Research Article

On Acyclic Structures with Greatest First Gourava Invariant

Mariam Imtiaz,1 Maria Naseem,2 Misbah Arshad,3 Salma Kanwal4, and Maria Liaqat4

1University of Engineering and Technology, KSK Campus, Lahore, Pakistan
2Department of Mathematics, Faculty of Science, University of Central Punjab, Lahore, Pakistan
3COMSATS University Islamabad, Sahiwal Campus, Pakistan
4Lahore College for Women University, Lahore, Pakistan

Correspondence should be addressed to Salma Kanwal; salma.kanwal055@gmail.com

Received 27 December 2021; Accepted 1 April 2022; Published 25 April 2022

Copyright © 2022 Mariam Imtiaz et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

1. Introduction

Topological index is very basic tool in chemical modeling. In molecular graph, atoms are considered as vertices and chemical bonds as edges. In short, the graph is a combination of vertices and edges. First chemical index was Wiener index introduced by Wiener [1] in 1947 to compare the boiling points of few alkanes isomers; he revealed that this index is highly agreed with the boiling point of molecules 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 given as

\[ W(\xi) = \sum_{(\mu, \eta)} d_\xi(\mu, \eta), \]

where \( d_\xi(\mu, \eta) \) indicates the distance between the vertices \( \mu \) and \( \eta \) in \( \xi \). The most studied degree-based indices, i.e., Zagreb indices introduced by Gutman and Das [2], are defined as follows

\[ M_1(\xi) = \sum_{\mu, \eta \in V(\xi)} (d_\xi(\mu))^2 = \sum_{\mu, \eta \in E(\xi)} (d_\xi(\mu) + d_\xi(\eta)), \]
\[ M_2(\xi) = \sum_{\mu, \eta \in E(\xi)} (d_\xi(\mu)d_\xi(\eta)). \]

Some properties about these indices are depicted in [3, 4]. The 1st and 2nd reformulated Zagreb indices were regener-ated by Miličević’ et al. [5] in terms of edge degree, defined as

\[ EM_1(\xi) = \sum_{f_i \in E(\xi)} \left( d_{f_i} \right)^2, \]
\[ EM_2(\xi) = \sum_{f_i \neq f_j} d_{f_i}d_{f_j}. \]

The 1st and 2nd Gourava indices were presented by V. R. Kulli in 2017 [6]. These indices are defined as

\[ GO_1(\xi) = \sum_{\mu, \eta \in E(\xi)} [d(\mu) + d(\eta) + d(\mu)d(\eta)], \]
\[ GO_2(\xi) = \sum_{\mu, \eta \in E(\xi)} [d(\mu) + d(\eta)][d(\mu)d(\eta)]. \]

A topological index is a mathematical formula, 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 3,000 topological invariants registered till now. All 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 1st and 2nd Gourava invariants highly correlate with entropy and acentric factor, respectively.

In [7], the graph operations for Gourava index are presented. In our present study, we considered that all graphs are simple and connected. For any graph, the degree of a vertex is defined as the number of edges attached to it. The smallest degree of graph $\xi$ is represented by $\delta(\xi)$. The vertex in a graph whose degree is one is known as pendant vertex. The neighborhood of a vertex $\mu$ is the set of all nodes attached with $\mu$, represented by $N(\mu)$. There are two types of neighborhood, open neighborhood and closed neighborhood. If $N(\mu)$ includes all the other nodes except $\mu$, then it is called open neighborhood, but if it includes the node $\mu$, then it is called closed neighborhood. Closed neighborhood is defined as $N[\mu] = N(\mu) \cup \{\mu\}$ (for further notations in graph theory, we refer [8]).

Some bounds of reformulated Zagreb indices are given in [9]. In 2012, Xu and Das [10] established some graph transformations that maximize or minimize the multiplicative sum Zagreb index of graphs and used these graph transformations to determine the extremal graphs among trees, unicyclic, and bicyclic graphs for multiplicative sum Zagreb index. Two years later, in 2014, Ji et al. [11] extended the work of Xu and Das [10] for the 1st reformulated Zagreb index. In 2017, Gao et al. [12] used the same graph transformations as given in [11] to compute the similar results as computed in [11] but for the hyper-Zagreb index.

Tomescu and Kanwal [13] in 2013 introduced some graph transformations to compute the general sum-connectivity index for acyclic connected graphs of given diameter, order, and pendant vertices and determined the corresponding extremal trees and gave the ordering of trees with minimum general sum-connectivity index. Illic et al. in 2011 [14] used some graph transformations to find the bounds for unicyclic and bicyclic graphs with respect to degree distance index. Liu et al. [15] analyzed the newly introduced chemical invariant termed as Mostar invariant for tree-like phenylenes and provided a detailed discussion for the obtained results. Liu et al. [16], provided an ordering of acyclic, bicyclic, and tricyclic structures with respect to recently introduced invariants Sombor and reduced Sombor invariants. In [17], Liu et al. determined some degree-based chemical invariants for octahedron networks. Qi et al. [18] put forward computations of several degree-based chemical invariants for rhombus-type silicate and oxide structures. In [19], the authors investigated several degree-based invariants for planar octahedron networks and made comparison of obtained numerical results. Hu et al. [20] analyzed certain distance-based invariants for chemical interconnection networks and analyzed their behavior.

In this work, we are aimed to determine the acyclic structures having maximum values of first Gourava invariant and put forward acyclic structures attaining first five greatest values of first Gourava invariant. Plan of work and methodology behind attaining main results of this work is to apply certain edge swapping transformations to acyclic graphs and observe the behavior of first Gourava invariant. We will see that it increased for the resultant graph and eventually leads us to acyclic structures with the first five bigger values of above-mentioned invariant.

2. Gourava Index and Graph Transformations

In this section, we use certain graph transformations presented by Ji et al. [11]. Further, we will notice that these transformations increase the $GO_1$ for trees. These transformations are narrated below.

In $B_1$-transformation, let $\xi$ be a nontrivial connected graph having vertices $\mu, \eta \in \xi$, such that $N(\eta) = \mu_i, \eta_1, \eta_2, \cdots, \eta_{1,h}$ and $N(\mu) = \eta_1, \mu_1, \mu_2, \cdots, \mu_{1,f}$, where $\eta_1$ and $\mu_1$ have no common neighbors in $\xi$, $f \geq 0$ and $h \geq 1$.

Let $\xi'$ be the graph obtained after applying $B_1$-transformation, such that $\xi' = \xi - \eta_1\eta_1, \eta_1\eta_2, \cdots, \eta_1\eta_{1,h} + \mu_1\mu_1, \mu_1\mu_2, \cdots, \mu_1\mu_{1,f}$ as explained in Figure 1.

Lemma 1. Let $\xi$ be a connected graph with no cycle and $\xi'$ be a graph obtained after applying $B_1$-transformation (as shown in Figure 1), and then, $GO_1(B_1(\xi)) = GO_1(\xi') > GO_1(\xi)$ for any $f, h \geq 1$.

Proof. From Figure 1, $d_\xi \cdot f = f + h + 1$ and $d_{\xi'}(\eta) = 1$. We can easily guess that degree of $\mu_i$ increases, while degree of $\eta_i$ decreases after applying transformation, and all other vertices preserve their degrees.

$$GO_1(\xi') - GO_1(\xi) = \sum_{i=1}^f \left\{ d_{\xi'}(\mu_{1,i}) + d_{\xi'}(\mu_{1}) + d_{\xi'}(\mu_{1,i})d_{\xi'}(\mu_{1}) \right\} + \sum_{j=1}^h \left\{ d_{\xi'}(\eta_{1,j}) + d_{\xi'}(\mu_{1}) + d_{\xi'}(\eta_{1,j})d_{\xi'}(\mu_{1}) \right\} + \left\{ d_{\xi'}(\mu_{1}) + d_{\xi'}(\eta_{1,i}) + d_{\xi'}(\mu_{1})d_{\xi'}(\eta_{1,i}) \right\} - \sum_{i=1}^f \left\{ d_{\xi'}(\mu_{1,i}) + d_{\xi'}(\mu_{1}) + d_{\xi'}(\mu_{1,i})d_{\xi'}(\mu_{1}) \right\} - \sum_{j=1}^h \left\{ d_{\xi'}(\eta_{1,j}) + d_{\xi'}(\eta_{1,i}) + d_{\xi'}(\eta_{1,j})d_{\xi'}(\eta_{1,i}) \right\} - \left\{ d_{\xi'}(\mu_{1}) + d_{\xi'}(\eta_{1,i}) + d_{\xi'}(\mu_{1})d_{\xi'}(\eta_{1,i}) \right\}.$$
Let \( B_2(\gamma, b) \) be an acyclic graph, and \( \gamma \) and \( b \) be obtained after applying \( B_2 \)-transformation (as shown in Figure 2) where \( d_\xi(y_1, b_1) \geq 1 \); then,

\[
GO_1(B_2(\xi)) = GO_1(\xi') > GO_1(\xi),
\]

for any \( f > 1 \) and \( h, \xi \geq 1 \).

**Lemma 2.** Let \( \xi \) be an acyclic graph, and \( \xi' \) is obtained after applying \( B_2 \)-transformation (as shown in Figure 2) where \( d_\xi(y_1, b_1) \geq 1 \); then,

\[
GO_1(B_2(\xi)) = GO_1(\xi') > GO_1(\xi),
\]

for any \( f > 1 \) and \( h, \xi \geq 1 \).

**Proof.** Here \( d_\xi'(\mu_{ij}) = d_\xi(\mu_{ij}) \), and \( d_\xi'(\eta_{ij}) = d_\xi(\eta_{ij}) \), and after transformation, \( d_\xi'(\mu_1) > d_\xi(\mu_1) \) and \( d_\xi'(\eta_1) < d_\xi(\eta_1) \).

\[
GO_1(\xi') > GO_1(\xi)
\]

\[
= \sum_{j=1}^{f} \left\{ \left( d_\xi'(\eta_{ij}) + d_\xi'(\mu_1) + d_\xi'(\mu_{ij})d_\xi'(\mu_1) \right) - \left( d_\xi(\mu_1) + d_\xi(\mu_{ij})d_\xi(\mu_1) \right) \right\} + \sum_{j=1}^{h} \left\{ \left( d_\xi'(\eta_{ij}) + d_\xi(\mu_1) + d_\xi(\eta_{ij})d_\xi(\mu_1) \right) - \left( d_\xi(\eta_{ij}) + d_\xi(\mu_{ij})d_\xi(\mu_1) \right) \right\}
\]

\[
= \sum_{j=1}^{f} \left\{ \left( d_\xi'(\mu_{ij}) + (f + h + 1)(f + h + 1)d_\xi'(\mu_{ij}) \right) - \left( d_\xi(\mu_{ij}) + (f + 1)(f + 1)d_\xi(\mu_{ij}) \right) \right\} + \sum_{j=1}^{h} \left\{ \left( d_\xi'(\eta_{ij}) + (f + h + 1)(f + h + 1)d_\xi'(\eta_{ij}) \right) + \left( d_\xi(\eta_{ij}) + (f + 1)(f + 1)d_\xi(\eta_{ij}) \right) \right\}
\]

\[
= \sum_{j=1}^{f} \left\{ h + h d_\xi(\mu_{ij}) \right\} + \sum_{j=1}^{h} \left\{ f + f d_\xi(\eta_{ij}) \right\} - fh
\]

\[
= \sum_{j=1}^{f} \left\{ h + h d_\xi(\mu_{ij}) \right\} + \sum_{j=1}^{h} \left\{ f + f d_\xi(\eta_{ij}) \right\} - fh
\]

\[
= \sum_{j=1}^{f} \left\{ h f d_\xi(\mu_{ij}) + h f d_\xi(\eta_{ij}) + h f \right\}
\]

\[
= \sum_{j=1}^{f} \left\{ h f d_\xi(\mu_{ij}) + d_\xi(\eta_{ij}) + 1 \right\} > 0 \Rightarrow GO_1(B_2(\xi))
\]

\[
GO_1(\xi') > GO_1(\xi)
\]

(5)

\[
□
\]
\[
\begin{align*}
\{ (f+1) + (h+2) + (f+1)(h+2) \} \\
+ \{ 2 + (\ell + 1) + 2(\ell + 1) \} \\
- \{ (h+2) + (\ell + 1) + (h+2)(\ell + 1) \}
\end{align*}
\]
\[
\sum_{j=1}^{h} \left[ h + h d_x (\mu_{1j}) \right] + \sum_{j=1}^{h} \left[ (f-1) + (f-1) d_x (\eta_{1j}) \right] + (h - hf) + (-2h - ht)
\]
\[
f \left[ h + h d_x (\mu_{1j}) \right] + h \left[ (f-1) + (f-1) d_x (\eta_{1j}) \right] + (h - hf) + (-2h - ht)
\]
\[
hf + hf + hf - h + hf - h + h - hf - 2h - ht
\]
\[
3hf - 3h - ht = h[3f - (\ell + 3)] > 0 \Rightarrow \text{GO}_1(B_2(\xi)) = \text{GO}_1(\xi).
\]

Lemma 3. Let \( \xi \) be an acyclic graph and \( B_2(\xi) = \xi' \) is obtained after applying \( B_2 \)-transformation (as shown in Figure 3), where \( d_x (\mu_{1j}, \eta_{ij}) = d_{B_2(\xi)} (\mu_{1j}, \eta_{ij}) \geq 2 \) and \( d_x (\gamma_{j1}, g_{j3}) = d_{B_2(\xi)} (\gamma_{j1}, g_{j3}) \geq 0 \). If \( f > 1, h, \ell \geq 1 \), then

\[
\text{GO}_1(B_2(\xi)) = \text{GO}_1(\xi') > \text{GO}_2(\xi)
\]

Proof. Like the previous lemma, we have

\[
\text{GO}_1(\xi) = \sum_{j=1}^{f} \left[ d_x (\mu_{1j}) + d_x (\mu_{1j}) + d_x (\mu_{1j}) d_x (\mu_{1j}) \right] + \sum_{j=1}^{h} \left[ d_x (\eta_{1j}) + d_x (\mu_{1j}) + d_x (\eta_{1j}) d_x (\mu_{1j}) \right] + d_x (\mu_{1j}) + d_x (\gamma_{j1}) + d_x (\eta_{1j}) d_x (\gamma_{j1}) - \sum_{j=1}^{f} [d_x (\mu_{1j}) + d_x (\mu_{1j}) + d_x (\mu_{1j}) d_x (\mu_{1j})]
\]

\[
\begin{align*}
- \sum_{j=1}^{h} \left\{ d_x (\eta_{1j}) + d_x (\eta_{1j}) + d_x (\eta_{1j}) d_x (\eta_{1j}) \right\} \\
- \{ d_x (\mu_{1j}) + d_x (\mu_{1j}) + d_x (\mu_{1j}) d_x (\mu_{1j}) \} \\
- \{ d_x (\mu_{1j}) + d_x (\mu_{1j}) + d_x (\mu_{1j}) d_x (\mu_{1j}) \}
\end{align*}
\]

\[
\begin{align*}
= \sum_{j=1}^{f} \left[ d_x (\mu_{1j}) + d_x (\mu_{1j}) + d_x (\mu_{1j}) d_x (\mu_{1j}) \right] + \sum_{j=1}^{h} \left[ d_x (\eta_{1j}) + d_x (\mu_{1j}) + d_x (\eta_{1j}) d_x (\mu_{1j}) \right] + d_x (\mu_{1j}) + d_x (\gamma_{j1}) + d_x (\eta_{1j}) d_x (\gamma_{j1}) - \sum_{j=1}^{f} [d_x (\mu_{1j}) + d_x (\mu_{1j}) + d_x (\mu_{1j}) d_x (\mu_{1j})]
\end{align*}
\]

\[
\begin{align*}
\text{GO}_1(B_2(\xi)) = \text{GO}_1(\xi') > \text{GO}_2(\xi)
\end{align*}
\]
\[ f(h) = fh + fh - h + fh - h + h = 4h - 4h = |h - hf - (l + 4)| > 0 \Rightarrow G_1(B_1(\xi)) > G_1(\xi) \]  

\[ G_1(\xi') > G_1(\xi) \]

\[ \text{Lemma 4: Let } \xi \text{ be acyclic connected graph, and } \xi' = B_1(\xi) \text{ is obtained after applying } B_j \text{-transformation (as shown in Figure 4) for any } f > (l - 1) \text{; we have } G_1(B_1(\xi)) = G_1(\xi') > G_1(\xi). \]

\[ \text{Proof. Since } d_j(\mu_1, y_{1}) \geq 1, \text{ and if } d_k(\mu_1, y_{1}) \geq 2, \text{ then } d_k(\mu_1) + d_{k'}(y_{1}) = (f + 1) + (\ell + 1) = d_k(\mu_1) + d_{k'}(y_{1}); \text{ now by using definition of } G_1(\xi), \text{ we have} \]

\[ G_1(\xi') - G_1(\xi) = \sum_{i=1}^{f} \left\{ d_{k'}(\mu_{1,i}) + d_{k}(\mu_{1,i}) + 2d_{k}(\mu_{1,i})d_{k'}(\mu_{1,i}) \right\} + \sum_{j=1}^{l-1} \left\{ d_{k'}(y_{1,j}) + d_{k}(y_{1,j}) + d_{k}(y_{1,j})d_{k'}(y_{1,j}) \right\} + \left\{ d_{k'}(y_{1}) + d_{k}(y_{1}) + d_{k}(y_{1})d_{k'}(y_{1}) \right\} + \left\{ d_{k'}(\mu_{1}) + d_{k}(\mu_{1}) + d_{k}(\mu_{1})d_{k'}(\mu_{1}) \right\} + \left\{ d_{k'}(g_{1}) + d_{k}(g_{1}) + d_{k}(g_{1})d_{k'}(g_{1}) \right\} + \left\{ d_{k'}(y_{1}) + d_{k}(y_{1}) + d_{k}(y_{1})d_{k'}(y_{1}) \right\} - \left\{ d_{k'}(y_{1}) + d_{k}(y_{1}) + d_{k}(y_{1})d_{k'}(y_{1}) \right\} - \left\{ d_{k'}(\mu_{1}) + d_{k}(\mu_{1}) + d_{k}(\mu_{1})d_{k'}(\mu_{1}) \right\} - \left\{ d_{k'}(g_{1}) + d_{k}(g_{1}) + d_{k}(g_{1})d_{k'}(g_{1}) \right\} \]

\[ = \sum_{i=1}^{f} \left\{ d_{k'}(\mu_{1,i}) + d_{k}(\mu_{1,i}) + d_{k}(\mu_{1,i})d_{k'}(\mu_{1,i}) \right\} + \sum_{j=1}^{l-1} \left\{ d_{k'}(y_{1,j}) + d_{k}(y_{1,j}) + d_{k}(y_{1,j})d_{k'}(y_{1,j}) \right\} + \left\{ d_{k'}(y_{1}) + d_{k}(y_{1}) + d_{k}(y_{1})d_{k'}(y_{1}) \right\} - \left\{ d_{k'}(y_{1}) + d_{k}(y_{1}) + d_{k}(y_{1})d_{k'}(y_{1}) \right\} - \left\{ d_{k'}(\mu_{1}) + d_{k}(\mu_{1}) + d_{k}(\mu_{1})d_{k'}(\mu_{1}) \right\} - \left\{ d_{k'}(g_{1}) + d_{k}(g_{1}) + d_{k}(g_{1})d_{k'}(g_{1}) \right\} \]

\[ = \sum_{i=1}^{f} \left\{ d_{k'}(\mu_{1,i}) + d_{k}(\mu_{1,i}) + d_{k}(\mu_{1,i})d_{k'}(\mu_{1,i}) \right\} + \sum_{j=1}^{l-1} \left\{ d_{k'}(y_{1,j}) + d_{k}(y_{1,j}) + d_{k}(y_{1,j})d_{k'}(y_{1,j}) \right\} + \left\{ d_{k'}(y_{1}) + d_{k}(y_{1}) + d_{k}(y_{1})d_{k'}(y_{1}) \right\} - \left\{ d_{k'}(y_{1}) + d_{k}(y_{1}) + d_{k}(y_{1})d_{k'}(y_{1}) \right\} - \left\{ d_{k'}(\mu_{1}) + d_{k}(\mu_{1}) + d_{k}(\mu_{1})d_{k'}(\mu_{1}) \right\} - \left\{ d_{k'}(g_{1}) + d_{k}(g_{1}) + d_{k}(g_{1})d_{k'}(g_{1}) \right\} \]

\[ \text{If } d_{k}(\mu_{1}, y_{1}) = 1, \text{ then} \]

\[ G_1(\xi') - G_1(\xi) = \sum_{i=1}^{f} \left\{ d_{k'}(\mu_{1,i}) + d_{k}(\mu_{1,i}) + d_{k}(\mu_{1,i})d_{k'}(\mu_{1,i}) \right\} + \sum_{j=1}^{l-1} \left\{ d_{k'}(y_{1,j}) + d_{k}(y_{1,j}) + d_{k}(y_{1,j})d_{k'}(y_{1,j}) \right\} + \left\{ d_{k'}(y_{1}) + d_{k}(y_{1}) + d_{k}(y_{1})d_{k'}(y_{1}) \right\} - \left\{ d_{k'}(y_{1}) + d_{k}(y_{1}) + d_{k}(y_{1})d_{k'}(y_{1}) \right\} - \left\{ d_{k'}(\mu_{1}) + d_{k}(\mu_{1}) + d_{k}(\mu_{1})d_{k'}(\mu_{1}) \right\} - \left\{ d_{k'}(g_{1}) + d_{k}(g_{1}) + d_{k}(g_{1})d_{k'}(g_{1}) \right\} \]
\[ + \{ d_i^\ell (y_{i,j}) + d_i^\ell (\mu_i) + d_i^\ell (\gamma_i) d_i^\ell (\mu_i) \} \\
- \sum_{j=1}^{\ell-1} \{ d_i^\ell (\mu_j) + d_i^\ell (\mu_i) d_i^\ell (\mu_j) \} \\
+ \{ d_i^\ell (y_{i,j}) + d_i^\ell (\gamma_i) d_i^\ell (y_{i,j}) \} \\
- \{ d_i^\ell (y_{i,j}) + d_i^\ell (\gamma_i) d_i^\ell (y_{i,j}) \} \\
+ \{ d_i^\ell (\mu_j) + d_i^\ell (\mu_i) d_i^\ell (\mu_j) \} \\
+ \{ d_i^\ell (y_{i,j}) + d_i^\ell (\gamma_i) d_i^\ell (y_{i,j}) \} \\
- \{ d_i^\ell (y_{i,j}) + d_i^\ell (\gamma_i) d_i^\ell (y_{i,j}) \} \\
\]

\[ = 4f - 4\ell + 4 \]

\[ = (f - (\ell - 1)) > 0 \Rightarrow GO_1(B_i(\xi)) \]

\[ = GO_1(\xi^i) > GO_1(\xi) \]

\[ \Box \]

3. Ordering Trees Having Maximum GO_1

In this section, we identify the trees having maximum first Gourava index, and also, we give a sequence of these trees having first five largest values of GO_1.

Theorem 5. Let \( T^* \) be a set of trees having order \( \lambda \) and diameter \( d^* \), where \( \lambda \geq 3 \) and \( 2 \leq d^* \leq \lambda - 1 \). Then, \( GO_1 \) is maximum value for \( T^* = S_{\lambda, \lambda-d^*+1} \).

Proof. First, we apply \( B_i \)-transformation to those vertices of \( T^* \) which are other than diametral path, and we observe that maximum value of \( GO_1 \) is obtained for \( MS(\lambda_1, \lambda_2, \ldots, \lambda_{d^*-1}) \).

Then, we apply all those transformations which are explained above, and we conclude that the maximum value is acquired only for \( \lambda_1 = \lambda - d^*, \lambda_2 = \lambda_3 = \cdots = 0, \lambda_{d^*-1} = 1 \) for \( S_{\lambda, \lambda-d^*+1} \).

Corollary 6. (a) Let \( T^* \) denotes the set of trees with order \( \lambda \).

Then,

\[ \max_{\text{diam}(T^*)=\ell} GO_1(T^*) > \max_{\text{diam}(T^*)=m} GO_1(T^*), \quad (12) \]

where \( 2 \leq \ell \leq m \leq \lambda - 1 \).

(b) Let the order of set of trees of \( T^* \) be \( \lambda \) with diameter \( 3 \leq d^* \leq \lambda - 2 \); then the greatest value of \( GO_1(T^*) \) for these graphs is in the following order: \( MS(\lambda - d^*, 0, \ldots, 0, 1), MS(\lambda - d^* - 1, 0, \ldots, 0, 2), \ldots, MS(\lfloor \lambda - d^* + 1/2 \rfloor, 0, \ldots, 0, \lfloor \lambda - d^* + 1/2 \rfloor) \).

Proof. We can achieve \( MS(\lambda - \ell, 0, \ldots, 0, 1) \) from \( MS(\lambda - m^*, 0, \ldots, 0, 1) \) by repeated use of first transformation (as described in Lemma 1).

(b) We use first three transformations (as explained in Lemmas 1 to 3, and then, we use the fourth transformation to multistars \( MS(g_1, 0, \ldots, 0, g_2) \) with order \( \lambda \) where \( g_1 + g_2 = \lambda - d^* + 1 \).

Theorem 7. For \( \lambda > 10 \), the trees having the greatest 1st Gourava index can be given in the following order (shown in Figure 5):

\[ GO_1(K_{1, \lambda-1}) > GO_1(BS(\lambda - 3, 1)) > GO_1(BS(\lambda - 4, 2)) > GO_1(S_{\lambda, \lambda-3}) > GO_1(BS(\lambda - 5, 3)). \]

(13)

Proof. In the family of trees having diameter 2, the star \( K_{1, \lambda-1} \) is the only tree which by above corollary possesses
the greatest 1st Gourava index. The second maximum value of 1st Gourava index reaches for $S^*_1\lambda -2 = BS(\lambda - 3, 1)$ for the trees having diameter 3. The third maximum value of this sequence can be obtained for $BS(\lambda - 4, 2)$ which also belongs to the class of trees having diameter 3. For $\lambda = 5$, the $BS(\lambda - 4, 2)$ coincides with $BS(\lambda - 3, 1)$. The next graph in the class of trees with diameter 3 is $BS(\lambda - 5, 3)$. The next maximum value is obtained by $S^*_1\lambda - 3$ which has diameter 4. We obtain

$$GO_1(BS(\lambda - 4, 2)) > GO_1(S^*_1\lambda - 3).$$

(14)

Applying $r_1$-transform to $S^*_1\lambda - 3$, we obtain $BS(\lambda - 4, 2)$. It follows that for $\lambda \geq 6$, the order of trees possessing maximum value is $GO_1(K_1\lambda - 2) > GO_1(BS(\lambda - 3, 1)) > GO_1(BS(\lambda - 4, 2))$. For the fourth term of this series, we have

$$GO_1(BS(\lambda - 5, 3) - GO_1(S^*_1\lambda - 3)) = [(\lambda - 5)(1 + \lambda - 4 + \lambda - 4) + (\lambda - 4 + 4 + 4(\lambda - 4)) + 3(4 + 1 + 4)] - [(\lambda - 4) + (1 + \lambda - 3 + \lambda - 3) + (3\lambda - 7) + 8 + 5] = [2\lambda^2 - 12\lambda + 46] - [2\lambda^2 - 10\lambda + 26] = 2[10 - \lambda] < 0$$

(15)

This implies that $GO_1(BS(\lambda - 5, 3) < GO_1(S^*_1\lambda - 3)$ for $\lambda > 10$. For $\lambda > 10$, the fourth member in the above constructed sequence is $S^*_1\lambda - 3$. For next member, we calculate

$$GO_1(BS(\lambda - 5, 3) - GO_1(MS(\lambda - 5, 0, 2)) = [(\lambda - 5)(1 + \lambda - 4 + \lambda - 4) + (\lambda - 4 + 4 + 4(\lambda - 4)) + 3(4 + 1 + 4)] - [(\lambda - 5)(1 + \lambda - 4 + \lambda - 4) + (\lambda - 4) + 2 + 2(\lambda - 4) + (2 + 3 + 6) + (2(1 + 3 + 3)]$$

$$= [(\lambda - 5)(2\lambda - 7) + (5\lambda - 16) + 3(9)] - [(\lambda - 5)(2\lambda - 7) + (3\lambda - 6) + 11 + 14] = [2\lambda^2 - 12\lambda + 46] - [2\lambda^2 - 14\lambda + 54] = 2(\lambda - 4) > 0.$$

(16)

For $\lambda > 4$, $MS(\lambda - 5, 0, 2)$ gets the 2nd maximum value of $GO_1$ in the set of trees of diameter 4. Applying $1st$ transformation (as described earlier) to $MS(\lambda - 5, 0, 2)$, we get $MS(\lambda - 5, 0, 1) < MS(\lambda - 5, 0, 2)$ which terminates the proof.

For example, for $\lambda = 12$, we see that

$$GO_1(K_1\lambda - 1) > GO_1(BS(\lambda - 3, 1)) > GO_1(BS(\lambda - 4, 2)) > GO_1(S^*_1\lambda - 3) > GO_1(BS(\lambda - 5, 3)),$$

(17)

which as a result verifies our main result of this work.

$$GO_1(K_1\lambda - 1) = \sum_{\mu \epsilon (E(K_1\lambda - 1))} [d(\mu) + d(\eta) + d(\mu)d(\eta)] = 11[11 + 11 + 1] = 25GO_1(BS(\lambda - 3, 1)) = \sum_{\mu \epsilon (E(BS(\lambda - 3, 1)))} [d(\mu) + d(\eta) + d(\mu)d(\eta)] = 9[10 + 10 + 10 + 10 + 20 + 21 + 2] = 226,$$

$$GO_1(BS(\lambda - 4, 2)) = \sum_{\mu \epsilon (E(BS(\lambda - 4, 2)))} [d(\mu) + d(\eta) + d(\mu)d(\eta)] = 8[1 + 9 + 9] + [9 + 3 + 27] + 2[1 + 3 + 3] = 205,$$

$$GO_1(S^*_1\lambda - 3) = \sum_{\mu \epsilon (E(S^*_1\lambda - 3))} [d(\mu) + d(\eta) + d(\mu)d(\eta)] = 8[1 + 9 + 9] + [9 + 2 + 18] + [8 + 4 + 32] + [2 + 2 + 4] + [8 + 2 + 2] = 194.$$
Table 1: Comparison of different values of \( GO_1(T^*_\lambda) \) for \( \lambda = 14 \).

| \( T^*_\lambda \) | \( GO_1(T^*_\lambda) \) |
|-----------------|-----------------|
| \( K_{1,13} \) | 351             |
| BS(11, 1)      | 318             |
| BS(10, 2)      | 291             |
| \( S_{14,11} \) | 278             |
| BS(9, 3)       | 270             |

\[
GO_1(\text{BS}(\lambda - 5, 3)) = \sum_{\mu \in (EBS(\lambda - 5, 3))} [d(\mu) + d(\eta) + d(\mu)d(\eta)]
= 7[1 + 8 + 8] + [8 + 4 + 32] + 3[1 + 4 + 4]
= 190. \tag{18}
\]

Hence proved

\[
GO_1(K_{1,13}) > GO_1(\text{BS}(\lambda - 3, 1)) > GO_1(\text{BS}(\lambda - 4, 2))
> GO_1(S_{14,11}) > GO_1(\text{BS}(\lambda - 5, 3)). \tag{19}
\]

Table 1 provides certain trees \( T^*_\lambda \) of order \( \lambda \), along with their value of \( GO_1 \).

**Theorem 8.** Let \( T^* \) be a tree having order \( \lambda \geq 5 \) with \( \alpha \)-leaf nodes, where \( 3 \leq \alpha \leq \lambda - 2 \). Then,

\[
GO_1(T^*) \leq 2\{\alpha^2 - 3\alpha + 4\lambda - 5\}. \tag{20}
\]

Equality holds if \( T^* = S_{\lambda,\alpha}^* \).

**Proof.** First under the supposition of theorem, we prove that if \( x' \) is a pendant node attached to a vertex \( y' \), then

\[
GO_1(T^*) - GO_1(T^* - x) \leq 4\alpha. \tag{21}
\]

Equality holds for \( S_{\lambda,\alpha}^* \) and for \( d(y') = \alpha \). Here, we notice that there exist a vertex \( \ell_0 \in N(y') \setminus \{x'\} \) such that \( d(\ell_0) \geq 2 \) since otherwise \( T^* \) would be a star, which is against the supposition of theorem. Now,

\[
GO_1(T^*) - GO_1(T^*)
= \left[d(y') + 1 + d(y') \right]
- \sum_{\ell \in N(y')\setminus\{x'\}} \left\{ \left( d(y') - 1 \right) + d(\ell) + \left( d(y') - 1 \right)d(\ell) \right\}
- \left\{ d(y') + d(\ell) + d(y')d(\ell) \right\}. \tag{22}
\]

Since \( d(\ell) \geq 2 \), we have

\[
\left\{ \left( d(y') - 1 \right) + d(\ell_0) + \left( d(y') - 1 \right)d(\ell_0) \right\}
- \left\{ d(y') + d(\ell_0) + d(y')d(\ell_0) \right\}
\leq \left\{ 3d(y') - 1 \right\} - \left\{ 3d(y') + 2 \right\}. \tag{23}
\]

For the remaining \( d(y') - 2 \) nodes \( \ell \in N(y') \setminus \{x', \ell_0\} \), we conclude that

\[
\left\{ \left( d(y') - 1 \right) + d(\ell) + \left( d(y') - 1 \right)d(\ell) \right\}
- \left\{ d(y') + d(\ell) + d(y')d(\ell) \right\}
\leq \left\{ 2d(y') - 1 \right\} - \left\{ 2d(y') + 1 \right\}. \tag{24}
\]

This implies that

\[
GO_1(T^*) - GO_1(T^*)
= \left[ 2d(y') + 1 \right] - \left[ \left\{ \left( d(y') - 1 \right) + d(\ell_0) + \left( d(y') - 1 \right)d(\ell_0) \right\} \right.
- \left\{ d(y') + d(\ell) + d(y')d(\ell) \right\}
- \left\{ d(y') + d(\ell) + d(y')d(\ell) \right\}
\leq \left[ 2d(y') + 1 \right] - \left[ \left\{ 3d(y') - 1 \right\} - \left\{ 3d(y') + 2 \right\} \right.
- \left\{ 2d(y') - 1 \right\} - \left\{ 2d(y') + 1 \right\} \right]. \tag{25}
\]

Since \( d(y') \leq \alpha \),

\[
\Rightarrow GO_1(T^*) - GO_1(T^*) \leq 4\alpha. \tag{26}
\]

Equality holds if \( d(y') = \alpha \), one neighbor of \( y' \) has degree two, while all the neighbor are leaf nodes, i.e., \( T^* = S_{\lambda,\alpha}^* \).

Now, the proof follows by induction on \( \lambda \). For \( \lambda = 5 \), we obtain \( \alpha = 3 \), and \( S_{3,5} = BS^*(1, 2) \) is a single tree of order 5 having three pendant nodes.

Let \( \alpha \geq 6 \) and suppose that the theorem is true for all the trees of order \( \lambda - 1 \) having \( \alpha \)-leaf nodes where \( 3 \leq \alpha \leq \lambda - 3 \). Let \( x' \) be the pendant node that is attached to node \( y' \). Here, we examine two subcases:

(a) When \( d(y') = 2 \)

(b) When \( d(y') \geq 3 \)
(a) For \(d(y') = 2\), we have

\[
\begin{align*}
GO_1(T^*) - GO_1\left(T^* - x'\right) \\
= (d(\ell) + 2 + 2d(\ell)) + (2 + 1 + 2) \\
- (d(\ell) + 1 + d(\ell))GO_1(T^*) - GO_1\left(T^* - x'\right) \\
= 6 + d(\ell)GO_1(T^*) \\
= 6 + d(\ell) + GO_1\left(T^* - x'\right)GO_1(T^*) \\
\leq 6 + d(\ell) + \{2\alpha^2 - 3\alpha + 4(\lambda - 1) - 5\} \\
= 2\{\alpha^2 - 3\alpha + 4(\lambda) - 5\} - 8 + 6 + d(\ell) \\
\implies GO_1(T^*) \leq S^*_\lambda, \alpha + d(\ell) - 2
\end{align*}
\]  
(27)

Equality holds for \(d(\ell) = 2\). If \(\alpha = \lambda - 2\), then \(T^* - x'\) has \(\lambda - 1\) nodes and \(\lambda - 2\) pendant nodes, i.e., \(T^* - x' = \kappa_{\lambda, \lambda - 2}\) and \(T^* = S^*_{\lambda, \lambda - 2} = S^*_\lambda, \alpha\).

(b) For \(d(y') \geq 3\), then \(T^* - x'\) has \(\lambda - 1\) nodes and \(\alpha - 1\) leaf nodes. Then, by induction, we obtain

\[
\begin{align*}
GO_1(T^*) \leq GO_1(T^*) + 4\alpha \leq S^*_{\lambda, \alpha - 1} + 4\alpha = S^*_\lambda, \alpha
\end{align*}
\]  
(28)

Equality holds if \(T^* - x' = S^*_{\lambda, \alpha - 1}\) and \(d(y') = \alpha\), i.e., \(T^* = S^*_\lambda, \alpha\). \(\square\)

Data Availability

The data used to support the findings of this study are cited at relevant places within the articles in references.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

References

[1] H. Wiener, “Structural determination of paraffin boiling points,” Journal of the American Chemical Society, vol. 69, no. 1, pp. 17–20, 1947.

[2] I. Gutman and K. C. Das, “The first Zagreb index 30 years after,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 50, no. 1, pp. 83–92, 2004.

[3] I. Gutman and N. Trinajstić, “Graph theory and molecular orbitals. Total \(\phi\)-electron energy of alternant hydrocarbons,” Chemical Physics Letters, vol. 17, no. 4, pp. 535–538, 1972.

[4] K. C. Das and I. Gutman, “Some properties of the second Zagreb index,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 52, no. 1, 2004.

[5] A. Miličević, S. Nikolić, and N. Trinajstić, “On reformulated Zagreb indices,” Molecular Diversity, vol. 8, pp. 393–399, 2004.

[6] V. R. Kulli, “The Gourava indices and coindices of graphs,” Annals of Pure and Applied Mathematics, vol. 14, no. 1, pp. 33–38, 2017.

[7] V. R. Kulli, “The Gourava index of four operations on graphs,” Mathematical Combinatorics, vol. 4, pp. 65–67, 2018.

[8] J. A. Bondy and U. S. R. Murty, Graph Theory, Springer, New York, 2008.

[9] N. De, “Some bounds of reformulated Zagreb indices,” Applied Mathematical Sciences, vol. 6, no. 101, pp. 5005–5012, 2012.

[10] K. Xu and K. C. Das, “Trees, unicyclic, and bicyclic graphs extremal with respect to multiplicative sum Zagreb index,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 68, pp. 257–272, 2012.

[11] S. Ji, X. Li, and B. Huo, “On reformulated Zagreb indices with respect to acyclic, unicyclic and bicyclic graphs,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 72, pp. 723–732, 2014.

[12] W. Gao, M. K. Jamil, A. Javed, M. R. Farahani, S. Wang, and J. B. Liu, “Sharp bounds of the hyper- Zagreb index on acyclic, unicyclic and bicyclic,” Discrete Dynamics in Nature and Society, vol. 2017, Article ID 6079450, 5 pages, 2017.

[13] I. Tomescu and S. Kanwal, “Ordering trees having small general sum- connectivity index,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 69, pp. 535–548, 2013.

[14] A. Ilić, D. Stevanović, L. Feng, G. Yu, and P. Dankelmann, “Degree distance of unicyclic and bicyclic graphs,” Discrete Applied Mathematics, vol. 159, pp. 779–788, 2011.

[15] H. Liu, H. Chen, Z. Tang, and L. You, “Ordering tree-like phenylenes by their Mostar indices,” 2021, https://arxiv.org/abs/2103.04018.

[16] H. Liu, L. You, and Y. Huang, “Ordering chemical graphs by Sombo indices and its applications,” MATCH Communications in Mathematical and in Computer Chemistry, vol. 87, no. 1, pp. 5–22, 2022.

[17] J. B. Liu, H. Ali, M. K. Shafiq, G. Dustigeer, and P. Ali, “On topological properties of planar octahedron networks,” Polycyclic Aromatic Compounds, vol. 42, pp. 1–17, 2021.

[18] R. Qi, H. Ali, U. Babar, J. B. Liu, and P. Ali, “On the Sum of Degree-Based Topological Indices of Rhombus-Type Silicate and Oxide Structures,” Journal of Mathematics, vol. 2021, Article ID 1100024, 16 pages, 2021.

[19] W. Zhen, P. Ali, H. Ali, G. Dustigeer, and J. B. Liu, “On Computation Degree-Based Topological Descriptors for Planar Octahedron Networks,” Journal of Mathematics, vol. 2021, Article ID 4880092, 12 pages, 2021.

[20] M. Hu, H. Ali, M. A. Binyamin, B. Ali, J. B. Liu, and C. Fan, “On Distance-Based Topological Descriptors of Chemical Interconnection Networks,” Journal of Mathematics, vol. 2021, Article ID 5520619, 10 pages, 2021.