Research Article
Valency-Based Descriptors for Silicon Carbides, Bismuth(III) Iodide, and Dendrimers in Drug Applications

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Silicon carbide (SiC), also called carborundum, is a semiconductor containing silicon and carbon. Dendrimers are repetitively branched molecules that are typically symmetric around the core and often adopt a spherical three-dimensional morphology. Bismuth(III) iodide is an inorganic compound with the formula BiI3. This gray-black solid is the product of the reaction between bismuth and iodine, which once was of interest in qualitative inorganic analysis. In chemical graph theory, we associate a graph to a compound and compute topological indices that help us in guessing properties of the understudy compound. A topological index is the graph invariant number, calculated from a graph representing a molecule. Most of the proposed topological indices are related either to a vertex adjacency relationship (atom-atom connectivity) in the graph or to topological distances in the graph. In this paper, we aim to compute the first and second Gourava indices and hyper-Gourava indices for silicon carbides, bismuth(III) iodide, and dendrimers.

1. Introduction
Mathematical chemistry provides tools such as polynomials and functions that depend upon the information hidden in the symmetry of graphs of chemical compounds and helps to predict properties of the understudy molecular compound without the use of quantum mechanics. A topological index is a numerical parameter of a graph and depicts its topology. It describes the structure of molecules numerically and are used in the development of qualitative structure activity relationships (QSARs). There are three kinds of topological indices, namely, degree-based, distance-based, and surface-based topological indices. Lot of research has been done on degree-based topological indices, for example, see [1–9]. Degree-based topological indices correlate the structure of the molecular compound with its various physical properties, biological activities, and chemical reactivity [10–14]. Boiling point, heat of formation, fracture toughness, strain energy, and rigidity of a molecule are strongly connected to its graphical structure.

The first topological index was introduced by Wiener when he was studying the boiling point of alkanes [15], which is now known as the Wiener index [16–20]. In 1975, Milan Randić introduced a simple topological index called the Randić index [21]. Many research papers and survey papers have been written on this graph invariant due to its interesting mathematical properties and valuable applications in chemistry [22–27]. The other oldest topological indices are Zagrebin indices defined by Gutman and Trinajstic in [28] and are one of the most studied topological indices [29–33]. Topological indices are helpful in guessing properties of concerned compounds and are used in QSARs [34–37]. There are more than 148 topological indices in the literature [38–42], but none of them are able to guess all the
properties of the concerned compound (together they do it to some extent). Therefore, there is always room to define new topological indices [43]. Recently, in 2017, the first and second Gourava indices [44] were defined as

\[
\begin{align*}
\text{GO}_1 (G) &= \sum_{uv \in E(G)} [(d_u + d_v) + (d_u d_v)], \\
\text{GO}_2 (G) &= \sum_{uv \in E(G)} [(d_u + d_v) + (d_u d_v)].
\end{align*}
\]

In the same year, the first and second hyper-Gourava indices [45] have been defined as

\[
\begin{align*}
\text{HGO}_1 (G) &= \sum_{uv \in E(G)} [(d_u + d_v) + (d_u d_v)]^2, \\
\text{HGO}_2 (G) &= \sum_{uv \in E(G)} [(d_u + d_v) + (d_u d_v)]^3.
\end{align*}
\]

Note that \( \text{GO}_1 (G) = M_1 (G) + M_2 (G) \), \( \text{GO}_2 (G) = M_1 (G) M_2 (G) \), \( \text{HGO}_1 (G) = H_1 (G) + H_2 (G) + 2M_1 (G) + M_2 (G) \), and \( \text{HGO}_2 (G) = H_1 (G) H_2 (G) \). In this paper, the aim is to compute Gourava indices and hyper-Gourava indices for silicone carbides, bismuth triiodide, and dendrimers and their graphical representations.

2. Methodology

To compute our results, first we constructed the graph of the concerned molecular compounds and counted the total number of vertices and edges. Secondly, we divided the edge set of concerned graphs into different classes based on the degrees of end vertices. By applying definitions of Gourava indices, we computed our desired results. We plotted our computed results by using Maple 2015 to see their dependencies on the involved parameters.

3. Gourava Indices

In this section, we present our main computational results. This section consists of three subsections. In Section 3.1, we present results about silicone carbides \( \text{Si}_2\text{C}_3 - \text{I}[p, q] \), \( \text{Si}_2\text{C}_3 - \text{II}[p, q] \), \( \text{Si}_2\text{C}_3 - \text{III}[p, q] \), and \( \text{SiC}_3 - \text{III}[p, q] \). In Section 3.2, we give results about the bismuth triiodide chain \( m - \text{Bi}_3 \) and the bismuth triiodide sheet \( \text{Bi}_3 (m \times n) \). In Section 3.3, we present results about four dendrimer structures: porphyrin dendrimer \( \text{D}_{n}\text{P}_{m} \), propyl ether imine dendrimer (PETIM), zinc-porphyrin dendrimer DPZ\(_n\), and Poly(ETHyleneAmidoAmine) dendrimer (PETAAA).

3.1. Gourava Indices for Silicon Carbides. Silicon carbide (SiC), also called carborundum, is a semiconductor containing silicon and carbon. It occurs in nature as the incredibly uncommon mineral Moissanite. Manufactured SiC powder has been created in mass since 1893 for use as an abrasive. Grains of silicon carbide are reinforced together by sintering to shape extremely hard ceramic production that are generally utilized in applications requiring high continuance, for example, vehicle brakes, vehicle clutches, and ceramic plates in impenetrable vests. Electronic utilisations of silicon carbide, for example, light-emitting diodes (LEDs) and locators in early radios, were first exhibited around 1907. SiC is utilized in semiconductor electronic devices that work at high temperatures or high voltages, or both. Huge single crystals of silicon carbide can be developed by the Lely technique, and they can be cut into gems known as manufactured Moissanite. SiC with a high surface zone can be created from SiO\(_2\) contained in the plant material. Due to huge amount of application, silicone carbides have been studied extensively [6, 42]. In this section, we computed Gourava indices for silicone carbides \( \text{Si}_3\text{C}_3 - \text{I}[p, q] \), \( \text{Si}_2\text{C}_3 - \text{II}[p, q] \), \( \text{Si}_2\text{C}_3 - \text{III}[p, q] \), and \( \text{SiC}_3 - \text{III}[p, q] \).

3.1.1. Gourava Indices for Silicon Carbide \( \text{Si}_2\text{C}_3 - \text{I}[p, q] \).

The molecular graphs of silicon carbide \( \text{Si}_2\text{C}_3 - \text{I}[p, q] \) are shown in Figures 1–4, where Figure 1 shows the unit cell of silicone carbide, Figure 2 shows \( \text{Si}_2\text{C}_3[p, q] \) for \( p = 4, q = 3 \), Figure 3 shows \( \text{Si}_2\text{C}_3[p, q] \) for \( p = 4, q = 1 \), and Figure 4 shows \( \text{Si}_2\text{C}_3[p, q] \) for \( p = 4, q = 3 \). The edge partition of the edge set of \( \text{Si}_2\text{C}_3 - \text{I}[p, q] \) based on the degree of the end vertex is given in Table 1.

Theorem 1. Let \( G \) be the graph of silicon carbide \( \text{Si}_2\text{C}_3\text{I}[p, q] \). Then, the first and second Gourava indices are

\[
\begin{align*}
(1) \text{GO}_1 (G) &= 225pq - 61p - 91q + 18, \\
(2) \text{GO}_2 (G) &= 810pq - 290p - 430q + 126.
\end{align*}
\]

Proof: From the edge partition of \( \text{Si}_2\text{C}_3[p, q] \) given in Table 1, we have

\[
\begin{align*}
(1) \text{GO}_1 (G) &= \sum_{uv \in E(G)} [(d_u + d_v) + (d_u d_v)] \\
&= [(1 + 2) + (1 \times 2)](1) + [(1 + 3) + (1 \times 3)](1) \\
&\quad + [(2 + 2) + (2 \times 2)](p + 2q) \\
&\quad + [(2 + 3) + (2 \times 3)](6p + 8q - 9) \\
&\quad + [(3 + 3) + (3 \times 3)](15pq - 9p - 13q + 7) \\
&= 225pq - 61p - 91q + 18. \\
(2) \text{GO}_2 (G) &= \sum_{uv \in E(G)} [(d_u + d_v)(d_u d_v)] \\
&= [(1 + 2) \times (1 + 2)](1) + [(1 + 3) \times (1 + 3)](1) \\
&\quad + [(2 + 2) \times (2 + 2)](p + 2q) \\
&\quad + [(2 + 3) \times (2 + 3)](6p + 8q - 9) \\
&\quad + [(3 + 3) \times (3 + 3)](15pq - 9p - 13q + 7) \\
&= 810pq - 290p - 430q + 126.
\end{align*}
\]
From the edge partition of Si$_2$C$_3$I, we have

\[
\text{Table 1: } \text{Degree-based edge partition of } \text{Si}_2\text{C}_3\text{I}[p,q].
\]

| $(d_u, d_v)$ | Frequency |
|-------------|------------|
| (1,2)       | 1          |
| (1,3)       | 1          |
| (2,2)       | $p + 2q$   |
| (2,3)       | $6p - 1 + 8(q - 1)$ |
| (3,3)       | $15pq - 9p - 13q + 7$ |

**Theorem 2.** Let $G$ be the graph of silicon carbide Si$_2$C$_3$I[p,q]. Then, the first and second hyper-Gourava indices are

1. $\text{HGO}_1(G) = 3375pq - 1235p - 1829q + 566$,
2. $\text{HGO}_2(G) = 43740pq - 20588p - 30196q + 12492$.

**Proof.** From the edge partition of Si$_2$C$_3$I[p,q] given in Table 1, we have

1. The first hyper-Gourava index for Si$_2$C$_3$I[p,q] is

\[
\text{HGO}_1(G) = \sum_{uv \in E(G)} \left[ (d_u + d_v) + (d_u, d_v)^2 \right] = [(1 \times 2) + (1 \times 2)]^2 (1) + [(1 \times 3) + (1 \times 3)]^2 (1) + [(2 \times 2) + (2 \times 2)]^2 (p + 2q) + [(2 \times 3) + (2 \times 3)]^2 (6p + 8q - 9) + [(3 \times 3) + (3 \times 3)]^2 (15pq - 9p - 13q + 7) = 3375pq - 1235p - 1829q + 566.
\]

(5)

2. The second hyper-Gourava index for Si$_2$C$_3$I[p,q] is

\[
\text{HGO}_2(G) = \sum_{uv \in E(G)} \left[ (d_u + d_v) + (d_u, d_v)^2 \right] = [(1 \times 2) \times (1 \times 2) + (1 \times 3) \times (1 \times 3)]^2 (1) + [(2 \times 2) \times (2 \times 2) + (2 \times 3) \times (2 \times 3)]^2 (p + 2q) + [(2 \times 3) \times (2 \times 3) + (3 \times 3) \times (3 \times 3)]^2 (6p + 8q - 9) + [(3 \times 3) \times (3 \times 3)]^2 (15pq - 9p - 13q + 7) = 43740pq - 20588p - 30196q + 12492.
\]

(6)

3.1.2. Gourava Indices for Silicon Carbide Si$_2$C$_3$ - II[p,q]. The molecular graphs of silicon carbide Si$_2$C$_3$ - II[p,q] are shown in Figures 5–8, where Figure 5 shows the unit cell of Si$_2$C$_3$ - II[p,q], Figure 6 shows Si$_2$C$_3$ - II[p,q] for $p = 3$, $q = 3$, Figure 7 shows Si$_2$C$_3$ - II[p,q] for $p = 3$, $q = 1$, and Figure 8 shows Si$_2$C$_3$ - II[p,q] for $p = 5$, $q = 2$. The edge partition of the edge set of Si$_2$C$_3$ - II[p,q] based on the degree of the end vertex is given in Table 2.

**Theorem 3.** Let $G$ be the graph of silicon carbide Si$_2$C$_3$ - II[p,q]. Then, the first and second Gourava indices are

1. $\text{GO}_1(G) = 225pq - 91p - 91q + 28$,
2. $\text{GO}_2(G) = 810pq - 430p - 430q + 198$.

**Proof.** From the edge partition of Si$_2$C$_3$ - II[p,q] given in Table 2, we have

1. The first Gourava index for Si$_2$C$_3$I[p,q] is

\[
\text{GO}_1(G) = \sum_{uv \in E(G)} \left[ (d_u + d_v) + (d_u, d_v) \right] = [(1 \times 2) + (1 \times 2)]^2 (1) + [(1 \times 3) + (1 \times 3)]^2 (1) + [(2 \times 2) + (2 \times 2)]^2 (p + 2q) + [(2 \times 3) + (2 \times 3)]^2 (6p + 8q - 9) + [(3 \times 3) + (3 \times 3)]^2 (15pq - 9p - 13q + 11) = 225pq - 91p - 91q + 28.
\]
Table 2: Degree-based edge partition of Si$_2$C$_3$ – II$[p, q]$. \\

| $(d_u, d_v)$ | Frequency |
|----------------|------------|
| (1, 2)         | 2          |
| (1, 3)         | 1          |
| (2, 2)         | $2p + 2q$  |
| (2, 3)         | $8p + 8q - 14$ |
| (3, 3)         | $15pq - 13p - 13q + 11$ |

(2) The second Gourava index for Si$_2$C$_3$ – II$[p, q]$ is

$$GO_2(G) = \sum_{uv \in E(G)} [(d_u + d_v)(d_u d_v)]$$

$$= [(1 + 2) \times (1 \times 2)]^2 (2) + [(1 + 3) \times (1 \times 3)]^2 (1)$$

$$+ [(2 + 2) \times (2 \times 2)]^2 (2p + 2q)$$

$$+ [(2 + 3) \times (2 \times 3)]^2 (8p + 8q - 14)$$

$$+ [(3 + 3) \times (3 \times 3)]^2 (15pq - 13p - 13q + 11)$$

$$= 1080pq - 680p - 680q + 396.$$  

(8) 

Theorem 4. Let $G$ be the graph of silicon carbide Si$_2$C$_3$ – II$[p, q]$. Then, the first and second hyper-Gourava indices are

1. $HGO_1(G) = 3375pq - 1829p - 1829q + 880,$
2. $HGO_2(G) = 43740pq - 30196p - 30196q + 19692.$

Proof. From the edge partition of Si$_2$C$_3$ – II$[p, q]$ given in Table 2, we have

(1) The first hyper-Gourava index for Si$_2$C$_3$ – II$[p, q]$ is

$$HGO_1(G) = \sum_{uv \in E(G)} [(d_u + d_v)(d_u + d_v)]$$

$$= [(1 + 2) \times (1 \times 2)]^2 (2) + [(1 + 3) \times (1 \times 3)]^2 (1)$$

$$+ [(2 + 2) \times (2 \times 2)]^2 (2p + 2q)$$

$$+ [(2 + 3) \times (2 \times 3)]^2 (8p + 8q - 14)$$

$$+ [(3 + 3) \times (3 \times 3)]^2 (15pq - 3p - 13q + 11)$$

$$= 3375pq - 1829p - 1829q + 880.$$  

(9)

(2) The second hyper-Gourava index for Si$_2$C$_3$ – II$[p, q]$ is

$$HGO_2(G) = \sum_{uv \in E(G)} [(d_u + d_v)(d_u d_v)]$$

$$= [(1 + 2) \times (1 \times 2)]^2 (2) + [(1 + 3) \times (1 \times 3)]^2 (1)$$

$$+ [(2 + 2) \times (2 \times 2)]^2 (2p + 2q)$$

$$+ [(2 + 3) \times (2 \times 3)]^2 (8p + 8q - 14)$$

$$+ [(3 + 3) \times (3 \times 3)]^2 (15pq - 13p - 13q + 11)$$

$$= 43740pq - 30196p - 30196q + 19692.$$  

(10) 

3.1.3. Gourava Indices for Silicon Carbide Si$_2$C$_3$ – III$[p, q]$. The unit cell of Si$_2$C$_3$III$[p, q]$ is shown in Figure 9. The 2D lattice graphs of Si$_2$C$_3$ – I[5, 1], Si$_2$C$_3$ – I[5, 2], and Si$_2$C$_3$ – I[5, 4] are shown in Figures 10–12, respectively. The edge partition of the edge set of Si$_2$C$_3$III$[p, q]$ based on the degrees of end vertices is given in Table 3.

Theorem 5. Let $G$ be the graph of silicon carbide Si$_2$C$_3$ – III$[p, q]$. Then, the first and second Gourava indices are

1. $GO_1(G) = 225pq - 62p - 91q + 18,$
2. $GO_2(G) = 810pq - 300p - 430q + 128.$

Proof. From the edge partition of Si$_2$C$_3$III$[p, q]$ given in Table 3, we have

(1) The first Gourava index for Si$_2$C$_3$III$[p, q]$ is

$$GO_1(G) = \sum_{uv \in E(G)} [(d_u + d_v)(d_u + d_v)]$$

$$= (1 \times 3)(1) + [(2 + 2) \times (2 \times 2)](2p + 2q)$$

$$+ [(2 + 3) \times (2 \times 3)] (8p + 8q - 14)$$

$$+ [(3 + 3) \times (3 \times 3)] (15pq - 13p - 13q + 11)$$

$$= 225pq - 62p - 91q + 18.$$  

(11)
Theorem 6. Let $G$ be the graph of silicon carbide $Si_2C_3III[p,q]$. Then, the first and second hyper-Gourava indices are

1. \( HGO_1(G) = 3375pq - 1282p - 1829q + 500, \)
2. \( HGO_2(G) = 43740pq - 21960p - 30196q + 13328. \)

Proof. From the edge partition of $Si_2C_3III[p,q]$ given in Table 3, we have

\[
(1) \quad HGO_1(G) = \sum_{uv \in E(G)} [(d_u + d_v)(d_u + d_v)] = [(1 + 3)(1 + 3) + (2 + 2)(2 + 2) + (8p + 8q - 14) + (15pq - 13p - 13q + 11)] \times 2 = 3375pq - 1282p - 1829q + 500.
\]

\[
(2) \quad HGO_2(G) = \sum_{uv \in E(G)} [(d_u + d_v)(d_u + d_v)] = [(1 + 3)(1 + 3) + (2 + 2)(2 + 2) + (8p + 8q - 14) + (15pq - 13p - 13q + 11)] \times 2 = 43740pq - 21960p - 30196q + 13328.
\]

\[
(13)
\]

3.1.4. Gourava Indices for Silicon Carbide $SiC_3III[p,q]$.

The unit cell of $SiC_3III[p,q]$ is shown in Figure 13. The 2D lattice graphs of $SiC_3III[p,q]$, $SiC_3III[p,q]$, and $SiC_3III[p,q]$ are shown in Figures 14–16, respectively. The edge partition of the edge set of $SiC_3III[p,q]$ based on the degrees of end vertices is given in Table 4.

Theorem 7. Let $G$ be the graph of silicon carbide $SiC_3III[p,q]$. Then, the first and second Gourava indices are

1. \( GO_1(G) = 480pq - 90p - 60q + 25, \)
2. \( GO_2(G) = 648pq - 420p - 280q + 168. \)

Proof. From the edge partition of the edge set of $SiC_3III[p,q]$ given in Table 4, we have

\[
(1) \quad GO_1(G) = \sum_{uv \in E(G)} [(d_u + d_v)(d_u + d_v)] = [(1 + 2)(1 + 3) + (2 + 2)(2 + 2) + (6p + 4q - 8) + (12pq - 12p - 8q + 8)] \times 2 = 480pq - 90p - 60q + 25.
\]

\[
(14)
\]

\[
(15)
\]
Figure 13: Unit cell.

Figure 14: SiC$_3$ – III[5, 1].

Figure 15: SiC$_3$ – III[5, 2].

Figure 16: SiC$_3$ – III[5, 4].

Table 4: Degree-based edge partition of SiC$_3$III[p, q].

| (d$_{u}$, d$_{v}$) | Frequency |
|---------------|-----------|
| (1, 2)        | 2         |
| (1, 3)        | 1         |
| (2, 2)        | 3$p + 2q - 3$ |
| (2, 3)        | 6$p + 4q - 8$ |
| (3, 3)        | 12$pq - 12p - 8q + 8$ |

Proof. From the edge partition of the edge set of SiC$_3$ III[p, q] given in Table 4, we have

(1) The first hyper-Gourava index for SiC$_3$III[p, q] is

$$HGO_1(G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_{u'}, d_{v'})]^2$$

$$= [(1 + 2) + (1 \times 2)]^2 (2) + [(1 + 3) + (1 \times 3)]^2 (1)$$

$$+ [(2 + 2) + (2 \times 2)]^2 (2p + 2q)$$

$$+ [(2 + 3) + (2 \times 3)]^2 (8p + 8q - 14)$$

$$+ [(3 + 3) + (3 \times 3)]^2 (15pq - 3p - 13q + 11)$$

$$= 2700pq - 1782p - 118q + 739.$$  \hspace{1cm} (17)

(2) The second hyper-Gourava index for SiC$_3$III[p, q] is

$$HGO_2(G) = \sum_{uv \in E(G)} [(d_u + d_v) . (d_{u'}, d_{v'})]^2$$

$$= [(1 + 2) \times (1 \times 2)]^2 (2) + [(1 + 3) \times (1 \times 3)]^2 (1)$$

$$+ [(2 + 2) \times (2 \times 2)]^2 (2p + 2q)$$

$$+ [(2 + 3) \times (2 \times 3)]^2 (8p + 8q - 14)$$

$$+ [(3 + 3) \times (3 \times 3)]^2 (15pq - 13p - 13q + 11)$$

$$= 34992pq - 28824p - 19216q + 15576.$$  \hspace{1cm} (18) \hspace{1cm} \square

3.1.5. Graphical Comparison of Results of Silicone Carbides. In Figures 17–20, we can observe that the behavior of all indices is exponentially increasing with respect to the involved parameters.

Codes for plotting the first and second Gourava indices for silicon carbide Si$_3$C$_1$[p, r] are given as follows:

```plaintext
plot3d(225 * p * q - 61 * p - 91 * q + 18, p = 0..1, q = 0..1, colour = red),
plot3d(810 * p * q - 290 * p - 430 * q + 126, p = 0..1, q = 0..1, colour = green).
```

3.2. Gourava Indices for Bismuth Triiodide. Bi$_3$I$_3$ is an inorganic compound which is the result of the reaction between iodine and bismuth, which inspired the enthusiasm for subjective inorganic investigations [46]. Bi$_3$I$_3$ is an excellent inorganic compound and is very useful in qualitative inorganic analysis [47]. It has been proven that Bi-doped glass optical strands are one of the most promising dynamic laser media. Different kinds of Bi-doped fiber strands have been created and have been used to construct Bi-doped fiber lasers and optical loudspeakers [48]. Layered Bi$_3$I$_3$ gemstones are considered to be a three-layered stack structure in which a plane of bismuth atoms is sandwiched between iodide.
particle planes to form a continuous plane [49]. The periodic superposition of the three layers forms diamond-shaped BiI₃ crystals with \( R - 3 \) symmetry [50, 51]. A progressive stack of I – Bi – I layers forms a hexagonal structure with symmetry [52]. A jewel of BiI₃ has been integrated in [46]. We referred to [6] for the topological study of bismuth triiodide.

3.2.1. Bismuth Triiodide Chain \( m – BiI₃ \). The molecular graph of the unit cell of \( m – BiI₃ \) is shown in Figure 21. From Figure 22, we can see that the molecular graph of \( m – BiI₃ \) has two types of edge sets. The edge partition of the edge set of \( m – BiI₃ \) is given in Table 5.

**Theorem 9.** Let \( G \) be the graph of the bismuth triiodide chain \( m – BiI₃ \). Then, the first and second Gourava indices are

1. \( GO₁(G) = 452m + 184 \),
2. \( GO₂(G) = 2088m + 720 \).

\[ q \]

**Figure 17:** Comparison of the first Gourava index.

**Figure 18:** Comparison of the second Gourava index.

**Figure 19:** Comparison of the first hyper-Gourava index.

**Figure 20:** Comparison of the second hyper-Gourava index.

**Figure 21:** Unit cell (bismuth triiodide).
Figure 22: The chain for $m = 3$ (bismuth triiodide).

Table 5: Degree-based edge partition of $m - \text{BiI}_3[m,n]$ of end vertices of each edge.

| $(d_u, d_v)$ | Frequency |
|------------|-----------|
| (1, 6)     | $4m + 8$  |
| (2, 6)     | $20m + 4$ |

**Proof.** From the edge partition of the edge set of $m - \text{BiI}_3$ given in Table 5, we have

1. The first Gourava index for $m - \text{BiI}_3$ is
   \[
   \text{GO}_1 (G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u, d_v)] 
   \]
   \[
   = [(1 + 6) + (1 \times 6)] (4m + 8) 
   + [(2 + 6) + (2 \times 6)] (20m + 4) 
   = 452m + 184. 
   \]

2. The second Gourava index for $m - \text{BiI}_3$ is
   \[
   \text{GO}_2 (G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u, d_v)] 
   \]
   \[
   = [(1 + 6) + (1 \times 6)] (4m + 8) 
   + [(2 + 6) + (2 \times 6)] (20m + 4) 
   = 2088m + 720. 
   \]

**Theorem 10.** Let $G$ be the graph of the bismuth triiodide chain $m - \text{BiI}_3$. Then, the first and second hyper-Gourava indices are

1. $\text{HGO}_1 (G) = 8676m + 2952$, 
2. $\text{HGO}_2 (G) = 191376m + 93376$.

**Proof.** From the edge partition of the edge set of $m - \text{BiI}_3$ given in Table 5, we have

1. The first hyper-Gourava index for $m - \text{BiI}_3$ is
   \[
   \text{HGO}_1 (G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u, d_v)]^2 
   \]
   \[
   = [(1 + 6) + (1 \times 6)]^2 (4m + 8) 
   + [(2 + 6) + (2 \times 6)]^2 (20m + 4) 
   = 8676m + 2952. 
   \]

2. The second hyper-Gourava index for $m - \text{BiI}_3$ is
   \[
   \text{HGO}_2 (G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u, d_v)] 
   \]
   \[
   = [(1 + 6) + (1 \times 6)] (4m + 8) 
   + [(2 + 6) + (2 \times 6)] (20m + 4) 
   = 191376m + 93376. 
   \]

**3.2.2. Bismuth Triiodide Sheet $\text{BiI}_3(m \times n)$**

The molecular graph of the bismuth triiodide sheet $\text{BiI}_3(m \times n)$ is shown in Figure 23. It can be observed from Figure 23 that the edge set of the bismuth triiodide sheet $\text{BiI}_3(m \times n)$ can be divided into three classes based on the degrees of end vertices as shown in Table 6.

**Theorem 11.** Let $G$ be the graph of the bismuth triiodide sheet $\text{BiI}_3(m \times n)$. Then, the first and second Gourava indices are

1. $\text{GO}_1 (G) = 402mn + 212m + 50n - 28$, 
2. $\text{GO}_2 (G) = 2124mn + 936m - 36n - 216$.

**Proof.** From the edge partition of the edge set of the bismuth triiodide sheet $\text{BiI}_3(m \times n)$ given in Table 6, we have

1. The first Gourava index for $\text{BiI}_3(m \times n)$ is
   \[
   \text{GO}_1 (G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u, d_v)] 
   \]
   \[
   = [(1 + 6) + (1 \times 6)] (4m + 4n + 4) 
   + [(2 + 6) + (2 \times 6)] (12mn + 8m + 8n - 4) 
   + [(3 + 6) + (3 \times 6)] (6mn - 6n) 
   = 402mn + 212m + 50n - 28. 
   \]

2. The second Gourava index for $\text{BiI}_3(m \times n)$ is
   \[
   \text{GO}_2 (G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u, d_v)] 
   \]
   \[
   = [(1 + 6) \times (1 \times 6)] (4m + 4n + 4) 
   + [(2 + 6) \times (2 \times 6)] (12mn + 8m + 8n - 4) 
   + [(3 + 6) \times (3 \times 6)] (6mn - 6n) 
   = 2124mn + 936m - 36n - 216. 
   \]

**Theorem 12.** Let $G$ be the graph of the bismuth triiodide sheet $\text{BiI}_3(m \times n)$. Then, the first and second hyper-Gourava indices are

1. $\text{HGO}_1 (G) = 9174mn + 3876m - 498n - 924$, 
2. $\text{HGO}_2 (G) = 268056mn + 80784m - 143036n - 29808$. 

Proof. From the edge partition of the edge set of the bismuth triiodides sheet \( \text{BiI}_3 \) \((m \times n)\) given in Table 6, we have

1. The first hyper-Gourava index for \( \text{BiI}_3 \) \((m \times n)\) is

\[
\text{HGO}_1(G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u d_v)]^2
\]

\[
= [(1 + 6) + (1 \times 6)]^2 (4m + 4n + 4)
+ [(2 + 6) + (2 \times 6)]^2 (12mn + 8m + 8n - 4)
+ [(3 + 6) + (3 \times 6)]^2 (6mn - 6n)
= 9174mn + 3876m - 498n - 924.
\]

(26)

2. The second hyper-Gourava index for \( \text{BiI}_3 \) \((m \times n)\) is

\[
\text{HGO}_2(G) = \sum_{uv \in E(G)} [(d_u + d_v) (d_u d_v)]^2
\]

\[
= [(1 + 6) \times (1 \times 6)]^2 (4m + 4n + 4)
+ [(2 + 6) \times (2 \times 6)]^2 (12mn + 8m + 8n - 4)
+ [(3 + 6) \times (3 \times 6)]^2 (6mn - 6n)
= 268056mn + 80784m - 143036n - 29808.
\]

(27)

\[\square\]

3.3. Graphical Representation. Graphical representation of computed topological indices for the bismuth triiodide chain is shown in Figures 24–27, and the graphical representation of the bismuth triiodide sheet is shown in Figures 28–31.

3.4. Gourava Indices for Dendrimers. In the medication mathematical model, the structure of the drug is addressed as an undirected graph, where each vertex exhibits a molecule and each edge addresses a bond between atoms. A huge number of new drugs have been made each year. From this time forward, it asks for a giant measure of work to choose the pharmacological compound and organic qualities of these new drugs, and such remaining tasks at hand end up being progressively specific and grouped. It requires enough reagent rigging and accomplices to test the exhibitions and the responses of new drugs. Nevertheless, in cut down poor countries and locales (for instance, certain urban networks and countries in South America, Southeast Asia, Africa, and India), there is no sufficient money to settle reagents and apparatus which can be used to gauge the biochemical properties. For topological study of dendrimers, we refer [53–66].
3.4.1. Gourava Indices of Porphyrin Dendrimer $D_nP_n$

The algebraic graph of porphyrin dendrimer $D_nP_n$ is shown in Figure 32. For porphyrin dendrimer $D_nP_n$, $|V(D_nP_n)| = 96n - 10$ and $|E(D_nP_n)| = 105n - 11$. There are six type of edges in the edge set of porphyrin dendrimer, based on the degree of end vertices. Degree-based partition of edges of porphyrin dendrimer $D_nP_n$ is given in Table 7.

**Theorem 13.** Let $G$ be the graph of porphyrin dendrimer $D_nP_n$. Then, the first and second Gourava indices are

1. $GO_1(G) = 1169n - 106$,
2. $GO_2(G) = 3478n - 260$.

**Proof.** From the edge partition of $D_nP_n$ given in Table 7, we have

1. The first Gourava index for $D_nP_n$ is

$$GO_1(G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u, d_v)]$$

   $$= [(1 + 3) + (1 \times 3)](2n) + [(1 + 4) + (1 \times 4)](24n)$$
   $$+ [(2 + 2) + (2 \times 2)](10n - 5)$$
   $$+ [(2 + 3) + (2 \times 3)](48n - 6)$$
   $$+ [(3 + 3) + (3 \times 3)](13n) + [(3 + 4) + (3 \times 4)](8n)$$

   $$= 1169n - 106.$$  \(\text{(28)}\)

2. The second Gourava index for $D_nP_n$ is
Theorem 14. Let $G$ be the graph of porphyrin dendrimer $D_n P_m$. Then, the first and second hyper-Gourava indices are

1. $HGO_1(G) = 13727n - 1046$,
2. $HGO_2(G) = 150004n - 6680$.

Proof. From the edge partition of $D_n P_m$ given in Table 7, we have

1. The first hyper-Gourava index for $D_n P_m$ is

\[
HGO_1(G) = \sum_{uv \in E(G)} \left((d_u + d_v)(d_u d_v)\right)^2 \\
= \left[(1+3)(1+3)(2n) + [(1+4)(1+4)](24n)
+ [(2+2)(2+2)](10n-5)
+ [(2+3)(2+3)](48n-6)
+ [(3+3)(3+3)](13n) + [(3+4)(3+4)](8n)\right] \\
= 3478n - 260.
\]

(29)

2. The second hyper-Gourava index for $D_n P_m$ is

\[
HGO_2(G) = \sum_{uv \in E(G)} \left((d_u + d_v)(d_u d_v)\right)^2 \\
= \left[(1+3)(1+3)(2n) + [(1+4)(1+4)](24n)
+ [(2+2)(2+2)](10n-5)
+ [(2+3)(2+3)](48n-6)
+ [(3+3)(3+3)](13n) + [(3+4)(3+4)](8n)\right] \\
= 13727n - 1046.
\]

(30)

\[
\begin{align*}
(1, 3) & \quad 2n \\
(1, 4) & \quad 124n \\
(2, 2) & \quad 10n - 5 \\
(2, 3) & \quad 48n - 6 \\
(3, 3) & \quad 13n \\
(3, 4) & \quad 8n \\
\end{align*}
\]

Table 7: Degree-based edge partition of $D_n P_m$. 

(31)
3.4.2. Propyl Ether Imine Dendrimer (PETIM). The algebraic graph of propyl ether imine dendrimer (PETIM) is shown in Figure 33. For propyl ether imine dendrimer (PETIM), \(|V(\text{PETIM})| = 24.2^n - 23\) and \(|E(\text{PETIM})| = 24.2^n - 24\). There are six type of edges in the edge set of porphyrin dendrimer, based on the degree of end vertices. Degree-based partition of edges of propyl ether imine dendrimer (PETIM) is given in Table 8.

**Theorem 15.** Let \(G\) be the graph of propyl ether imine dendrimer (PETIM). Then, the first and second Gourava indices are

\[
(1) \quad G_{01}(G) = 66.2^n + 5n^{n+1} + 8.2^{n+4} - 232, \\
(2) \quad G_{02}(G) = 18.2^n + 6.6^{n+1} + 16.2^{n+4} - 528.
\]

**Proof.** From the edge partition of PETIM given in Table 8, we have

(1) The first Gourava index for PETIM is
\[
G_{01}(\text{PETIM}) = \sum_{uv \in E(\text{PETIM})} [(d_u + d_v) + (d_u d_v)] \\
= [(1 + 2) + (1 \times 2)](2^{n+1}) \\
+ [(2 + 2) + (2 \times 2)](2^{n+4} - 18) \\
+ [(2 + 3) + (2 \times 3)](6.2^n - 6) \\
= 66.2^n + 5n^{n+1} + 8.2^{n+4} - 232.
\]

(2) The second Gourava index for PETIM is
\[
G_{02}(\text{PETIM}) = \sum_{uv \in E(\text{PETIM})} [(d_u + d_v) + (d_u d_v)] \\
= [(1 + 2) \times (1 \times 2)](2^{n+1}) \\
+ [(2 + 2) \times (2 \times 2)](2^{n+4} - 18) \\
+ [(2 + 3) \times (2 \times 3)](6.2^n - 6) \\
= 18.2^n + 6.6^{n+1} + 16.2^{n+4} - 528.
\]

**Theorem 16.** Let \(G\) be the graph of propyl ether imine dendrimer (PETIM). Then, the first and second hyper-Gourava indices are

\[
(1) \quad HGO_{1}(G) = 726.2^n + 25.6^{n+1} + 64.2^{n+4} - 2120, \\
(2) \quad HGO_{2}(G) = 5400.2^n + 36.6^{n+1} + 256.2^{n+4} - 11808.
\]

**Proof.** From the edge partition of PETIM given in Table 8, we have

(1) The first hyper-Gourava index for PETIM is
\[
HGO_{1}(G) = \sum_{uv \in E(\text{PETIM})} [(d_u + d_v)\cdot (d_u d_v)] \\
= [(1 + 2) + (1 \times 2)](2^{n+1}) \\
+ [(2 + 2) + (2 \times 2)](2^{n+4} - 18) \\
+ [(2 + 3) + (2 \times 3)](6.2^n - 6) \\
= 726.2^n + 25.6^{n+1} + 64.2^{n+4} - 2120.
\]

(2) The second hyper-Gourava index for PETIM is
\[
HGO_{2}(G) = \sum_{uv \in E(\text{PETIM})} [(d_u + d_v)\cdot (d_u d_v)] \\
= [(1 + 2) \times (1 \times 2)](2^{n+1}) \\
+ [(2 + 2) \times (2 \times 2)](2^{n+4} - 18) \\
+ [(2 + 3) \times (2 \times 3)](6.2^n - 6) \\
= 5400.2^n + 36.6^{n+1} + 256.2^{n+4} - 11808.
\]

3.4.3. Zinc-Porphyrin Dendrimer DPZ. The algebraic graph of zinc-porphyrin dendrimer DPZ is shown in Figure 34. There are six type of edges in the edge set of porphyrin dendrimer, based on the degree of end vertices. Degree-based partition of edges of zinc-porphyrin dendrimer DPZ is given in Table 9.
Theorem 17. Let $G$ be the graph of zinc-porphyrin dendrimer $DPZ_n$. Then, the first and second Gourava indices are

(1) $GO_1(G) = 688.2^n - 372$
(2) $GO_2(G) = 1888.2^n - 1072$

Proof. From the edge partition of $DPZ_n$ given in Table 9, we have

(1) The first Gourava index for $DPZ_n$ is

$$GO_1(G) = \sum_{u\in E(G)} [(d_u + d_v) + (d_u, d_v)]$$
$$= [(2 + 2) + (2 \times 2)](16.2^n - 4)$$
$$+ [(2 + 3) + (2 \times 3)](40.2^n - 16)$$
$$+ [(3 + 3) + (3 \times 3)](8.2^n - 16)$$
$$+ [(3 + 4) + (3 \times 4)](4)$$
$$= 688.2^n - 372.$$  

(2) The second Gourava index for $DPZ_n$ is

$$GO_2(G) = \sum_{u\in E(G)} [(d_u + d_v)(d_u, d_v)]$$
$$= [(2 + 2) \times (2 \times 2)](16.2^n - 4)$$
$$+ [(2 + 3) \times (2 \times 3)](40.2^n - 16)$$
$$+ [(3 + 3) \times (3 \times 3)](8.2^n - 16)$$
$$+ [(3 + 4) \times (3 \times 4)](4)$$
$$= 1888.2^n - 1072.$$  

Theorem 18. Let $G$ be the graph of zinc-porphyrin dendrimer $DPZ_n$. Then, the first and second hyper-Gourava indices are

(1) $HGO_1(G) = 7664n^n - 5716$
(2) $HGO_2(G) = 63424.2^n - 33856$

Proof. From the edge partition of $DPZ_n$ given in Table 9, we have

(1) The first hyper-Gourava index for $DPZ_n$ is

$$HGO_1(G) = \sum_{u\in E(G)} [(d_u + d_v) + (d_u, d_v)]^2$$
$$= [(2 + 2) + (2 \times 2)]^2(16.2^n - 4)$$
$$+ [(2 + 3) + (2 \times 3)]^2(40.2^n - 16)$$
$$+ [(3 + 3) + (3 \times 3)]^2(8.2^n - 16)$$
$$+ [(3 + 4) + (3 \times 4)]^2(4)$$
$$= 7664n^n - 5716.$$  

(2) The second hyper-Gourava index for $DPZ_n$ is

$$HGO_2(G) = \sum_{u\in E(G)} [(d_u + d_v)(d_u, d_v)]^2$$
$$= [(2 + 2) \times (2 \times 2)]^2(16.2^n - 4)$$
$$+ [(2 + 3) \times (2 \times 3)]^2(40.2^n - 16)$$
$$+ [(3 + 3) \times (3 \times 3)]^2(8.2^n - 16)$$
$$+ [(3 + 4) \times (3 \times 4)]^2(4)$$
$$= 63424.2^n - 33856.$$  

3.4.4. Poly(ETHyleneAmidoAmine) Dendrimer (PETA). The algebraic graph of Poly(ETHyleneAmidoAmine) dendrimer (PETA) is shown in Figure 35. For Poly(ETHyleneAmidoAmine) dendrimer (PETA), $|V(PETA)| = 44.2^n - 18$ and $|E(PETA)| = 44.2^n - 19$. There are six type of edges in the edge set of porphyrin dendrimer, based on the degree of end vertices. Degree-based partition of edges of Poly(ETHyleneAmidoAmine) dendrimer (PETA) is given in Table 10.

Theorem 19. Let $G$ be the graph of Poly(ETHylene Amido Amine) dendrimer (PETA). Then, the first and second Gourava indices are

(1) $GO_1(G) = 369.2^n - 177$
(2) $GO_2(G) = 928.2^n - 422$

Proof. From the edge partition of PETA given in Table 10, we have

(1) The first Gourava index for PETA is
Theorem 20. Let $G$ be the graph of Poly(ETHylene Amide Amine) dendrimer (PETAA). Then, the first and second hyper-Gourava indices are

$$
\text{GO}_1 (G) = \sum_{uv \in E(G)} \left[(d_u + d_v) + (d_u \cdot d_v)\right] \\
= \left[(1 + 2) \times (1 \times 2)\right](4.2^n) \\
+ \left[(1 + 3) \times (1 \times 3)\right](4.2^n - 2) \\
+ \left[(2 + 2) \times (2 \times 2)\right](16.2^n - 8) \\
+ \left[(2 + 3) \times (2 \times 3)\right](20.2^n - 9) \\
= 369.2^n - 177.
$$

(2) The second Gourava index for PETAA is

$$
\text{GO}_2 (\text{PETAA}) = \sum_{uv \in E(G)} \left[(d_u + d_v) \cdot (d_u \cdot d_v)\right] \\
= \left[(1 + 2) \times (1 \times 2)\right](4.2^n) \\
+ \left[(1 + 3) \times (1 \times 3)\right](4.2^n - 2) \\
+ \left[(2 + 2) \times (2 \times 2)\right](16.2^n - 8) \\
+ \left[(2 + 3) \times (2 \times 3)\right](20.2^n - 9) \\
= 928.2^n - 422.
$$
Proof. From the edge partition of PETAA given in Table 10, we have

\( HGO_1 (G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u d_v)]^2 \)

\[ = [(1 + 2) + (1 \times 2)]^2 (4.2^n) \]
\[ + [(1 + 3) + (1 \times 3)]^2 (4.2^n - 2) \]
\[ + [(2 + 2) + (2 \times 2)]^2 (16.2^n - 8) \]
\[ + [(2 + 3) + (2 \times 3)]^2 (20.2^n - 9) \]
\[ = 3740.2^n - 1699. \]

(2) The second hyper-Gourava index for PETAA is

\( HGO_2 (G) = \sum_{uv \in E(G)} [(d_u + d_v) (d_u d_v)]^2 \)

\[ = [(1 + 2) \times (1 \times 2)]^2 (4.2^n) \]
\[ + [(1 + 3) \times (1 \times 3)]^2 (4.2^n - 2) \]
\[ + [(2 + 2) \times (2 \times 2)]^2 (16.2^n - 8) \]
\[ + [(2 + 3) \times (2 \times 3)]^2 (20.2^n - 9) \]
\[ = 22816.2^n - 10436. \]

\[ \square \]

3.4.5. Graphical Comparison. In this section, we will present the graphical comparison of first, second, first hyper-, and second hyper-Gourava indices for porphyrin dendrimer \( D_n P_n \), propyl ether imine dendrimer (PETIM), zinc-porphyrin dendrimer \( DPZ_n \) and Poly(EthyleneAmidoAmine) dendrimer (PETAA). Figures 36–39 show the all indices are linearly increasing with respect to involved parameters.

4. Conclusions and Future Works

It is important to calculate topological indices of dendrimers because it is a proved fact that topological indices help to predict many properties without going to the wet lab. There are more than around 148 topological indices, but none of them can completely describe all properties of a chemical compound. Therefore, there is always room to define and study new topological indices. Gourava indices are one step in this direction and are very close to Zagreb indices. Zagreb indices are very well studied by chemists and mathematicians due to their huge applications in chemistry. It is an interesting problem for researchers to study chemical properties and bonds of Gourava indices.

Data Availability

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

Conflicts of Interest

The authors of this paper declare that they have no conflicts of interest.

Authors’ Contributions

All authors have equal contribution.

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