Asia Pac. J. Math. 2026 **13**:146

STRUCTURAL CHARACTERIZATION AND ZAGREB INDEX OF LINKED BICYCLIC MOLECULAR GRAPHS: AN APPLICATION TO CYCLOPENTYLCYCLOHEXANE

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Received Jun. 18, 2026

Abstract. Molecular graph theory provides a rigorous mathematical framework for analyzing the structural connectivity of chemical compounds through graph-theoretic representations. Motivated by the molecular structure of cyclopentylcyclohexane, this study investigates a linked bicyclic molecular graph constructed by joining two cycle graphs with a single bridge edge. The main objective is to characterize the structural properties of this graph and to derive its Zagreb-type topological indices. Explicit formulas are obtained for several fundamental structural parameters, including order, size, vertex degrees, distance-related properties, and diameter. Furthermore, Zagreb-type topological indices are derived to describe the degree-based invariant behavior of the linked bicyclic molecular graph. The molecular graph of cyclopentylcyclohexane is presented as a representative case, illustrating the applicability of the proposed framework to a concrete linked bicyclic chemical structure. The results contribute to the structural characterization of linked cyclic molecular graphs and provide useful graph invariants for further studies in chemical graph theory and molecular topology.

2020 Mathematics Subject Classification. 05C50; 05C92; 92E10.

Key words and phrases. linked bicyclic graph; molecular graph; spectral graph theory; cyclopentylcyclohexane; computational molecular modeling.

1. Introduction

Molecular graph theory provides a rigorous mathematical framework for representing and analyzing the structural connectivity of chemical compounds. In this representation, atoms are modeled as vertices

DOI: 10.28924/APJM/13-146

and chemical bonds as edges, allowing molecular structures to be studied using graph-theoretical and spectral methods [8]. Such methods lead to molecular descriptors that quantitatively characterize structural features of chemical graphs [5].

Structural parameters such as vertex degree, distance, and diameter describe the connectivity pattern of a molecular graph and provide fundamental information about its topological structure. In particular, degree-based parameters play an important role in defining Zagreb-type topological indices, which are widely used to quantify molecular branching and connectivity. The first Zagreb index, second Zagreb index, and hyper-Zagreb index are among the invariants commonly employed to capture structural information encoded by vertex degrees and edge adjacencies. Related graph invariants, including energy-based, Laplacian-type, and closeness-energy parameters, have also been investigated in various graph classes [10,11]. These graph-theoretical parameters may support molecular comparison, structural classification, and preliminary computational analysis of related chemical structures.

A linked bicyclic molecular graph is obtained by joining two cycle graphs through a single connecting edge. Unlike fused or condensed bicyclic graphs, the two cycles in a linked bicyclic graph do not share vertices or edges. Thus, this class of graphs provides a simple but structurally meaningful model for molecular systems consisting of two cyclic units connected by a single bond.

Cyclopentylcyclohexane provides a representative example of a linked bicyclic molecular structure, since it consists of a cyclopentane ring and a Cyclohexane ring connected by a single bond. In the corresponding molecular graph, atoms are treated as vertices and chemical bonds as edges, so the structure can be modeled as C_5^6. This compound is selected as a case study because its ring-linked bicyclic structure provides a concrete molecular example for examining the structural and spectral properties of linked bicyclic molecular graphs.

Ring systems constitute important structural components of pharmaceutical compounds because they influence molecular architecture and provide scaffolds for molecular optimization [12]. Molecular structures can also be represented computationally as graphs, allowing relationships between atomic connectivity and molecular properties to be examined using graph-based methods [9,14]. Cyclopentylcyclohexane has been reported in GC–MS analysis of *Caesalpinia sappan* extract; however, its individual cytotoxic activity remains unconfirmed because the reported assay was performed on the complete extract rather than the purified compound [4].

Although cycle graphs and several classes of bicyclic graphs have been widely investigated, a systematic characterization of linked bicyclic molecular graphs, particularly in terms of both structural and spectral properties, remains limited. Motivated by this gap, this study develops structural and spectral characterizations of linked bicyclic molecular graphs. Explicit results are derived for the order, size, vertex degree, distance function, diameter, first Zagreb, second Zagreb, and hyper Zagreb indices.

Finally, the obtained theoretical results are applied to the molecular graph of Cyclopentylcyclohexane, represented by C_5^6. This application illustrates how the proposed framework can be used to analyze a concrete linked bicyclic molecular structure.

2. Preliminaries

The molecule is modeled as a simple graph $G = (V, E)$, where vertices $V(G) = \{v_1, v_2, \cdots, v_n\}$ represent atoms and edges $E(G)$ represents chemical bonds.

The number of vertices that adjacent to v is the degree of v, denoted by $deg_G(v)$. For each unordered pair of vertices $\{u, v\}$, let $d_G(u, v)$ denote the shortest path distance between u and v, and let $\alpha_G(u, v)$ denote the number of shortest paths connecting these two vertices. The diameter of G is defined by

$$\operatorname{diam}(G) = \max_{u,v \in V(G)} d_G(u, v).$$

Furthermore, the molecular graph can be associated with several Zagreb-based topological indices, which are useful for describing structural and chemical properties of the molecule. The first Zagreb index is defined as the sum of the squares of the degrees of all vertices in a graph [3]:

$$M_1(G) = \sum_{v \in V} \left(\deg_G(v)\right)^2. \tag{2.1}$$

The second Zagreb index is defined as the sum, taken over all edges (u,v), of the product of the degrees of the two incident vertices [1]:

$$M_2(G) = \sum_{uv \in E} \deg_G(u) \cdot \deg_G(v). \tag{2.2}$$

The hyper-Zagreb index is defined as the sum, over all edges (u,v), of the square of the sum of the degrees of the two incident vertices [13]:

$$HM(G) = \sum_{uv \in E} \left(\deg_G(u) + \deg_G(v)\right)^2. \tag{2.3}$$

3. Structural Properties of Linked Bicyclic Molecular Graphs

A cycle graph is obtained by joining the terminal vertices of a path graph. Consequently, every vertex in a cycle graph has degree two. A cycle graph with n vertices is denoted by C_n.

Let C_{n_1} and C_{n_2} be two distinct cycle graphs with vertex sets $V(C_{n_1}) = \{r_1, r_2, \ldots, r_{n_1}\}$ and $V(C_{n_2}) = \{s_1, s_2, \ldots, s_{n_2}\}$, respectively, for natural numbers $n_1, n_2 \geq 2$. The linked bicyclic graph, denoted by $C_{n_1}^{n_2}$, is obtained by adding a single edge (r_1, s_1) between the vertices $r_1 \in V(C_{n_1})$ and $s_1 \in V(C_{n_2})$, as illustrated in Figure 1.

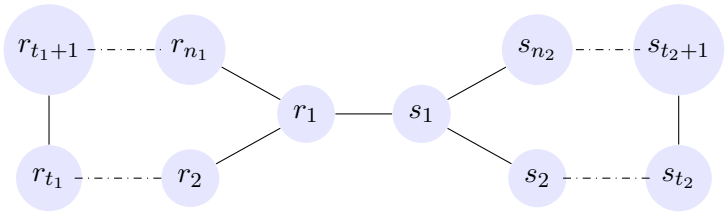

FIGURE 1. Clustered graph G

Theorem 3.1. *Let $G = C_{n_1}^{n_2}$ be a linked bicyclic graph obtained by joining two cycle graphs C_{n_1} and C_{n_2} through the edge (r_1, s_1), where $V(C_{n_1}) = \{r_1, r_2, \ldots, r_{n_1}\}$ and $V(C_{n_2}) = \{s_1, s_2, \ldots, s_{n_2}\}$. Then the degree of each vertex $v \in V(G)$ is given by*

$$deg_G(v) = \begin{cases} 3, & \text{if } v = r_1 \text{ or } v = s_1 \\ 2, & \text{if } v \in V(C_{n_1}) \backslash r_1 \text{ and } v \in V(C_{n_2}) \backslash s_1 \end{cases}.$$

Proof. In a cycle graph, every vertex has degree two. In the linked bicyclic graph $C_{n_1}^{n_2}$, the graph is obtained by adding a single edge (r_1, s_1) between the two cycle graphs C_{n_1} and C_{n_2}. Hence, the vertices r_1 and s_1 each receive one additional incident edge. Since both vertices originally have degree two in their respective cycles, we obtain

$$\deg_G(r_1) = \deg_G(s_1) = 3.$$

All other vertices are not incident with the linking edge (r_1, s_1). Therefore, their degrees remain equal to two. Thus,

$$\deg_G(v) = 2$$

for every $v \in (V(C_{n_1}) \setminus \{r_1\}) \cup (V(C_{n_2}) \setminus \{s_1\})$. This completes the proof. □

Theorem 3.2. *Let $G = C_{n_1}^{n_2}$ be a linked bicyclic graph obtained by joining two cycle graphs C_{n_1} and C_{n_2} through the edge (r_1, s_1), where $V(C_{n_1}) = \{r_1, r_2, \ldots, r_{n_1}\}$ and $V(C_{n_2}) = \{s_1, s_2, \ldots, s_{n_2}\}$. Then the distance between two vertices u and v in G is*

$$d_G(u,v) = \begin{cases} \min\{|i-j|,\ n_1 - |i-j|\}, & \text{if } u = r_i,\ v = r_j, \\ \min\{|i-j|,\ n_2 - |i-j|\}, & \text{if } u = s_i,\ v = s_j, \\ \min\{i-1,\ n_1 - i + 1\} + \\ 1 + \min\{j-1,\ n_2 - j + 1\}, & \text{if } u = r_i,\ v = s_j. \end{cases}$$

Proof. If $u = r_i$ and $v = r_j$ lie in C_{n_1}, then the shortest path between them is contained in C_{n_1}. Hence,

$$d_G(r_i, r_j) = \min\{|i-j|,\ n_1 - |i-j|\}.$$

Similarly, if $u = s_i$ and $v = s_j$ lie in C_{n_2}, then

$$d_G(s_i, s_j) = \min\{|i-j|,\ n_2 - |i-j|\}.$$

It remains to consider the case $u = r_i$ and $v = s_j$. Since (r_1, s_1) is the only edge joining the two cycles, every path from r_i to s_j must pass through this edge. Therefore,

$$d_G(r_i, s_j) = d_{C_{n_1}}(r_i, r_1) + 1 + d_{C_{n_2}}(s_1, s_j).$$

Now,

$$d_{C_{n_1}}(r_i, r_1) = \min\{i - 1,\ n_1 - i + 1\}$$

and

$$d_{C_{n_2}}(s_1, s_j) = \min\{j - 1,\ n_2 - j + 1\}.$$

Thus,

$$d_G(r_i, s_j) = \min\{i - 1,\ n_1 - i + 1\} + 1 + \min\{j - 1,\ n_2 - j + 1\}.$$

This completes the proof. □

Theorem 3.3. *Let $G = C_{n_1}^{n_2}$ be a linked bicyclic graph obtained by joining two cycle graphs C_{n_1} and C_{n_2} through the edge (r_1, s_1), where $V(C_{n_1}) = \{r_1, r_2, \ldots, r_{n_1}\}$ and $V(C_{n_2}) = \{s_1, s_2, \ldots, s_{n_2}\}$. Then the diameter of G is*

$$diam_G = \left\lfloor \frac{n_1}{2} \right\rfloor + \left\lfloor \frac{n_2}{2} \right\rfloor + 1.$$

Proof. Let $x \in V(C_{n_1})$ and $y \in V(C_{n_2})$. Since the only edge joining the two cycles is (r_1, s_1), every path from x to y must pass through this edge. Hence,

$$d_G(x, y) = d_{C_{n_1}}(x, r_1) + 1 + d_{C_{n_2}}(s_1, y).$$

For $x = r_i$, we have

$$d_{C_{n_1}}(x, r_1) = \min\{i - 1, n_1 - i + 1\} \leq \left\lfloor \frac{n_1}{2} \right\rfloor.$$

Similarly, for $y = s_j$,

$$d_{C_{n_2}}(s_1, y) = \min\{j - 1, n_2 - j + 1\} \leq \left\lfloor \frac{n_2}{2} \right\rfloor.$$

Thus,

$$d_G(x, y) \leq \left\lfloor \frac{n_1}{2} \right\rfloor + 1 + \left\lfloor \frac{n_2}{2} \right\rfloor.$$

This upper bound is attained by choosing x and y such that

$$d_{C_{n_1}}(x, r_1) = \left\lfloor \frac{n_1}{2} \right\rfloor \quad \text{and} \quad d_{C_{n_2}}(s_1, y) = \left\lfloor \frac{n_2}{2} \right\rfloor.$$

Moreover, the distance between any two vertices in the same cycle is at most the diameter of that cycle. Therefore, the largest distance in G occurs between vertices lying in different cycles. Consequently,

$$\text{diam}(G) = \left\lfloor \frac{n_1}{2} \right\rfloor + \left\lfloor \frac{n_2}{2} \right\rfloor + 1.$$

□

Theorem 3.4. *Let $G = C_{n_1}^{n_2}$ be a linked bicyclic graph obtained by joining two cycle graphs C_{n_1} and C_{n_2} through the edge (r_1, s_1), where*

$$V(C_{n_1}) = \{r_1, r_2, \ldots, r_{n_1}\} \quad \textit{and} \quad V(C_{n_2}) = \{s_1, s_2, \ldots, s_{n_2}\}.$$

Then the number of edges of G is

$$|E(G)| = n_1 + n_2 + 1.$$

Proof. The cycle graph C_{n_1} has n_1 edges, and the cycle graph C_{n_2} has n_2 edges. Since G is obtained by adding exactly one edge (r_1, s_1) between the two cycles, the total number of edges is

$$|E(G)| = |E(C_{n_1})| + |E(C_{n_2})| + 1 = n_1 + n_2 + 1.$$

This completes the proof.

□

4. Zagreb-Type Topological Indices of Linked Bicyclic Molecular Graphs

Having established the structural formulation of the linked bicyclic molecular graph, we next examine its degree-based topological behavior through Zagreb-type indices. This section focuses on how the linkage structure influences the values of the first Zagreb index, second Zagreb index, and related Zagreb-type descriptors.

Theorem 4.1. *Let $G = C_{n_1}^{n_2}$ be a linked bicyclic graph obtained by joining two cycle graphs C_{n_1} and C_{n_2} through the edge (r_1, s_1), where*

$$V(C_{n_1}) = \{r_1, r_2, \ldots, r_{n_1}\} \quad \textit{and} \quad V(C_{n_2}) = \{s_1, s_2, \ldots, s_{n_2}\}.$$

Then the first Zagreb of G is

$$M_1(G) = 4(n_1 + n_2) + 10.$$

Proof. Based on Equation 2.1, we have

$$\begin{aligned}
M_1(G) &= \sum_{v \in V} (\deg_G(v))^2 \\
&= \sum_{v \in V(C_{n_1}) \setminus r_1, v \in V(C_{n_2}) \setminus s_1} (\deg_G(v))^2 + \sum_{v = r_1, s_1} (\deg_G(v))^2 \\
&= \sum_{v \in V(C_{n_1}) \setminus r_1, v \in V(C_{n_2}) \setminus s_1} (2)^2 + \sum_{v = r_1, s_1} (3)^2 \\
&= ((n_1 - 1) + (n_2 - 1))(2)^2 + (2)(3)^2 \\
&= 4(n_1 + n_2 - 2) + 18 \\
&= 4(n_1 + n_2) + 10.
\end{aligned}$$

□

Theorem 4.2. *Let $G = C_{n_1}^{n_2}$ be a linked bicyclic graph obtained by joining two cycle graphs C_{n_1} and C_{n_2} through the edge (r_1, s_1), where*

$$V(C_{n_1}) = \{r_1, r_2, \ldots, r_{n_1}\} \quad \textit{and} \quad V(C_{n_2}) = \{s_1, s_2, \ldots, s_{n_2}\}.$$

Then the second Zagreb of G is

$$M_2(G) = 4(n_1 + n_2) + 17.$$

Proof. Based on Equation 2.2, we have

$$\begin{aligned} M_2(G) &= \sum_{uv \in E} \deg_G(u) \cdot \deg_G(v) \\ &= (n_1 + n_2 - 4)2 \cdot 2 + 4 \cdot 2 \cdot 3 + 1 \cdot 3 \cdot 3 \\ &= 4(n_1 + n_2 - 4) + 24 + 9 \\ &= 4(n_1 + n_2) + 17. \end{aligned}$$

□

Theorem 4.3. *Let $G = C_{n_1}^{n_2}$ be a linked bicyclic graph obtained by joining two cycle graphs C_{n_1} and C_{n_2} through the edge (r_1, s_1), where*

$$V(C_{n_1}) = \{r_1, r_2, \ldots, r_{n_1}\} \quad \textit{and} \quad V(C_{n_2}) = \{s_1, s_2, \ldots, s_{n_2}\}.$$

Then the hyper Zagreb of G is

$$HM(G) = 4(n_1 + n_2) + 10.$$

Proof. Based on Equation 2.3, we have

$$\begin{aligned} HM(G) &= \sum_{uv \in E} \left(\deg_G(u) + \deg_G(v)\right)^2 \\ &= (n_1 + n_2 - 4)(2 + 2)^2 + 4(2 + 3)^2 + 1(3 + 3)^2 \\ &= 16(n_1 + n_2 - 4) + 100 + 36 \\ &= 16(n_1 + n_2) + 72. \end{aligned}$$

□

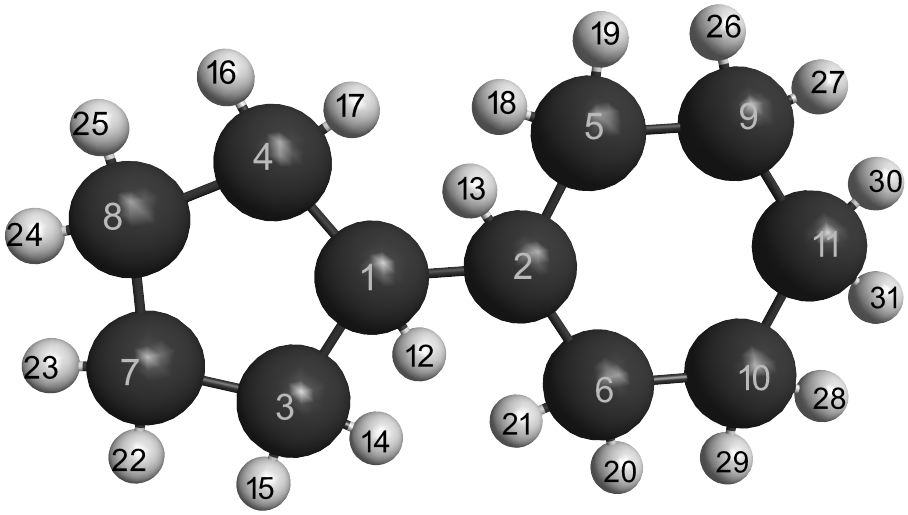

FIGURE 2. Cyclopentylcyclohexane (compound) $C_{11}H_{20}$

5. Cyclopentylcyclohexane Compound

Cyclopentylcyclohexane is considered in this study as an example of a linked bicyclic molecular graph, where the cyclopentane and cyclohexane rings are modeled as two cycle graphs connected by a single edge.

This construction yields a connected graph consisting of two cycle graphs joined by a single edge, and hence forms a simple linked bicyclic graph. In this study, Cyclopentylcyclohexane is modeled as such a molecular graph, where its 11 methylene groups are represented as vertices and the chemical bonds between adjacent methylene groups are represented as edges. Then we denote this compound as a linked bicyclic graph C_5^6.

The degree of each vertex in the linked bicyclic graph C_5^6 can be determined by counting the number of edges incident to that vertex. Since vertices v_1 and v_2 connect the two cycles, they are adjacent to three vertices each. The remaining vertices belong only to their respective cycles and therefore have degree two. Hence, $d(v_1) = d(v_2) = 3$,
$d(v_3) = d(v_4) = d(v_5) = d(v_6) = d(v_7) = d(v_8) = d(v_9) = d(v_{10}) = d(v_{11}) = 2$.

Moreover, the graph C_5^6 is obtained by joining a cycle graph C_5 and a cycle graph C_6 with a single connecting edge. Since C_5 contains 5 edges and C_6 contains 6 edges, the total number of edges in C_5^6 is

$$|E(C_5^6)| = 5 + 6 + 1 = 12.$$

The longest shortest path is attained between a vertex at maximum distance from v_1 in the cycle C_5 and a vertex at maximum distance from v_2 in the cycle C_6. Since the maximum distance from v_1 to any vertex of C_5 is 2, the distance between v_1 and v_2 is 1, and the maximum distance from v_2 to any vertex of C_6 is 3, it follows that

$$\operatorname{diam}(C_5^6) = 2 + 1 + 3 = 6.$$

The first Zagreb index of a graph C_5^6 is defined by

$$M_1(C_5^6) = \sum_{v \in V(C_5^6)} d(v)^2.$$

Since the graph C_5^6 has two vertices of degree 3 and nine vertices of degree 2, we obtain the first Zagreb index of C_5^6 as follows.

$$\begin{aligned} M_1(C_5^6) &= 3^2 + 3^2 + 2^2 + 2^2 + 2^2 + 2^2 + 2^2 + 2^2 + 2^2 + 2^2 + 2^2 \\ &= 2(3^2) + 9(2^2) \\ &= 2(9) + 9(4) \\ &= 18 + 36 \\ &= 54. \end{aligned}$$

The second Zagreb index of a graph C_5^6 is defined as

$$M_2(C_5^6) = \sum_{uv \in E(C_5^6)} d(u)d(v).$$

For the graph C_5^6, there is one edge of type $(3,3)$, four edges of type $(3,2)$, and seven edges of type $(2,2)$. Therefore, the second Zagreb index of C_5^6 is

$$\begin{aligned} M_2(C_5^6) &= \sum_{uv \in E(C_5^6)} d(u)d(v) \\ &= 1(3 \cdot 3) + 4(3 \cdot 2) + 7(2 \cdot 2) \\ &= 9 + 24 + 28 \\ &= 61. \end{aligned}$$

The Hyper Zagreb index of a graph C_5^6 is defined as

$$HM(C_5^6) = \sum_{uv \in E(C_5^6)} \left(d(u) + d(v)\right)^2.$$

For the graph C_5^6, there is one edge of type $(3,3)$, four edges of type $(3,2)$, and seven edges of type $(2,2)$. Therefore, the Hyper Zagreb index of C_5^6 is

$$\begin{aligned} HM(C_5^6) &= \sum_{uv \in E(C_5^6)} (d(u) + d(v))^2 \\ &= 1(3+3)^2 + 4(3+2)^2 + 7(2+2)^2 \\ &= 1(36) + 4(25) + 7(16) \\ &= 36 + 100 + 112 \\ &= 248. \end{aligned}$$

6. Discussion

The increasing trends are consistent with the degree-based nature of Zagreb-type indices, which encode structural information through vertex degrees and adjacent degree interactions. The hyper-Zagreb index grows faster because it uses the squared sum of adjacent vertex degrees, making it more sensitive to structural expansion than the first and second Zagreb indices.

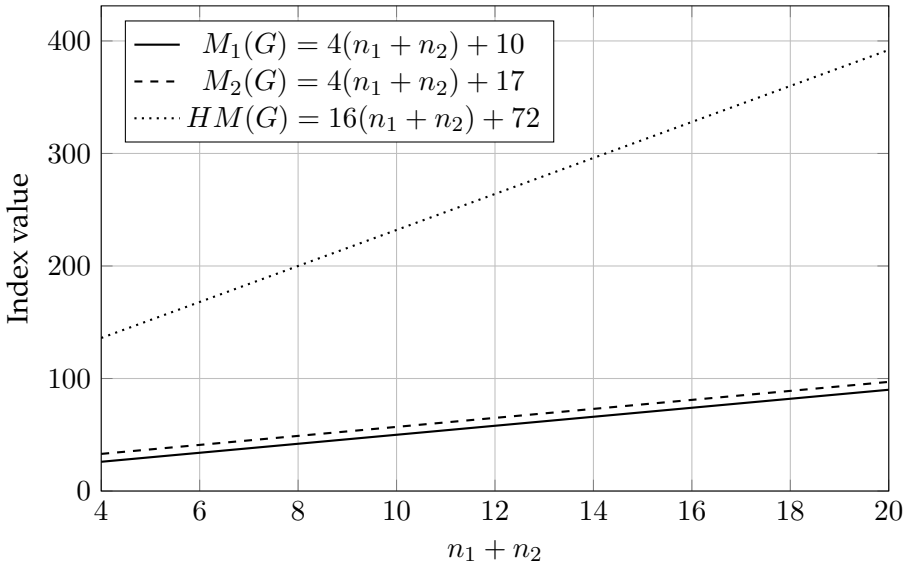

Figure 3. Comparison of the First Zagreb, Second Zagreb, and Hyper Zagreb indices of the linked bicyclic graph $C_{n_1}^{n_2}$.

The graphical comparison shows that the index values increase consistently as $n_1 + n_2$ becomes larger. This result is theoretically reasonable because Zagreb-type indices are degree-based topological descriptors; therefore, their values are strongly affected by the number of vertices, edge arrangement, pendant vertices, and degree distribution of the graph. Zhao and Li [15] emphasized that the first and second Zagreb indices reflect the extent of branching in the underlying molecular structure and demonstrated that, in bicyclic graphs, their sharp bounds depend on the number of pendant vertices. This supports the present finding that increasing the structural parameter $n_1 + n_2$ produces a corresponding increase in the observed index values.

The relatively close behavior of $M_1(G)$ and $M_2(G)$ is also consistent with previous studies showing that both indices are controlled by vertex-degree contributions in bicyclic graphs. Li and Zhao [6] showed that the extremal values of Zagreb indices in bicyclic graphs depend on structural restrictions such as matching number, perfect matching, pendant vertices, and the arrangement of cycles. Thus, the linear growth observed in Figure 3 can be interpreted as a consequence of systematic expansion in the graph structure rather than a purely numerical pattern.

Furthermore, the higher growth of $HM(G)$ compared with $M_1(G)$ and $M_2(G)$ indicates that this index is more sensitive to changes in adjacent vertex-degree contributions. This interpretation is in line with [2], who showed that variants of the second Zagreb index, especially those giving stronger weights to adjacent degree products, distinguish extremal unicyclic and bicyclic graphs more sharply. Similarly, Li and Zhang [7] confirmed that the second Zagreb index and its reciprocal form are powerful tools for characterizing extremal bicyclic graphs, particularly because they depend directly on degree interactions along edges.

Therefore, the present result is supported by the literature: as the graph expands through $n_1 + n_2$, the degree-based structural information increases, causing all indices to rise. The larger magnitude of $HM(G)$ suggests that it captures structural expansion more strongly than the classical Zagreb indices, making it more responsive to changes in the graph's degree-based configuration.

Acknowledgements. This research is funded by the University of Mataram under the PNBP Program 2026 (Grant No. 1716/UN18.L1/PP/2026).

Conflicts of Interest. The authors declare that there are no conflicts of interest regarding the publication of this paper.

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