree [10]. Similarly, if we remove a subset (say) X' of vertex set of cardinality q from G and it results in a tree, then G is known as q -apex tree, provided that the removal of any other subset of vertex set whose cardinality is less than q does not form a tree [10]. A tree is known as trivial apex tree or 0-apex tree.

Therefore, a non-trivial apex tree is one which is not a tree itself but it can be converted into a tree by removing a single or number of vertices. In short, 1-apex tree is a graph which can be made a tree by removing single vertex as shown in Figure 1 (2-apex tree can be converted into a tree by removing 2 vertices as shown in Figure 2) and so on. In fact, apex trees are quasitrees which were introduced by Xu et al. [11]. Xu et al. [12] determined bounds on harary indices in case of apex trees. In 2018, Akhter et al. determined k -apex trees with extremal first reformulated Zagreb index [13].

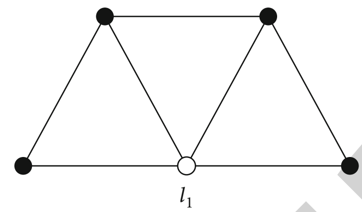

Figure 1: 1-apex tree.

2. Upper Bound of GO_2 for q-Apex Trees

Let $\lambda \geq 3$, $q \geq 1$, and $T^*(\lambda)$, and $T^*_q(\lambda)$ denotes the set of all no-trivial apex trees and q-apex trees on λ vertices, respectively.

Lemma 1. *Let T^* be a tree of order λ, and then*

$$GO_2(T^*) \leq (\lambda - 1)^2 \lambda \tag{4}$$

with equality holds if and only if $T^* = S_\lambda$.

Proof. Since T^* is a tree, it follows that for any edge $\theta\vartheta \in E$ (T^*), we have $N(\theta) \cap N(\vartheta) = \varnothing$. Hence, $d_{T^*}(\theta) + d_{T^*}(\vartheta) = |N(\theta)| + |N(\vartheta)| \leq \lambda$. Now, using the value of $d_{T^*}(\theta) + d_{T^*}(\vartheta)$ in the definition of second Gourava index, we get

$$GO_2(T^*) = \sum_{\theta\vartheta \in E(T^*)} (d(\theta) + d(\vartheta)) d(\theta) d(\vartheta) \leq \lambda \sum_{\theta\vartheta \in E(T^*)} d(\theta) d(\vartheta) \leq \lambda(\lambda - 1)^2. \tag{5}$$

□

Example 2. Let BS (a, b) be bistar graph obtained by joining the apex vertices of two star graph $K_{1,a}$ and $K_{1,b}$ on different vertices with $a, b \geq 1$, and $S_{\lambda,a}$ be the graph obtained by joining a $-$ 1 pendent edges to the end vertex of path $P_{\lambda-a+1}$. Figure 3 depicts the graphs of BS(4, 4) and S^*_{10}, respectively. By definition of second Gourava index, we have $GO_2(S^*_{10}) = 810 > GO_2(BS(4, 4)) = 490$. In Table 1, we have computed the second Gourava index of some classes of trees on 8 vertices. Observe that $GO_2(S^*_8)$ has the maximum value among all other trees.

Lemma 3. *Let $u', v' \in V(G)$ be two nonadjacent vertices of G, and then*

$$GO_2\left(G + u'v'\right) > GO_2(G). \tag{6}$$

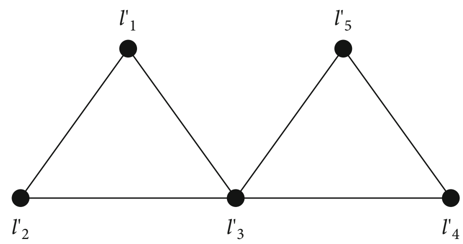

Figure 2: 2-apex tree.

Proof. By definition of $GO_2(G)$, we have

$$GO_2(G) = \sum_{\theta\vartheta\in E(G)} [d(\theta) + d(\vartheta)]d(\theta)d(\vartheta),$$
$$GO_2\left(G + u'v'\right) = \sum_{\theta\vartheta\in E(G)} [d(\theta) + d(\vartheta)]d(\theta)d(\vartheta) + \left[d\left(u'\right) + d\left(v'\right)\right]d\left(u'\right)d\left(v'\right). \quad (7)$$

Since $d(u'), d(v') > 0$, it follows that $\mathrm{GO}_2(G + u'v') > GO_2(G)$. □

Lemma 4. *Let $G \in T^*(\lambda)$ with maximum GO_2 value, and let $x' \in V(G)$ be an apex vertex, and then*

$$\delta(G) = 2, \quad (8)$$

$$d\left(x'\right) = \lambda - 1. \quad (9)$$

Proof.

(1) Suppose $\delta(G) = 1$ and y' is a leaf node in G, then $x'y'$ is not an edge in G and $G + x'y' \in T^*(\lambda)$. Then, by Lemma 3, $\mathrm{GO}_2(G + x'y') > GO_2(G)$ is a contradiction. Next, we prove that $\delta(G) > 2$ is not possible. Suppose $d(\theta) \geq 3$ for all $\theta \in V(G)$, then for any $\theta \in V(G)$, the degree of all vertices in $G - \theta$ is greater or equal to two. This implies that $G - \theta$ is not a tree. Hence, $\delta(G) = 2$.

(2) Suppose $d(x') < (\lambda - 1)$, then there exists a vertex $y' \in V(G)$ with $x'y' \notin EG$. Now, $G + x'y' \in T^*(\lambda)$ and $\mathrm{GO}_2(G + x'y') > GO_2(G)$ are a contradiction. Hence, $d(x') = (\lambda - 1)$.

□

Lemma 5. *Let G_1 and G_2 be two graphs on disjoint vertex sets with $|V(G_1)| = \pi_1$, $|V(G_2)| = \pi_2$, $|E(G_1)| = \varpi_1$, and $|E(G_2)| = \varpi_2$. Then,*

$$\begin{aligned} GO_2(G_1 + G_2) = {} & GO_2(G_1) + GO_2(G_2) + 4\pi_2 M_2(G_1) \\ & + 4\pi_1 M_2(G_2) + 3\pi_2{}^2 M_1(G_1) + 3\pi_1{}^2 M_1(G_2) \\ & + 2\pi_2{}^3 \varpi_1 + 2\pi_1{}^3 \varpi_2 + F(G_1)\pi_2 + F(G_2)\pi_1 \\ & + 2M_1(G_1)\varpi_2 + 2M_1(G_2)\varpi_1 + \pi_1\pi_2[M_1(G_1) \\ & + M_1(G_2)] + 8\varpi_1\varpi_2[\pi_1 + \pi_2] + 4\pi_1\pi_2[\varpi_1\pi_2 \\ & + \varpi_2\pi_1] + 2\pi_1\pi_2[\varpi_1\pi_1 + \varpi_2\pi_2] + \pi_1{}^2\pi_2{}^2[\pi_1 + \pi_2]. \end{aligned} \quad (10)$$

Proof. By definition of second Gourava index,

$$GO_2(G_1 + G_2) = \sum_{\theta\vartheta\in E(G_1+G_2)} \left[d_{G_1+G_2}(\theta) + d_{G_1+G_2}(\vartheta)\right]\left(d_{G_1+G_2}(\theta)d_{G_1+G_2}(\vartheta)\right). \quad (11)$$

Now, using the definition of joint of two graphs having disjoint vertex sets, we get

$$\begin{aligned} GO_2(G_1 + G_2) = {} & \sum_{\theta\vartheta\in E(G_1)} \left[d_{G_1+G_2}(\theta) + d_{G_1+G_2}(\vartheta)\right] d_{G_1+G_2}(\theta)d_{G_1+G_2}(\vartheta) \\ & + \sum_{\theta\vartheta\in E(G_2)} \left[d_{G_1+G_2}(\theta) + d_{G_1+G_2}(\vartheta)\right] d_{G_1+G_2}(\theta)d_{G_1+G_2}(\vartheta) \\ & + \sum_{\{\theta\vartheta;\theta\in V(G_1),\vartheta\in V(G_2)\}} \left[d_{G_1+G_2}(\theta) + d_{G_1+G_2}(\vartheta)\right] d_{G_1+G_2}(\theta)d_{G_1+G_2}(\vartheta). \end{aligned} \quad (12)$$

Let

$$A_1 = \sum_{\theta\vartheta\in E(G_1)} \left[d_{G_1+G_2}(\theta) + d_{G_1+G_2}(\vartheta)\right]\left(d_{G_1+G_2}(\theta)d_{G_1+G_2}(\vartheta)\right),$$

$$B_1 = \sum_{\theta\vartheta\in E(G_2)} \left[d_{G_1+G_2}(\theta) + d_{G_1+G_2}(\vartheta)\right]\left(d_{G_1+G_2}(\theta)d_{G_1+G_2}(\vartheta)\right),$$

$$C_1 = \sum_{\theta\vartheta\in\{\theta\vartheta;\theta\in V(G_1),\vartheta\in V(G_2)\}} \left[d_{G_1+G_2}(\theta) + d_{G_1+G_2}(\vartheta)\right]\left(d_{G_1+G_2}(\theta)d_{G_1+G_2}(\vartheta)\right). \quad (13)$$

Now, using the fact $d_{G_1+G_2}(\theta) = \begin{cases} d_{G_1}(\theta) + \pi_2\,; \theta \in V(G_1) \\ d_{G_2}(\theta) + \pi_1\,; \vartheta \in V(G_2) \end{cases}$ the value of A_1 can be computed

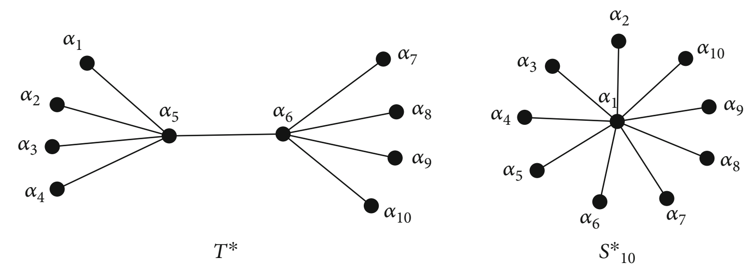

Figure 3: Trees of order 10.

as

$$
\begin{aligned}
A_1 &= \sum_{\theta\vartheta\in E(G_1)} \left[d_{G_1+G_2}(\theta) + d_{G_1+G_2}(\vartheta)\right] d_{G_1+G_2}(\theta) d_{G_1+G_2}(\vartheta) \\
&= \sum_{\theta\vartheta\in E(G_1)} \left[d_{G_1}(\theta) + d_{G_1}(\vartheta) + 2\pi_2\right]\left(d_{G_1}(\theta) + \pi_2\right)\left(d_{G_1}(\vartheta) + \pi_2\right) \\
&= \sum_{\theta\vartheta\in E(G_1)} \left[d_{G_1}{}^2(\theta) d_{G_1}(\vartheta) + d_{G_1}(\theta)^2 \pi_2 + d_{G_1}(\theta) d_{G_1}(\vartheta)\pi_2\right. \\
&\quad + d_{G_1}(\theta)\pi_2{}^2 + d_{G_1}{}^2(\vartheta) d_{G_1}(\theta) + d_{G_1}(\theta) d_{G_1}(\vartheta)\pi_2 + d_{G_1}{}^2(\vartheta)\pi_2 \\
&\quad \left.+ d_{G_1}(\theta)\pi_2{}^2 + 2\pi_2 d_{G_1}(\theta) d_{G_1}(\vartheta) + 2\pi_2{}^2 d_{G_1}(\theta) + 2\pi_2{}^2 d_{G_1}(\vartheta) + 2\pi_2\right] \\
&= \sum_{\theta\vartheta\in E(G_1)} \left[d_{G_1}{}^2(\theta) d_{G_1}(\vartheta) + d_{G_1}{}^2(\vartheta) d_{G_1}(\theta)\right] + \pi_2 \sum_{\theta\vartheta\in E(G_1)} \left[d_{G_1}{}^2(\theta) + d_{G_1}{}^2(\vartheta)\right] \\
&\quad + 4\pi_2 \sum_{\theta\vartheta\in E(G_1)} \left[d_{G_1}(\theta) d_{G_1}(\vartheta)\right] + 3\pi_2{}^2\left[d_{G_1}(\theta) + d_{G_1}(\vartheta)\right] + 2\pi_2{}^3 \sum_{\theta\vartheta\in E(G_1)} .
\end{aligned}
\tag{14}
$$

Similarly,

$$
B_1 = GO_2(G_2) + \pi_1 F(G_2) + 4\pi_1 M_2(G_2) + 3\pi_1{}^2 M_1(G_2) + 2\pi_1{}^3 \varpi_2. \tag{15}
$$

The value of C_1 can be calculated as

$$
\begin{aligned}
C_1 &= \sum_{\theta\vartheta\in\{\theta\vartheta;\theta\in V(G_1),\vartheta\in V(G_2)\}} \left[d_{G_1+G_2}(\theta) + d_{G_1+G_2}(\vartheta)\right]\left(d_{G_1+G_2}(\theta) d_{G_1+G_2}(\vartheta)\right) \\
&= \sum_{\theta\in V(G_1),\vartheta\in V(G_2)} \left[d_{G_1}(\theta) + \pi_2 + d_{G_2}(\vartheta) + \pi_1\right]\left(\left(d_{G_1}(\theta) + \pi_2\right)\left(d_{G_2}(\vartheta) + \pi_1\right)\right) \\
&= \sum_{\theta\in V(G_1),\vartheta\in V(G_2)} \left[d_{G_1}{}^2(\theta) d_{G_2}(\vartheta) + d_{G_1}{}^2(\theta)\pi_1 + d_{G_2}(\vartheta) d_{G_1}(\theta)\pi_2\right. \\
&\quad + d_{G_1}(\theta)\pi_2\pi_1 + d_{G_1}(\theta) d_{G_2}{}^2(\vartheta) + d_{G_1}(\theta) d_{G_2}(\vartheta)\pi_1 + d_{G_2}{}^2(\vartheta)\pi_2 \\
&\quad + d_{G_2}(\vartheta)\pi_1\pi_2 + d_{G_1}(\theta) d_{G_2}(\vartheta)\pi_1 + d_{G_1}(\theta)\pi_1{}^2 + d_{G_2}(\vartheta)\pi_1\pi_2 + \pi_1{}^2\pi_2 \\
&\quad + d_{G_1}(\theta) d_{G_2}(\vartheta)\pi_2 + d_{G_1}(\theta)\pi_1\pi_2 + d_{G_2}(\vartheta)\pi_2{}^2 + \pi_1\pi_2{}^2 = 2M_1(G_1)\varpi_2 \\
&\quad + 2M_1(G_2)\varpi_1 + \pi_1\pi_2[M_1(G_1) + M_1(G_2)] + 8\varpi_1\varpi_2[\pi_1 + \pi_2] \\
&\quad + 4\pi_1\pi_2[\varpi_1\pi_2 \quad + \varpi_2\pi_1] + 2\pi_1\pi_2[\varpi_1\pi_1 + \varpi_2\pi_2] + \pi_1{}^2\pi_2{}^2[\pi_1 + \pi_2].
\end{aligned}
\tag{16}
$$

Table 1: $GO_2(T^*)$ of certain trees T^* of order 8.

T^*	$GO_2(T^*)$
S_8	392
BS (5, 1)	312
BS (4, 2)	264
BS (3, 3)	248
$S_{8,5}$	212
$S_{8,4}$	146
$S_{8,3}$	108

Now, using the values of A_1, B_1, and C_1 in Equation (2), we get

$$
\begin{aligned}
GO_2(G_1 + G_2) = {} & GO_2(G_1) + GO_2(G_2) + 4\pi_2 M_2(G_1) + 4\pi_1 M_2(G_2) \\
& + 3\pi_2{}^2 M_1(G_1) + 3\pi_1{}^2 M_1(G_2) + 2\pi_2{}^3\varpi_1 + 2\pi_1{}^3\varpi_2 \\
& + F(G_1)\pi_2 + F(G_2)\pi_1 + 2M_1(G_1)\varpi_2 + 2M_1(G_2)\varpi_1 \\
& + \pi_1\pi_2[M_1(G_1) + M_1(G_2)] + 8\varpi_1\varpi_2[\pi_1 + \pi_2] \\
& + 4\pi_1\pi_2[\varpi_1\pi_2 + \varpi_2\pi_1] + 2\pi_1\pi_2[\varpi_1\pi_1 + \varpi_2\pi_2] \\
& + \pi_1{}^2\pi_2{}^2[\pi_1 + \pi_2].
\end{aligned}
\tag{17}
$$

□

Theorem 6. *Let $G \in T^*(\lambda)$ and $\lambda \geq 5$, and then*

$$
GO_2(G) \leq 6\lambda^3 - 14\lambda^2 + 2\lambda + 6, \tag{18}
$$

with equality holds if $G = \kappa_1 + S_{\lambda-1}$.

Proof. Let $G \in T^*(\lambda)$ with maximum GO_2 value. By Lemma 4, we have $G = \kappa_1 + T^*_{\lambda-1}$. Let the cardinality of vertex sets of κ_1 and $T^*_{\lambda-1}$ be ρ_1 and ρ_2 where cardinality of their edge sets is ς_1 and ς_2, respectively. Now by, using Lemma 1., we

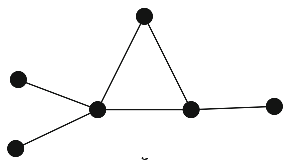

Figure 4: 1-apex tree.

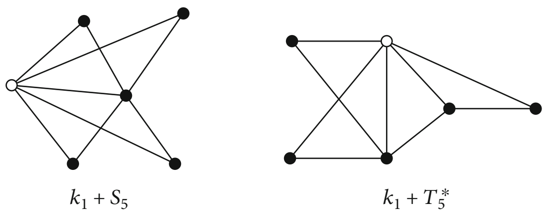

Figure 5: 1-apex tree.

Table 2: GO_2 value of some 1-apex trees of order 8.

$\kappa_1 + T^*_{(\lambda-1)}$	$GO_2\left(\kappa_1 + T^*_{(\lambda-1)}\right)$
$\kappa_1 + S_7$	2198
$\kappa_1 + BS(4,1)$	1962
$\kappa_1 + S_{7,4}$	1758
$\kappa_1 + S_{7,3}$	1634
$\kappa_1 + BS(3,2)$	1277

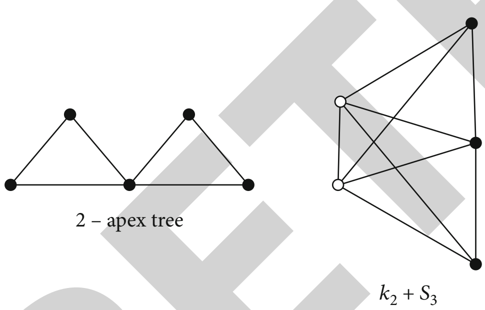

Figure 6: 1-apex tree.

Table 3: GO_2 values of some 2-apex trees on 9 vertices.

$\kappa_2 + T^*_{(\lambda-2)}$	$GO_2\left(\kappa_2 + T^*_{(\lambda-2)}\right)$
$\kappa_2 + S_7$	7824
$\kappa_2 + BS(4,1)$	7344
$\kappa_2 + S_{7,4}$	7108
$\kappa_2 + S_{7,3}$	6712
$\kappa_2 + BS(3,2)$	6684

have

$$\begin{aligned}GO_2(\kappa_1 + T^*_{\lambda-1}) &= GO_2(\kappa_1) + GO_2(T^*_{\lambda-1}) + 4\rho_2 M_2(\kappa_1)\\ &+ 4\rho_1 M_2(T^*_{\lambda-1}) + 3\rho_2{}^2 M_1(\kappa_1) + 3\rho_1{}^2 M_1(T^*_{\lambda-1})\\ &+ 2\rho_2{}^3\varsigma_1 + 2\rho_1{}^3\varsigma_2 + F(\kappa_1)\rho_2 + F(T^*_{\lambda-1})\rho_1\\ &+ 2M_1(\kappa_1)\varsigma_2 + 2M_1(T^*_{\lambda-1})\varsigma_1 + \rho_1\rho_2[M_1(\kappa_1)\\ &+ M_1(T^*_{\lambda-1})] + 8\varsigma_1\varsigma_2[\rho_1 + \rho_2] + 4\rho_1\rho_2[\varsigma_1\rho_2 + \varsigma_2\rho_1]\\ &+ 2\rho_1\rho_2[\varsigma_1\rho_1 + \varsigma_2\rho_2] + \rho_1{}^2\rho_2{}^2[\rho_1 + \rho_2] \le (\lambda-1)^2(\lambda+3)\\ &+ 7\left(\lambda^2 - 3\lambda + 2\right) + \left(3\lambda^3 - 12\lambda^2 + 15\lambda - 6\right)\\ &+ \left(\lambda^3 - 6\lambda^2 + 15\lambda - 14 + \left(\lambda^3 - 2\lambda^2 + \lambda = 6\lambda^3 - 14\lambda^2 + 2\lambda + 6.\right.\right.\end{aligned} \tag{19}$$

□

Example 7. Let $G_1 = \kappa_1 + S_{6-1}$, $G_2 = \kappa_1 + T_5^*$ as depicted in Figure 4 and G_3 be 1 -apex tree of order 6 as shown in Figure 5. Then, the values of second Gourava index of these 1-apex trees are $GO_2(G_1) = 810$, $GO_2(G_1) = 720$, and $GO_2(G_1) = 214$. Table 2 depicts the values second Gourava index of some graphs in the class of 1-apex trees of order 8. Observe that GO_2 *of* $\kappa_1 + S_7$ is maximum among all other graphs.

Theorem 8. *Let $q \ge 2$, $\lambda \ge 5$, and $G \in T_q^*(\lambda)$, and then*

$$GO_2(G) \le \left(q + q^2\right)(\lambda - 1)^3 + (\lambda + q)(\lambda - 1)\left(\lambda(q+1)^2 - (q+1)^3\right) \tag{20}$$

with equality holds if $G = \kappa_q + S_{\lambda-q}$

Proof. We prove it by induction the value of q. For $q = 1$, the result follows from Theorem 6. Suppose the result is true for $q - 1$ apex trees, let $G \in T_q^*(\lambda)$ with maximum GO_2 and $V_q \subset V(G)$ be the set of q-apex vertices. Since $GO_2(G + u'v') > GO_2(G)$ for any nonadjacent edges $u', v' \in V(G)$, it follows that V_q is a clique in G. Hence, $d(u') = \lambda - 1$ for all $u' \in V_q$, and the number of edges m' of the graph G is

$$m' = \frac{1}{2}\left(q^2 + q\right) + (q+1)\lambda - (q+1)^2. \tag{21}$$

Let x' be an apex vertex and $V_{q-1} = V_q - x'$. Observe that $d(x') = \lambda - 1$ and $G - x'$ are an $(q-1)$-apex tree. Then,

$$GO_2\left(G - x'\right) = \sum_{\theta\vartheta\in E\left(G-x'\right)(d_G(\theta) - 1 + d_G(\vartheta) - 1)((d_G(\theta) - 1)}$$

$$(d_G(\vartheta) - 1)) = \sum_{\theta\vartheta\in E(G-x')} [(d_G(\theta) + d_G(\vartheta) - 2)(d_G(\theta)d_G(\vartheta) -$$

$$d_G(\theta) - d_G(\vartheta) + 1)] = \sum_{\theta\vartheta\in E(G-x')} [d_G^2(\theta)d_G(\vartheta) - (d_G^2(\theta) - d_G(\theta)$$

$$d_G(\vartheta) + d_G(\theta) + d_G(\theta)d_G^2(\vartheta) - d_G(\theta)d_G(\vartheta) - d_G^2(\vartheta) + d_G(\vartheta)$$

$$-2d_G(\theta)d_G(\vartheta) + 2d_G(\theta) + 2d_G(\vartheta) - 2] = \sum_{\theta\vartheta\in E(G-x')} [d_G^2(\theta)d_G($$

$$\vartheta) + d_G(\theta)d_G^2(\vartheta)] - \sum_{\theta\vartheta\in E(G-x')} (d_G^2(\theta) + d_G^2(\vartheta)) - 4\sum_{\theta\vartheta\in E(G-x')} (d_G$$

$$(\theta)d_G(\vartheta)) + 3\sum_{\theta\vartheta\in E(G-x')}(d_G(\theta)+d_G(\vartheta)) - \sum_{\theta\vartheta\in E(G-x')} = \sum_{\theta\vartheta\in E(G-x')}[d_G^2(\theta)d_G(\vartheta)+d_G(\theta)d_G^2(\vartheta)] - \sum_{\theta\vartheta\in E(G-x')}(d_G^2(\theta)+d_G^2(\vartheta)) + \sum_{x'\theta\in E(G)}[(\lambda-1)^2 d_G(\theta)+(\lambda-1)d_G^2(\theta)] - \sum_{x'\theta\in E(G)}[(\lambda-1)^2 + d_G^2(\theta)] - \sum_{x'\theta\in E(G)}[(\lambda-1)^2 d_G(\theta)+(\lambda-1)d_G^2(\theta)] + \sum_{x'\theta\in E(G)}[(\lambda-1)^2 + d_G^2(\theta)] - 4\sum_{\theta\vartheta\in E(G-x')}(d_G(\theta)d_G(\vartheta)) + 3\sum_{\theta\vartheta\in E(G-x')}(d_G(\theta)+d_G(\vartheta)) - 4\sum_{x'\theta\in E(G)}(\lambda-1)d_G(\theta) + 3\sum_{x'\theta\in E(G)}((\lambda-1)+d_G(\theta)) + 4\sum_{x'\theta\in E(G)}(\lambda-1)d_G(\theta) - 3\sum_{x'\theta\in E(G)}((\lambda-1)+d_G(\theta)) - 2(m'-\lambda+1) = \sum_{\theta\vartheta\in E(G)}[d_G^2(\theta)d_G(\vartheta)+d_G(\theta)d_G^2(\vartheta)] - \sum_{\theta\vartheta\in E(G)}(d_G^2(\theta)+d_G^2(\vartheta)) - 4\sum_{\theta\vartheta\in E(G)}(d_G(\theta)d_G(\vartheta)) + 3\sum_{\theta\vartheta\in E(G)}(d_G(\theta)+d_G(\vartheta)) - \sum_{x'\theta\in E(G)}[(\lambda-1)^2 d_G(\theta)+(\lambda-1)d_G^2(\theta)] + \sum_{x'\theta\in E(G)}[(\lambda-1)^2+d_G^2(\theta)] + 4\sum_{x'\theta\in E(G)}(\lambda-1)d_G(\theta) - 3\sum_{x'\theta\in E(G)}((\lambda-1)+d_G(\theta)) - 2(m'-\lambda+1). \tag{22}$$

$$GO_2\left(G-x'\right) = GO_2(G) - F(G) - 4M_2(G)$$

$$+3M_1(G) - (\lambda-1)^2\Big(\sum_{\theta\in V(G-x')}(d_G(\theta)) + (\lambda-1) - (\lambda-1) - (\lambda-1)\Big)\Big[\sum_{\theta\in V(G-x')} d_G^2(\theta) + (\lambda-1)^2 - (\lambda-1)^2\Big] + (\lambda-1)^3 + \Big[\sum_{\theta\in V(G-x')} d_G^2(\theta) + (\lambda-1)^2 - (\lambda-1)^2\Big] + 4(\lambda-1)\Big(\sum_{\theta\in V(G-x')}(d_G(\theta)) + (\lambda-1) - (\lambda-1)\Big) - 3(\lambda-1)^2 - 3\Big(\sum_{\theta\in V(G-x')}(d_G(\theta)) + (\lambda-1) - (\lambda-1)\Big) - 2(m'-\lambda+1) = GO_2(G) - F(G) - 4M_2(G) + 3M_1(G) - (\lambda-1)^2\Big(\sum_{\theta\in V(G)}(d_G(\theta)) - (\lambda-1)\Big) - (\lambda-1)\Big[\sum_{\theta\in V(G)} d_G^2(\theta) - (\lambda-1)^2\Big] + (\lambda-1)^3\Big[\sum_{\theta\in V(G)} d_G^2(\theta) - (\lambda-1)^2\Big] + 4(\lambda-1)\Big(\sum_{\theta\in V(G)}(d_G(\theta))(\lambda-1)\Big) - 3(\lambda-1)^2 - 3\Big(\sum_{\theta\in V(G-x')}(d_G(\theta)) - (\lambda-1)\Big) - 2(m'-\lambda+1) = GO_2(G) - F(G) - 4M_2(G) + 3M_1(G) - (\lambda-1)^2(2m'-\lambda+1) - (\lambda-1)[M_1(G) - (\lambda-1)^2] + (\lambda-1)^3 + [M_1(G) - (\lambda-1)^2] + 4(\lambda-1)(2m'-\lambda+1) - 3(\lambda-1)^2 - 3(2m'-\lambda+1) - 2(m'-\lambda+1) = GO_2(G) - F(G) - 4M_2(G) + M_1(G)(5-\lambda) + 3(\lambda-1)^3 - 8(\lambda-1)^2 + 8m'\lambda - 16m' + 5\lambda - 5 - 2(\lambda-1)^2 m'.$$

Hence, we get

$$GO_2(G) = GO_2\left(G-x'\right) + F(G) + 4M_2(G)(\lambda-5)M_1(G) - 3(\lambda-1)^3 + 8(\lambda-1)^2 - 8m'\lambda + 16m' - 5\lambda + 5 + 2(\lambda-1)^2 m'. \tag{24}$$

Since $GO_2(G-x') = (q^2-q)(\lambda-1)^3 + (\lambda-q-1)(\lambda+q-2)(q^2\lambda-2q)$ and for $q\geq 2, \lambda\geq 5$, we have

$$M_1(G) \leq (q+1)\left(\lambda^2-2\lambda+1\right) + \lambda(q+1)^2 - (q+1)^3, \tag{25}$$

$$M_2(G) \leq \frac{1}{2}\left(q^2+q\right)\left(\lambda^2-2\lambda+1\right) + (\lambda-1)\left(\lambda(q+1)^2-(q+1)^3\right), \tag{26}$$

$$F(G) \leq (q+1)\left(\lambda^3-3\lambda^2+3\lambda-1\right) + \left(\lambda(q+1)^3-(q+1)^4 m' = \frac{1}{2}\left(q^2+q\right) + (q+1)\lambda - (q+1)^2.\right. \tag{27}$$

Using all the values in the above equation, we get

$$\begin{aligned} GO_2(G) \leq{}& \left(q^2-q\right)(\lambda-1)^3 + (\lambda-q-1)(\lambda+q-2)\left(q^2\lambda-2q\right) \\ &+ (q+1)\left(\lambda^3-3\lambda^2+3\lambda-1\right) + \left(\lambda(q+1)^3-(q+1)^4\right. \\ &+ 4\left(\frac{1}{2}\left(q^2+q\right)\left(\lambda^2-2\lambda+1\right) + (\lambda-1)\left(\lambda(q+1)^2-(q+1)^3\right)\right) \\ &+ (\lambda-5)(q+1)\left(\lambda^2-2\lambda+1\right) + \lambda(q+1)^2 - (q+1)^3 - 3(\lambda-1)^3 \\ &+ 8(\lambda-1)^2 - 8\lambda\left(\frac{1}{2}\left(q^2+q\right) + (q+1)\lambda - (q+1)^2\right) \\ &+ 16\left(\frac{1}{2}\left(q^2+q\right) + (q+1)\lambda - (q+1)^2\right) \\ &- 5\lambda + 5 + 2(\lambda-1)^2\left(\frac{1}{2}\left(q^2+q\right) + (q+1)\lambda - (q+1)^2\right). \end{aligned} \tag{28}$$

After simplification, we have

$$GO_2(G) \leq \left(q+q^2\right)(\lambda-1)^3 + (\lambda+q)(\lambda-1)\left(\lambda(q+1)^2-(q+1)^3\right) \tag{29}$$

□

Example 9. Let G_1 and $G_2 = \kappa_2 + S_{5-2}$ be 2 *-apex trees of* order 5 as shown in Figure 6. Then, $GO_2(G_1) = 224$ and $GO_2(G_2) = 888$. Table 3 depicts the values of some 2 apex trees on 9 vertices. Observe that GO_2 value of $\kappa_2 + S_7$ is the maximum among all others.

3. Conclusion

In our present discussion, we have determined the maximum value of second Gourava invariant for q-apex trees. In future, it would be interesting to find the same results for those chemical invariants which are not investigated till now.

Data Availability

No data is required to support the study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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