

Mostar index of certain classes of bicyclic graphs

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ABSTRACT

The Mostar index (MoI) of a finite and connected graph G is a measure of asymmetry, focusing on the edge-based structure of the graph. For an edge xy in G , let γ_{xy} and γ_{yx} denote the cardinalities of the sets of vertices closer to x and y respectively, then the Mostar index is defined as: $\text{MoI}(G) = \sum_{xy \in E(G)} |\gamma_{xy} - \gamma_{yx}|$ where the summation is taken over all edges $xy \in G$. This edge-wise difference reflects how asymmetrically the graph is structured around each edge and summing these differences across all edges yields the Mostar index for the graph. In this article, we compute the MoI for certain classes of bicyclic graphs that are of particular interest due to their moderately complex structure, lying between acyclic and polycyclic graphs. We classify bicyclic graphs into three distinct types, namely $\mathcal{B}^1(m, n)$, $\mathcal{B}^2(l, m, n)$ and $\mathcal{B}^1(l, m)$, based on their cycle arrangements and then provide explicit formulas for calculating the exact value of the Mostar index.

Keywords: topological index, Mostar index, bicyclic graph

1. Introduction

Graph theory offers the fundamental framework for analyzing and optimizing the structure and dynamics of complex networks. The topological index TI is a numerical quantity associated with a underlying structure of a graph [14, 13]. The study of these invariants has become increasingly significant in understanding the structural properties of various classes of graphs [4]. The distance-based topological index was introduced by Wiener, captured various structural features of a graph based on the distances between its vertices and correlated with several physicochemical properties of compounds [17, 16]. Subsequently, additional distance-based TIs such as Hosoya, Shultz and Szeged index were introduced to study branching patterns, asymmetry and connectivity [6, 11].

Vertices and edges integrate to form a graph G , having vertex set $V(G)$ and edge set $E(G)$. The

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Received 01 December 2024; Revised 10 April 2025; Accepted 19 April 2025; Published Online 12 May 2025.

DOI: [10.61091/jcmcc125-29](https://doi.org/10.61091/jcmcc125-29)

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degree of node x , represented by d_x , is defined as the count of incident links. The notation $d(x, y)$ represents the distance between the nodes, which is defined as the number of edges in the shortest path connecting x and y in G . The set of all nodes closer to x than y for each edge $xy \in E(G)$ is denoted by $\gamma(x, y)$ and the cardinality of set $\gamma(x, y)$ is denoted by $\gamma(xy)$.

In graph-theoretic approach, structures are essential because they define relationships and connectivity within graphs, influencing their properties and behavior. An important structure in graph theory is a graph with cycles, which are closed paths formed by a sequence of edges and vertices that create a loop. The cyclic graphs are critical for understanding complex network behaviors, such as feedback loops in control systems and redundancies in communication networks. Graphs with cycles can exhibit both symmetric and asymmetric behaviors. The study of asymmetry in these graphs is important, as it focuses on measuring how the structure deviates from symmetry.

The physicochemical properties of graphs can also be determined by quantifying their structural asymmetry. In this regard, Došlić et al. introduced the Mostar index, a novel distance-based topological index that measures asymmetry in edge neighborhoods [3]. It is calculated by summing the absolute differences between the cardinalities γ_{xy} and γ_{yx} for each edge xy in the graph G :

$$\text{MoI}(G) = \sum_{xy \in E(G)} |\gamma_{xy} - \gamma_{yx}|, \quad (1)$$

where

$$\text{MoI}(xy) = |\gamma_{xy} - \gamma_{yx}|. \quad (2)$$

Many researchers have studied the structural asymmetry of various classes of graphs. This includes investigating its properties, computational methods and applications in areas such as mathematical chemistry and network analysis. Recently, Mostar index and edge Mostar index of carbon structures and maximum Mostar index of all n -vertex cacti with its upper bound is also computed (see [1, 7]). The application of Mostar index in identifying vulnerable links has been discussed (see [2]). The difference between the Mostar index of the graph alongwith its irregularity has studied (see [5]). Extremal hexagonal chains with respect to Mostar index are characterised and some conjectures about the bicyclic graphs have been proved (see [8, 12]).

A graph that contains exactly two cycles is called a bicyclic graph such that $|E(G)| = |V(G)| + 1$. These two cycles can be connected by a path, an edge, or a common vertex. Bicyclic graphs have interesting structural aspects that allow researchers to analyze how size or connectivity of cycles influence the graph's overall properties. Recently, minimum Wiener index and extremal arithmetic-geometric index of bicyclic graphs are investigated (see [9, 10]). The upper bounds of the edge Mostar index with respect to bicyclic graphs and extremal bicyclic graphs with respect to Mostar index are studied (see [12, 15]). This motivates us to compute Mostar index for the following classes of bicyclic graphs.

1.1. Mostar index of Bicyclic graph of class-I ($\mathcal{B}^1(m, n)$)

The bicyclic graph $\mathcal{B}^1(m, n)$ is obtained from a cycle C_m by joining its two vertices at distance $n - 1$. The vertex set and edge set of $\mathcal{B}^1(m, n)$ are $V(\mathcal{B}^1(m, n)) = \{v_1, v_2, \dots, v_m\}$ and $E(\mathcal{B}^1(m, n)) = \{v_i v_{i+1} \mid 1 \leq i \leq m\} \cup \{v_1 v_n\}$ with cardinalities $|V(G)| = m$ and $|E(G)| = m + 1$ respectively and subscripts are taken as mod m . The bicyclic graph of class-I $\mathcal{B}^1(12, 6)$ is shown in Figure 1.

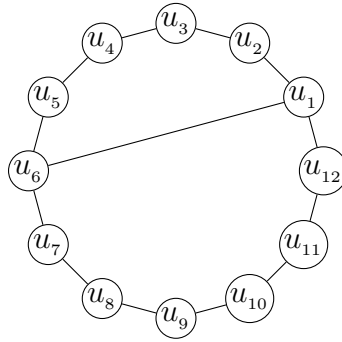


Fig. 1. Bicyclic graph of class-I ($\mathcal{B}^1(12, 6)$)

In the following Lemmas, Mostar index corresponding to edge partitions for the graph $\mathcal{B}^1(m, n)$ for different values of m and n is shown in Table 1 is computed.

Table 1. Edge partitions for the graph $\mathcal{B}^1(m, n)$ for different values of m and n

	$m = \text{odd}, n = \text{even}$	$m = \text{odd}, n = \text{odd}$	$m = \text{even}, n = \text{even}$	$m = \text{even}, n = \text{odd}$
$E_1(\mathcal{B}^1(m, n))$	$v_{\frac{n}{2}} v_{\frac{n+2}{2}}$	$v_{\frac{n}{2}} v_{\frac{n+2}{2}}$	$v_{\frac{n}{2}} v_{\frac{n+2}{2}}$	$v_{\frac{n-1}{2}} v_{\frac{n+1}{2}}, v_{\frac{n+1}{2}} v_{\frac{n+3}{2}}$
$E_2(\mathcal{B}^1(m, n))$	$v_i v_{i+1},$ $1 \leq i \leq \frac{n-2}{2},$ $\frac{n+2}{2} \leq i \leq n-1.$	$v_i v_{i+1},$ $1 \leq i \leq \frac{n-3}{2},$ $\frac{n+3}{2} \leq i \leq n-1.$	$v_i v_{i+1},$ $1 \leq i \leq \frac{n-2}{2},$ $\frac{n+2}{2} \leq i \leq n-1.$	$v_i v_{i+1},$ $1 \leq i \leq \frac{n-3}{2},$ $\frac{n+3}{2} \leq i \leq n-1.$
$E_3(\mathcal{B}^1(m, n))$	$v_{\frac{m+n-1}{2}} v_{\frac{m+n+1}{2}},$ $v_{\frac{m+n+1}{2}} v_{\frac{m+n+3}{2}}$	$v_{\frac{m+n}{2}} v_{\frac{m+n+2}{2}}$	$v_{\frac{m+n}{2}} v_{\frac{m+n+2}{2}}$	$v_{\frac{m+n-1}{2}} v_{\frac{m+n+1}{2}},$ $v_{\frac{m+n+1}{2}} v_{\frac{m+n+3}{2}}$
$E_4(\mathcal{B}^1(m, n))$	$v_{\frac{m+n-3}{2}} v_{\frac{m+n-1}{2}},$ $v_{\frac{m+n+3}{2}} v_{\frac{m+n+5}{2}}$	$v_{\frac{m+n-2}{2}} v_{\frac{m+n}{2}},$ $v_{\frac{m+n+2}{2}} v_{\frac{m+n+4}{2}}$	$v_{\frac{m+n-2}{2}} v_{\frac{m+n}{2}},$ $v_{\frac{m+n}{2}} v_{\frac{m+n+2}{2}}$	$v_{\frac{m+n-3}{2}} v_{\frac{m+n-1}{2}},$ $v_{\frac{m+n+3}{2}} v_{\frac{m+n+5}{2}}$
$E_5(\mathcal{B}^1(m, n))$	$v_i v_{i+1},$ $t \leq i \leq \frac{m+n-5}{2},$ $\frac{m+n+5}{2} \leq i \leq m.$	$v_i v_{i+1},$ $t \leq i \leq \frac{m+n-4}{2},$ $\frac{m+n+4}{2} \leq i \leq m.$	$v_i v_{i+1},$ $n \leq i \leq \frac{m+n-4}{2},$ $\frac{m+n+2}{2} \leq i \leq m.$	$v_i v_{i+1},$ $n \leq i \leq \frac{m+n-4}{2},$ $\frac{m+n+2}{2} \leq i \leq n.$
$E_6(\mathcal{B}^1(m, n))$	$v_1 v_n$	$v_1 v_n$	$v_1 v_n$	$v_1 v_n$

Lemma 1.1. Let $xy \in E(\mathcal{B}^1(m, n))$ for m is odd, n is even and $4 \leq n < \frac{m+3}{2}$, then

$$\text{MoI}(xy) = \begin{cases} 0, & \text{if } xy \in E_1(\mathcal{B}^1(m, n)), \\ m - n, & \text{if } xy \in E_2(\mathcal{B}^1(m, n)), \\ \frac{n-2}{2}, & \text{if } xy \in E_3(\mathcal{B}^1(m, n)), \\ n - 2, & \text{if } xy \in E_4(\mathcal{B}^1(m, n)), \\ n - 2, & \text{if } xy \in E_5(\mathcal{B}^1(m, n)), \\ 0, & \text{if } xy \in E_6(\mathcal{B}^1(m, n)). \end{cases}$$

Proof. Case i. For $xy \in E_1(\mathcal{B}^1(m, n))$.

Let $x = v_{\frac{n}{2}}$ and $y = v_{\frac{n+2}{2}}$, then $\gamma(v_{\frac{n}{2}}, v_{\frac{n+2}{2}}) = \{v_1, \dots, v_{\frac{n}{2}}, v_{\frac{m+n+3}{2}}, \dots, v_m\}$ and $(v_{\frac{n+2}{2}}, v_{\frac{n}{2}}) = \{v_{\frac{n+2}{2}}, \dots, v_{\frac{m+n-1}{2}}\}$. Hence, $\gamma_{v_{\frac{n}{2}} v_{\frac{n+2}{2}}} = \gamma_{v_{\frac{n+2}{2}} v_{\frac{n}{2}}} = \frac{m-1}{2}$. Therefore, in view of Eq. (2), $\text{MoI}(v_{\frac{n}{2}} v_{\frac{n+2}{2}}) = 0$.

Case ii. For $xy \in E_2(\mathcal{B}^1(m, n))$.

Let $x = v_i$ and $y = v_{i+1}$ for $1 \leq i \leq \frac{n-2}{2}$, then $\gamma(v_i, v_{i+1}) = \{v_1, \dots, v_i, v_{\frac{n+2i+2}{2}}, \dots, v_m\}$ and $\gamma(v_{i+1}, v_i) = \{v_{i+1}, \dots, v_{\frac{n+2i}{2}}\}$. Hence, $\gamma_{v_i v_{i+1}} = \frac{2m-n}{2}$, and $\gamma_{v_{i+1} v_i} = \frac{n}{2}$. Therefore, Eq. (2) implies $\text{MoI}(v_i v_{i+1}) = m - n$.

Case iii. For $xy \in E_3(\mathcal{B}^1(m, n))$.

Let $x = v_{\frac{n+n-1}{2}}$ and $y = v_{\frac{m+n+1}{2}}$, then $\gamma(v_{\frac{n+n-1}{2}}, v_{\frac{m+n+1}{2}}) = \{v_{\frac{n+2}{2}}, \dots, v_{\frac{n+n-1}{2}}\}$ and $\gamma(v_{\frac{m+n+1}{2}}, v_{\frac{n+n-1}{2}}) = \{v_{\frac{m+n+1}{2}}, \dots, v_m\}$. Hence, $\gamma_{v_{\frac{n+n-1}{2}} v_{\frac{m+n+1}{2}}} = \frac{m-1}{2}$, and $\gamma_{v_{\frac{m+n+1}{2}} v_{\frac{n+n-1}{2}}} = \frac{m-n+1}{2}$. Therefore, applying Eq. (2), $\text{MoI}(v_{\frac{n+n-1}{2}} v_{\frac{m+n+1}{2}}) = \frac{n-2}{2}$.

Case iv. For $xy \in E_4(\mathcal{B}^1(m, n))$.

Let $x = v_{\frac{m+n-3}{2}}$ and $y = v_{\frac{n+n-1}{2}}$, then $\gamma(v_{\frac{m+n-3}{2}}, v_{\frac{n+n-1}{2}}) = \{v_1, \dots, v_{\frac{m+n-3}{2}}\}$ and $\gamma(v_{\frac{n+n-1}{2}}, v_{\frac{m+n-3}{2}}) = \{v_{\frac{n+n-1}{2}}, \dots, v_{m-1}\}$. Therefore, $\gamma_{v_{\frac{m+n-3}{2}} v_{\frac{n+n-1}{2}}} = \frac{m+n-3}{2}$, and $\gamma_{v_{\frac{n+n-1}{2}} v_{\frac{m+n-3}{2}}} = \frac{m-n+1}{2}$. Hence, using Eq. (2), $\text{MoI}(v_{\frac{m+n-3}{2}} v_{\frac{n+n-1}{2}}) = n - 2$.

Case v. For $xy \in E_5(\mathcal{B}^1(m, n))$.

Let $x = v_i$ and $y = v_{i+1}$ for $n \leq i \leq \frac{m+n-5}{2}$, the resolving neighbourhoods of (v_i, v_{i+1}) and (v_{i+1}, v_i) are $\{v_1, \dots, v_i, v_{\frac{m-n+2i+4}{2}}, \dots, v_m\}$ and $\{v_{i+1}, \dots, v_{\frac{m-n+2i+2}{2}}\}$ respectively. Hence, $\gamma_{v_i v_{i+1}} = \frac{m+n-2}{2}$ and $\gamma_{v_{i+1} v_i} = \frac{m-n+2}{2}$. Therefore, in view of Eq. (2), $\text{MoI}(v_i v_{i+1}) = n - 2$.

Case vi. For $xy \in E_6(\mathcal{B}^1(m, n))$.

Let $x = v_1$ and $y = v_n$, then we have $\gamma(v_1, v_n) = \{v_1, \dots, v_{\frac{n}{2}}, v_{\frac{m+n+3}{2}}, \dots, v_m\}$ and $\gamma(v_n, v_1) = \{v_{\frac{n+2}{2}}, \dots, v_{\frac{n+n-1}{2}}\}$. Hence, $\gamma_{v_1 v_n} = \gamma_{v_n v_1} = \frac{m-1}{2}$. Therefore, using Eq. (2), $\text{MoI}(v_1 v_n) = 0$. $\square$

Lemma 1.2. Let $xy \in E(\mathcal{B}^1(m, n))$ where m, n are odd and $3 \leq n \leq \frac{m+1}{2}$, then

$$\text{MoI}(xy) = \begin{cases} \frac{m-n}{2}, & \text{if } xy \in E_1(\mathcal{B}^1(m, n)), \\ m-n, & \text{if } xy \in E_2(\mathcal{B}^1(m, n)), \\ 0, & \text{if } xy \in E_3(\mathcal{B}^1(m, n)), \\ n-2, & \text{if } xy \in E_4(\mathcal{B}^1(m, n)), \\ n-2, & \text{if } xy \in E_5(\mathcal{B}^1(m, n)), \\ 0, & \text{if } xy \in E_6(\mathcal{B}^1(m, n)). \end{cases}$$

Proof. *Case i.* For $xy \in E_1(\mathcal{B}^1(m, n))$.

Let $x = v_{\frac{n-1}{2}}$ and $y = v_{\frac{n+1}{2}}$, then $\gamma(v_{\frac{n-1}{2}}, v_{\frac{n+1}{2}}) = \{v_1, \dots, v_{\frac{n-1}{2}}, v_{\frac{m+n+2}{2}}, \dots, v_m\}$ and $\gamma(v_{\frac{n+1}{2}}, v_{\frac{n-1}{2}}) = \{v_{\frac{n+1}{2}}, \dots, v_{n-1}\}$. Hence, $\gamma_{v_{\frac{n-1}{2}} v_{\frac{n+1}{2}}} = \frac{m-1}{2}$, and $\gamma_{v_{\frac{n+1}{2}} v_{\frac{n-1}{2}}} = \frac{n-1}{2}$. Therefore, using Eq. (2), $\text{MoI}(v_{\frac{n-1}{2}} v_{\frac{n+1}{2}}) = \frac{m-n}{2}$.

Case ii. For $xy \in E_2(\mathcal{B}^1(m, n))$.

Let $x = v_i$ and $y = v_{i+1}$ for $1 \leq i \leq \frac{n-3}{2}$, then $\gamma(v_i, v_{i+1}) = \{v_1, \dots, v_i, v_{\frac{n+2i+3}{2}}, \dots, v_m\}$ and $\gamma(v_{i+1}, v_i) = \{v_{i+1}, \dots, v_{\frac{n+2i-1}{2}}\}$. Hence, $\gamma_{v_i v_{i+1}} = \frac{2m-n-1}{2}$ and $\gamma_{v_{i+1} v_i} = \frac{n-1}{2}$. Therefore, in view of Eq. (2) implies $\text{MoI}(v_i v_{i+1}) = m - n$.

Case iii. For $xy \in E_3(\mathcal{B}^1(m, n))$.

Let $x = v_{\frac{m+n}{2}}$ and $y = v_{\frac{m+n+2}{2}}$, then $\gamma(v_{\frac{m+n}{2}}, v_{\frac{m+n+2}{2}}) = \{v_1, \dots, v_{\frac{n-1}{2}}, v_{\frac{m+n+2}{2}}, \dots, v_m\}$ and $\gamma(v_{\frac{m+n+2}{2}}, v_{\frac{m+n}{2}}) = \{v_{\frac{n+3}{2}}, \dots, v_{\frac{m+n}{2}}\}$. Hence, $\gamma_{v_{\frac{m+n}{2}} v_{\frac{m+n+2}{2}}} = \frac{m-1}{2}$ and $\gamma_{v_{\frac{m+n+2}{2}} v_{\frac{m+n}{2}}} = \frac{m-1}{2}$. Hence, Eq. (2) implies $\text{MoI}(v_{\frac{m+n}{2}} v_{\frac{m+n+2}{2}}) = 0$.

Case iv. For $xy \in E_4(\mathcal{B}^1(m, n))$.

Let $x = v_{\frac{m+n-2}{2}}$ and $y = v_{\frac{m+n}{2}}$, then $\gamma(v_{\frac{m+n-2}{2}}, v_{\frac{m+n}{2}}) = \{v_1, \dots, v_{\frac{m+n-2}{2}}\}$ and $\gamma(v_{\frac{m+n}{2}}, v_{\frac{m+n-2}{2}}) =$

$\{v_{\frac{m+n}{2}}, \dots, v_m\}$. Therefore, $\gamma_{v_{\frac{m+n-2}{2}} v_{\frac{m+n}{2}}} = \frac{m+n-2}{2}$ and $\gamma_{v_{\frac{m+n}{2}} v_{\frac{m+n-2}{2}}} = \frac{m-n+2}{2}$. Henceforth, applying Eq. (2), $\text{MoI}(v_{\frac{m+n-2}{2}} v_{\frac{m+n}{2}}) = n - 2$.

Case v. For $xy \in E_5(\mathcal{B}^1(m, n))$.

Let $x = v_i$ and $y = v_{i+1}$ where $n \leq i \leq \frac{m+n-4}{2}$, then $v_i v_{i+1} = \{v_1, \dots, v_i, v_{\frac{m-n+2i+4}{2}}, \dots, v_m\}$ and $v_{i+1} v_i = \{v_{i+1}, \dots, v_{\frac{m-n+2i+2}{2}}\}$. Hence, $\gamma_{v_i v_{i+1}} = \frac{m+n-2}{2}$ and $\gamma_{v_{i+1} v_i} = \frac{m-n+2}{2}$. Therefore, using Eq. (2), $\text{MoI}(v_i v_{i+1}) = n - 2$.

Case vi. The proof is same as discussed in Lemma 1.1 case i. $\square$

Lemma 1.3. Let $xy \in E(\mathcal{B}^l(m, n))$ for m and n are even where $4 \leq n \leq \frac{m+2}{2}$, then

$$\text{MoI}(xy) = \begin{cases} 0, & \text{if } xy \in E_1(\mathcal{B}^l(m, n)), \\ m - n, & \text{if } xy \in E_2(\mathcal{B}^l(m, n)), \\ 0, & \text{if } xy \in E_3(\mathcal{B}^l(m, n)), \\ n - 2, & \text{if } xy \in E_4(\mathcal{B}^l(m, n)), \\ n - 2, & \text{if } xy \in E_5(\mathcal{B}^l(m, n)), \\ 0, & \text{if } xy \in E_6(\mathcal{B}^l(m, n)). \end{cases}$$

Proof. *Case i.* For $xy \in E_1(\mathcal{B}^1(m, n))$.

Let $x = v_{\frac{n}{2}}$ and $y = v_{\frac{n+2}{2}}$, then $\gamma(v_{\frac{n}{2}}, v_{\frac{n+2}{2}}) = \{v_1, \dots, v_{\frac{n}{2}}, v_{\frac{m+n+2}{2}}, \dots, v_m\}$ and $\gamma(v_{\frac{n+2}{2}}, v_{\frac{n}{2}}) = \{v_{\frac{n+2}{2}}, \dots, v_{\frac{m+n}{2}}\}$. Hence, $\gamma_{v_{\frac{n}{2}} v_{\frac{n+2}{2}}} = \frac{m}{2}$ and $\gamma_{v_{\frac{n+2}{2}} v_{\frac{n}{2}}} = \frac{m}{2}$. Therefore, using Eq. (2), $\text{MoI}(v_{\frac{n}{2}} v_{\frac{n+2}{2}}) = 0$.

Case ii. For $xy \in E_2(\mathcal{B}^1(m, n))$.

Let $x = v_i$ and $y = v_{i+1}$ for $1 \leq i \leq \frac{n-2}{2}$, then $\gamma(v_i, v_{i+1}) = \{v_1, \dots, v_i, v_{\frac{n+2i+2}{2}}, \dots, v_m\}$ and $\gamma(v_{i+1}, v_i) = \{v_{i+1}, \dots, v_{\frac{n+2i}{2}}\}$. Therefore, $\gamma_{v_i v_{i+1}} = \frac{2m-n}{2}$ and $\gamma_{v_{i+1} v_i} = \frac{n}{2}$. Hence, Eq. (2) implies $\text{MoI}(v_i v_{i+1}) = m - n$.

Case iii. For $xy \in E_3(\mathcal{B}^1(m, n))$.

Let $x = v_{\frac{m+n}{2}}$ and $y = v_{\frac{m+n+2}{2}}$, then $\gamma(v_{\frac{m+n}{2}}, v_{\frac{m+n+2}{2}}) = \{v_{\frac{n+2}{2}}, \dots, v_{\frac{m+n}{2}}\}$ and $\gamma(v_{\frac{m+n+2}{2}}, v_{\frac{m+n}{2}}) = \{v_1, \dots, v_{\frac{n}{2}}, v_{\frac{m+n+2}{2}}, \dots, v_m\}$. Therefore, $\gamma_{v_{\frac{m+n}{2}} v_{\frac{m+n+2}{2}}} = \frac{m}{2}$ and $\gamma_{v_{\frac{m+n+2}{2}} v_{\frac{m+n}{2}}} = \frac{m}{2}$. Hence, applying Eq. (2), $\text{MoI}(v_{\frac{m+n}{2}} v_{\frac{m+n+2}{2}}) = 0$.

Case iv. For $xy \in E_4(\mathcal{B}^1(m, n))$.

Let $x = v_{\frac{m+n-2}{2}}$ and $y = v_{\frac{m+n}{2}}$, then $\gamma(v_{\frac{m+n-2}{2}}, v_{\frac{m+n}{2}}) = \{v_1, \dots, v_{\frac{m+n-2}{2}}\}$ and $\gamma(v_{\frac{m+n}{2}}, v_{\frac{m+n-2}{2}}) = \{v_{\frac{m+n}{2}}, \dots, v_m\}$. Hence, $\gamma_{v_{\frac{m+n-2}{2}} v_{\frac{m+n}{2}}} = \frac{m+n-2}{2}$ and $\gamma_{v_{\frac{m+n}{2}} v_{\frac{m+n-2}{2}}} = \frac{m-n+2}{2}$. Therefore, in view of Eq. (2), $\text{MoI}(v_{\frac{m+n-2}{2}} v_{\frac{m+n}{2}}) = n - 2$.

Case v. For $xy \in E_5(\mathcal{B}^1(m, n))$.

Let $x = v_i$ and $y = v_{i+1}$ for $n \leq i \leq \frac{m+n-4}{2}$, then $\gamma(v_i, v_{i+1}) = \{v_1, \dots, v_i, v_{\frac{m-n+2i+4}{2}}, \dots, v_m\}$ and $\gamma(v_{i+1}, v_i) = \{v_{i+1}, \dots, v_{\frac{m-n+2i+2}{2}}\}$. Hence, $\gamma_{v_i v_{i+1}} = \frac{m+n-2}{2}$ and $\gamma_{v_{i+1} v_i} = \frac{m-n+2}{2}$. Therefore, $\text{MoI}(v_i, v_{i+1}) = n - 2$.

Case vi. The proof is same as discussed in Lemma 1.1 case i. $\square$

Lemma 1.4. Let $xy \in E(\mathcal{B}^1(m, n))$ for m is even and n is odd where $3 \leq n \leq \frac{m+2}{2}$, then

$$\text{MoI}(xy) = \begin{cases} \frac{m-n+1}{2}, & \text{if } xy \in E_1(\mathcal{B}^1(m, n)), \\ m-n, & \text{if } xy \in E_2(\mathcal{B}^1(m, n)), \\ \frac{n-1}{2}, & \text{if } xy \in E_3(\mathcal{B}^1(m, n)), \\ n-2, & \text{if } xy \in E_4(\mathcal{B}^1(m, n)), \\ m-n-3, & \text{if } xy \in E_5(\mathcal{B}^1(m, n)), \\ 0, & \text{if } xy \in E_6(\mathcal{B}^1(m, n)). \end{cases}$$

Proof. *Case i.* For $xy \in E_1(\mathcal{B}^1(m, n))$.

Let $x = v_{\frac{n-1}{2}}$ and $y = v_{\frac{n+1}{2}}$, then $\gamma(v_{\frac{n-1}{2}}, v_{\frac{n+1}{2}}) = \{v_1, \dots, v_{\frac{n-1}{2}}, v_{\frac{m+n+1}{2}}, \dots, v_m\}$ and $\gamma(v_{\frac{n+1}{2}}, v_{\frac{n-1}{2}}) = \{v_{\frac{n+1}{2}}, \dots, v_{n-1}\}$. Hence, $\gamma_{v_{\frac{n-1}{2}} v_{\frac{n+1}{2}}} = \frac{m}{2}$ and $\gamma_{v_{\frac{n+1}{2}} v_{\frac{n-1}{2}}} = \frac{n-1}{2}$. Therefore, using Eq. (2), $\text{MoI}(v_{\frac{n-1}{2}} v_{\frac{n+1}{2}}) = 2 \left(\frac{m-n+1}{2} \right) = \frac{m-n+1}{2}$.

Case ii. For $xy \in E_2(\mathcal{B}^1(m, n))$.

Let $x = v_i$ and $y = v_{i+1}$ for $1 \leq i \leq \frac{n-3}{2}$, then $\gamma(v_i, v_{i+1}) = \{v_1, \dots, v_i, v_{\frac{n+2i+3}{2}}, \dots, v_m\}$ and $\gamma(v_{i+1}, v_i) = \{v_{i+1}, \dots, v_{\frac{n+2i-1}{2}}\}$. Hence, $\gamma_{v_i v_{i+1}} = \frac{2m-n-1}{2}$ and $\gamma_{v_{i+1} v_i} = \frac{n-1}{2}$. Therefore, in view of Eq. (2), $\text{MoI}(v_i v_{i+1}) = m-n$.

Case iii. For $xy \in E_3(\mathcal{B}^1(m, n))$.

Let $x = v_{\frac{n+n-1}{2}}$ and $y = v_{\frac{m+n+1}{2}}$, then $\gamma(v_{\frac{n+n-1}{2}}, v_{\frac{m+n+1}{2}}) = \{v_{\frac{n+1}{2}}, \dots, v_{\frac{n+n-1}{2}}\}$ and $\gamma(v_{\frac{m+n+1}{2}}, v_{\frac{n+n-1}{2}}) = \{v_{\frac{m+n+1}{2}}, \dots, v_n\}$. Therefore, $\gamma_{v_{\frac{n+n-1}{2}} v_{\frac{m+n+1}{2}}} = \frac{m}{2}$ and $\gamma_{v_{\frac{m+n+1}{2}} v_{\frac{n+n-1}{2}}} = \frac{m-n+1}{2}$. Hence, Eq. (2) implies $\text{MoI}(v_{\frac{n+n-1}{2}} v_{\frac{m+n+1}{2}}) = 2 \left(\frac{n-1}{2} \right) = \frac{n-1}{2}$.

Case iv. For $xy \in E_4(\mathcal{B}^1(m, n))$.

Let $x = v_{\frac{m+n-3}{2}}$ and $y = v_{\frac{n+n-1}{2}}$, we have $\gamma(v_{\frac{m+n-3}{2}}, v_{\frac{n+n-1}{2}}) = \{v_1, \dots, v_{\frac{m+n-3}{2}}\}$ and $\gamma(v_{\frac{n+n-1}{2}}, v_{\frac{m+n-3}{2}}) = \{v_{\frac{n+n-1}{2}}, \dots, v_{m-1}\}$. Hence, $\gamma_{v_{\frac{m+n-3}{2}} v_{\frac{n+n-1}{2}}} = \frac{m+n-3}{2}$ and $\gamma_{v_{\frac{n+n-1}{2}} v_{\frac{m+n-3}{2}}} = \frac{m-n+1}{2}$. Therefore, applying Eq. (2), $\text{MoI}(v_{\frac{m+n-3}{2}} v_{\frac{n+n-1}{2}}) = n-2$.

Case v. For $xy \in E_5(\mathcal{B}^1(m, n))$.

Let $x = v_i$ and $y = v_{i+1}$ where $n \leq i \leq \frac{m+n-5}{2}$, then $(v_i, v_{i+1}) = \{v_1, \dots, v_i, v_{\frac{m-n+2i+5}{2}}, \dots, v_n\}$ and $(v_{i+1}, v_i) = \{v_{i+1}, \dots, v_{\frac{m-n+2i+1}{2}}\}$. Hence, $\gamma_{v_i v_{i+1}} = \frac{m+n-3}{2}$ and $\gamma_{v_{i+1} v_i} = \frac{m-n+1}{2}$. Therefore, using Eq. (2), $\text{MoI}(v_i v_{i+1}) = n-2$.

Case vi. The proof is same as discussed in Lemma 1.1 case i. □

The following theorem computes Mostar index of bicyclic graph of class-I $\mathcal{B}^1(m, n)$.

Theorem 1.5. Let $\mathcal{B}^1(m, n)$ be a bicyclic graph where $m \geq 9$ and $n \geq 3$, then

$$\text{MoI}(\mathcal{B}^1(m, n)) = \begin{cases} 2(n-2)(m-n), & \text{if } m \text{ is odd,} \\ 2(n-2)(m-n), & \text{if } m \text{ is even, } n \text{ is odd,} \\ 2(n-2)(m-n) + 2, & \text{if } m \text{ is even, } n \text{ is even.} \end{cases}$$

Proof. *Case i.* When $m = \text{odd}$.

Using Lemma 1.1 and Eq. (1), we have

$$\begin{aligned}
 \text{MoI}(\mathcal{B}^1(m, n)) &= \sum_{xy \in E_1(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_3(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| \\
 &\quad + \sum_{xy \in E_4(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_5(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_6(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| \\
 &= 1 \times 0 + (t-2) \times (n-t) + 2 \times \frac{(t-2)}{2} + 2 \times (t-2) \\
 &\quad + (n-t-3) \times (t-2) + 1 \times 0 \\
 &= 2(n-2)(m-n).
 \end{aligned}$$

Case ii. When $m = \text{even}$, $n = \text{odd}$.

In view of Lemma 1.3 and Eq. (1),

$$\begin{aligned}
 \text{MoI}(\mathcal{B}^1(m, n)) &= \sum_{xy \in E_1(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_3(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| \\
 &\quad + \sum_{xy \in E_4(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_5(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_6(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| \\
 &= 1 \times 0 + (t-2) \times (n-t) + 2 \times \frac{(t-2)}{2} + 2 \times (t-2) \\
 &\quad + (n-t-3) \times (t-2) + 1 \times 0 \\
 &= 2(n-2)(m-n).
 \end{aligned}$$

Case iii. When $m = \text{even}$, $n = \text{even}$.

By using Lemma 1.4 and Eq. (1),

$$\begin{aligned}
 \text{MoI}(\mathcal{B}^1(m, n)) &= \sum_{xy \in E_1(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_3(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| \\
 &\quad + \sum_{xy \in E_4(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_5(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_6(\mathcal{B}^1(m, n))} |\gamma_{xy} - \gamma_{yx}| \\
 &= 2 \times \frac{n-t+1}{2} + (t-3) \times (n-t) + 2 \times \frac{(t-1)}{2} + 2 \times (t-2) \\
 &\quad + (n-t-3) \times (t-2) + 1 \times 0 \\
 &= 2(n-2)(m-n) + 2.
 \end{aligned}$$

□

1.2. Mostar index of Bicyclic graph of class-II $\mathcal{B}^2(l, m, n)$

The bicyclic graph $\mathcal{B}^2(l, m, n)$ has two cycles of lengths l and n connected by a path of a length m where $l, n \geq 3$, $m \geq 1$ and $l \geq n$. The vertex set of $\mathcal{B}^2(l, m, n)$ is given by $\{u_a \mid 0 \leq a \leq l-1\} \cup \{v_b \mid 0 \leq b \leq n-1\} \cup \{w_c \mid 0 \leq c \leq m-2\}$ and $|V(\mathcal{B}^2(l, m, n))| = l + m + n - 2$. The edge set of $\mathcal{B}^2(l, m, n)$ is defined as: $E(\mathcal{B}^2(l, m, n)) = \{u_a u_{(a+1)}, u_{l-1} u_0, \mid 0 \leq a \leq l-2\} \cup \{v_b v_{(b+1)}, v_{n-1} v_0 \mid 0 \leq b \leq n-2\} \cup \{u_0 w_0, w_{m-2} v_0, w_{c-1} w_c \mid 1 \leq c \leq m-2\}$ and $|E(\mathcal{B}^2(l, m, n))| = l + m + n$. The graph $\mathcal{B}^2(9, 3, 7)$ is shown in Figure 2.

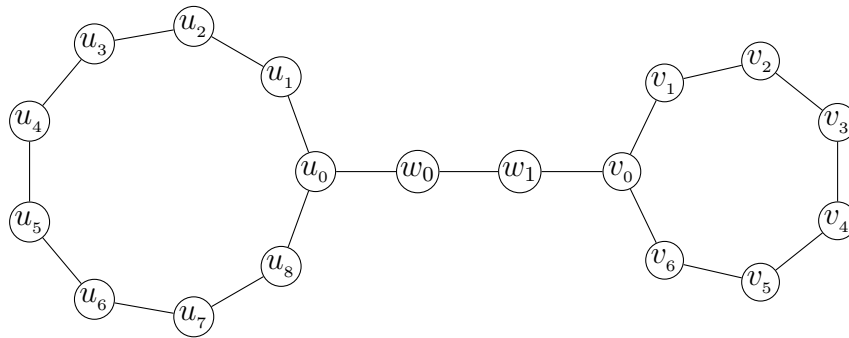


Fig. 2. Bicyclic graph of class-II ($\mathcal{B}^2(9, 3, 7)$)

In bicyclic graph $\mathcal{B}^2(l, m, n)$, the parameter j play an important role in computing its Mostar index. It affects the structural properties of $\mathcal{B}^2(l, m, n)$ under two conditions: $m \geq l - n + 2$ and $m < l - n + 2$. Further, assuming $l \geq n$ simplifies our computations.

Now, we will provide proof of lemmas to compute the Mostar index of bicyclic graph of class-II $\mathcal{B}^2(l, m, n)$ for the case $m \geq l - n + 2$.

Lemma 1.6. For $xy \in E_1(\mathcal{B}^2(l, m, n))$ where $l, n \geq 3$, $m \geq 1$ then $\text{MoI}(xy) = |m + n - 1|$.

Proof. The proof is divided into the following two cases:

Case i. When l is even.

The graph's symmetry helps us to compute the Mostar index for the following types of edges: $\{u_{\frac{l-2}{2}}u_{\frac{l}{2}}, u_{l-1}u_l \mid 1 \leq l \leq \lceil \frac{l-2}{2} \rceil\}$. Let $xy \in E_1(\mathcal{B}^2(l, m, n))$ where $x = u_{\frac{l-2}{2}}$ and $y = u_{\frac{l}{2}}$ then $\gamma(u_{\frac{l-2}{2}}, u_{\frac{l}{2}}) = \{u_0, \dots, u_{\frac{l-2}{2}}\} \cup \{x_0, \dots, x_{n-1}\} \cup \{w_0, \dots, w_{m-2}\}$ and $\gamma(u_{\frac{l}{2}}, u_{\frac{l-2}{2}}) = \{u_{\frac{l}{2}}, \dots, u_{l-1}\}$. Hence, $\gamma(u_{\frac{l-2}{2}}u_{\frac{l}{2}}) = \frac{l}{2} + n + m - 1$ and $\gamma(u_{\frac{l}{2}}u_{\frac{l-2}{2}}) = \frac{l}{2}$. Let $xy \in \{u_{l-1}u_l \mid 1 \leq l \leq \lceil \frac{l-2}{2} \rceil\}$, then $\gamma(u_{l-1}, u_l) = \{u_0, \dots, u_{l-1}, u_{\frac{l+2}{2}}, \dots, u_{l-1}\} \cup \{v_0, \dots, v_n\} \cup \{w_0, \dots, w_{m-2}\}$ and $\gamma(u_l, u_{l-1}) = \{u_l, \dots, u_{\frac{l}{2}+l-1}\}$. It can be seen, $\gamma(u_{l-1}u_l) = \frac{l}{2} + n + m - 1$ and $\gamma(u_l, u_{l-1}) = \frac{l}{2}$. Hence, for $xy \in E_1(\mathcal{B}^2(l, m, n))$, $\text{MoI}(xy) = |\frac{l}{2} + n + m - 1 - \frac{l}{2}| = |n + m - 1|$. Therefore, using Eq. (2), $\text{MoI}(xy) = |n + m - 1|$.

Case ii. When l is odd.

The graph's symmetry helps us to compute the Mostar index for the following types of edges: $\{u_{\frac{l-1}{2}}u_{\frac{l+1}{2}}, u_{i-1}u_i \mid 1 \leq i \leq \lceil \frac{l-2}{2} \rceil\}$. Let $xy \in E_1(\mathcal{B}^2(l, m, n))$ where $x = u_{\frac{l-1}{2}}$, $y = u_{\frac{l+1}{2}}$, then $\text{MoI}(xy) = 0$. If $xy \in \{u_{i-1}u_i \mid 1 \leq i \leq \lceil \frac{l-2}{2} \rceil\}$, the proof will be the same as discussed in case i i.e. $\text{MoI}(xy) = |n + m - 1|$. $\square$

Lemma 1.7. For $xy \in E_2(\mathcal{B}^2(l, m, n))$ where $l, n \geq 3$ and $m \geq 1$ then $\text{MoI}(xy) = |l + m - 1|$.

Proof. The proof is divided into the following two cases:

Case i. When n is even.

The graph's symmetry helps us to compute the Mostar index for the following types of edges: $\{v_{\frac{n-2}{2}}v_{\frac{n}{2}}, v_{l-1}v_l \mid 1 \leq l \leq \lceil \frac{n-2}{2} \rceil\}$. Let $xy \in E_2(\mathcal{B}^2(l, m, n))$ where $x = v_{\frac{n-2}{2}}$ and $y = v_{\frac{n}{2}}$ then $\gamma(v_{\frac{n-2}{2}}, v_{\frac{n}{2}}) = \{v_0, \dots, v_{\frac{n-2}{2}}\} \cup \{u_0, \dots, u_{l-1}\} \cup \{w_0, \dots, w_{m-2}\}$ and $\gamma(v_{\frac{n}{2}}, v_{\frac{n-2}{2}}) = \{v_{\frac{n}{2}}, \dots, v_{n-1}\}$. Hence, $\gamma(v_{\frac{n-2}{2}}v_{\frac{n}{2}}) = l + \frac{n}{2} + m - 1$ and $\gamma(v_{\frac{n}{2}}v_{\frac{n-2}{2}}) = \frac{n}{2}$. Let $xy \in \{v_{l-1}v_l \mid 1 \leq l \leq \lceil \frac{n-2}{2} \rceil\}$, then $\gamma(v_{l-1}, v_l) = \{v_0, \dots, v_{l-1}, v_{\frac{n+2}{2}}, \dots, v_{n-1}\} \cup \{u_0, \dots, u_{l-1}\} \cup \{w_0, \dots, w_{m-2}\}$ and $\gamma(v_l, v_{l-1}) =$

$\{v_l, \dots, v_{\frac{n}{2}+l-1}\}$. It can be seen, $\gamma(v_{l-1}v_l) = l + \frac{n}{2} + m - 1$ and $\gamma(v_{l-1}v_l) = \frac{n}{2}$. Hence, for $xy \in E_2(\mathcal{B}^2(l, m, n))$, $\text{MoI}(xy) = \left| \frac{l}{2} + n + m - 1 - \frac{l}{2} \right| = |l + m - 1|$.

Case ii. When n is odd.

The graph's symmetry helps us to compute the Mostar index for the following types of edges; $\left\{ v_{\frac{n-1}{2}}v_{\frac{n+1}{2}}, v_{i-1}v_i \mid 1 \leq i \leq \left\lceil \frac{n-2}{2} \right\rceil \right\}$. Let $xy \in E_2(\mathcal{B}^2(l, m, n))$ where $x = v_{\frac{n-1}{2}}$, $y = v_{\frac{n+1}{2}}$, then $\text{MoI}(xy) = 0$. If $xy \in \{v_{i-1}v_i \mid 1 \leq i \leq \left\lceil \frac{n-2}{2} \right\rceil\}$, the proof will be same as discussed in case i i.e. $\text{MoI}(xy) = |l + m - 1|$. $\square$

Lemma 1.8. Let $xy \in E_3(\mathcal{B}^2(l, m, n))$ for $l, n \geq 3$ and $m \geq 1$ then $\text{MoI}(xy) = |l - m - n + 2p + 1|$.

Proof. Let $xy \in E_3(\mathcal{B}^2(l, m, n))$ where $x = u_0$ and $y = w_0$ then $\gamma(u_0w_0) = \{u_0, \dots, u_{l-1}\}$ and $\gamma(w_0u_0) = \left\{ w_0, \dots, w_{\frac{m+2p+n-l-1}{2}} \right\} \cup \{v_0, \dots, v_{n-1}\}$. Let $xy \in E_3(\mathcal{B}^2(l, m, n))$ where $x = w_{p-1}$ and $y = w_p$ then $\gamma(w_{p-1}w_p) = \{u_0, \dots, u_{l-1}\} \cup \{w_0, \dots, w_{p-1}\}$ and $\gamma(w_pw_{p-1}) = \{v_0, \dots, v_{n-1}\} \cup \{w_p, \dots, w_{m-2}\}$. It can be seen, $\gamma(w_{p-1}w_p) = p + l$ and $\gamma(w_{p-1}w_p) = |m + n - p - 1|$. Hence, for $xy \in E_3(\mathcal{B}^2(l, m, n))$, $\text{MoI}(xy) = |l - m - n + 2p + 1|$. $\square$

The following theorem computes Mostar index of bicyclic graph of class-II $\mathcal{B}^2(l, m, n)$ for $m < l - n + 2$.

Theorem 1.9. For a bicyclic graph $\mathcal{B}^2(l, m, n)$ where $l, n \geq 3$ and $m \geq 1$, the following holds:

$$\text{MoI}(\mathcal{B}^2(l, m, n)) = \begin{cases} \left\lceil \frac{(l+m+n)^2 - 2l - 2n - 1}{2} \right\rceil, & \text{if } l = \text{even}, n = \text{even} \\ \left\lceil \frac{(l+m+n)^2 - 2(2l+n+m)+1}{2} \right\rceil, & \text{if } l = \text{even}, n = \text{odd} \\ \left\lceil \frac{(l+m+n)^2 - 4(l+n+m)+3}{2} \right\rceil, & \text{if } l = \text{odd}, n = \text{odd} \\ \left\lceil \frac{(l+m+n)^2 - 2(l+m+2n)+1}{2} \right\rceil, & \text{if } l = \text{odd}, n = \text{even}. \end{cases}$$

Proof. *Case i.* When $l = \text{even}, n = \text{even}$.

In view of Lemmas 1.6-1.8 and Eq. (1), we have

$$\begin{aligned} \text{MoI}(\mathcal{B}^2(l, m, n)) &= \sum_{xy \in E_1(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_3(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| \\ &= l(n + m - 1) + n(l + m - 1) + \left\lceil \frac{l^2 + m^2 + n^2 - 2ln - 1}{2} \right\rceil \\ &= \left\lceil \frac{(l + m + n)^2 - 2l - 2n - 1}{2} \right\rceil. \end{aligned}$$

Case ii. When $l = \text{even}, n = \text{odd}$.

With reference to Lemmas 1.6-1.8 and Eq. (1), we have

$$\begin{aligned}
\text{MoI}(\mathcal{B}^2(l, m, n)) &= \sum_{xy \in E_1(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_3(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| \\
&= l(n + m - 1) + (n - 1)(l + m - 1) + \left\lceil \frac{l^2 + m^2 + n^2 - 2ln - 1}{2} \right\rceil \\
&= \left\lceil \frac{(l + m + n)^2 - 2(2l + n + m) + 1}{2} \right\rceil.
\end{aligned}$$

Case iii. When $l = \text{odd}, n = \text{odd}$.

Using Lemmas 1.6-1.8 and Eq. (1), we have

$$\begin{aligned}
\text{MoI}(\mathcal{B}^2(l, m, n)) &= \sum_{xy \in E_1(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_3(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| \\
&= (l - 1)(n + m - 1) + (n - 1)(l + m - 1) + \left\lceil \frac{l^2 + m^2 + n^2 - 2ln - 1}{2} \right\rceil \\
&= \left\lceil \frac{(l + m + n)^2 - 4(l + n + m) + 3}{2} \right\rceil.
\end{aligned}$$

Case iv. When $l = \text{odd}, n = \text{even}$.

With reference to Lemmas 1.6-1.8 and Eq. (1), we have

$$\begin{aligned}
\text{MoI}(\mathcal{B}^2(l, m, n)) &= \sum_{xy \in E_1(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_3(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| \\
&= (l - 1)(n + m - 1) + n(l + m - 1) + \left\lceil \frac{l^2 + m^2 + n^2 - 2ln - 1}{2} \right\rceil \\
&= \left\lceil \frac{(l + m + n)^2 - 2(l + m + 2n) + 1}{2} \right\rceil.
\end{aligned}$$

□

Now, we will provide proof of lemmas to compute the Mostar index of bicyclic graph of class-I $\mathcal{B}^2(l, m, n)$ for the case $m < l - n + 2$.

Lemma 1.10. For $xy \in E_1(\mathcal{B}^2(l, m, n))$ where $i, k \geq 3$ and $j \geq 1$ then $\text{MoI}(E_1(\mathcal{B}^2(l, m, n))) = |k + j - 1|$.

Proof. The proof follows directly from the arguments established in Lemma 1.6. □

Lemma 1.11. For $xy \in E_2(\mathcal{B}^2(l, m, n))$ where $i, k \geq 3$ and $j \geq 1$ then $\text{MoI}(E_2(\mathcal{B}^2(l, m, n))) = |i + j - 1|$.

Proof. The proof follows directly from the arguments established in Lemma 1.7. □

Lemma 1.12. For $xy \in E_3(\mathcal{B}^2(l, m, n))$ where $i, k \geq 3$ and $j \geq 1$, then $\text{MoI}(E_3(\mathcal{B}^2(l, m, n))) = |i - k - j + 1| + |i + j - k - 1| + (j - 2)(|i - k - j + 1|) + j^2 - 3j + 2$.

Proof. Let $xy \in E_3(\mathcal{B}^2(l, m, n))$, where $x = u_0$, and $y = w_0$, then, $\gamma(u_0, w_0) = \{u_0, \dots, u_{l-1}\}$ and $\gamma(w_0, u_0) = \{v_0, \dots, v_{n-1}\} \cup \{w_0, \dots, w_{m-2}\}$. Hence, $\gamma(u_0 w_0) = l$ and $\gamma(w_0 u_0) = n + m - 1$. Using Eq. $\text{MoI}(u_0 w_0) = |l - n - m + 1|$. Now, let $x = w_{m-2}$, and $y = v_0$. Then, $\gamma(w_{m-2}, v_0) = \{u_0, \dots, u_{l-1}\} \cup \{w_0, \dots, w_{m-2}\}$ and $\gamma(v_0, w_{m-2}) = \{v_0, \dots, v_{n-1}\}$. Hence, $\gamma(w_{m-2}, v_0) = l + m - 1$ and $\gamma(v_0 w_{m-2}) = n$. Using Eq. $\text{MoI}(w_{m-2} v_0) = |l + m - n - 1|$. Also, for $xy \in \{w_{d-1} w_d \mid 1 \leq d \leq m - 2\}$ then $\gamma(w_{d-1} w_d) = \{u_0, \dots, u_{l-1}\} \cup \{w_0, \dots, w_{d-1}\}$ and $\gamma(w_d w_{d-1}) = \{v_0, \dots, v_{n-1}\} \cup \{w_d, \dots, w_{m-2}\}$. It can be seen, $\gamma(w_{d-1} w_d) = l + d$ and $\gamma(w_d w_{d-1}) = n + m - d - 1$ and $\text{MoI}(w_{d-1} w_d) = |l - n - m + 2d + 1|$. $\square$

The following theorem computes Mostar index of class-II $\mathcal{B}^2(l, m, n)$ for $j < i - k + 2$.

Theorem 1.13. Let $\mathcal{B}^2(l, m, n)$ be a bicyclic graph where $i, k \geq 3$ and $j \geq 1$ then

$$\text{MoI}(\mathcal{B}^2(l, m, n)) = \begin{cases} 2ik + ij + kj - i - k + \text{MoI}(E_3(\mathcal{B}^2(l, m, n))), & \text{if } i = \text{even}, k = \text{even} \\ 2ik + ij + kj - 2i - j - k + 1 + \text{MoI}(E_3(\mathcal{B}^2(l, m, n))), & \text{if } i = \text{even}, k = \text{odd} \\ 2ik + ij + kj - i - 2k - j + 1 + \text{MoI}(E_3(\mathcal{B}^2(l, m, n))), & \text{if } i = \text{odd}, k = \text{odd} \\ 2ik + ij + kj - 2i - 2k - 2j + 2 + \text{MoI}(E_3(\mathcal{B}^2(l, m, n))), & \text{if } i = \text{odd}, k = \text{even}. \end{cases}$$

Proof. Case i. When $i = \text{even}, k = \text{even}$.

With reference to Lemmas 1.10-1.11 and Eq. (1), we have

$$\begin{aligned} \text{MoI}(\mathcal{B}^2(l, m, n)) &= \sum_{xy \in E_1(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_3(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| \\ &= 2ln + lm + mn - l - n + |l - n - m + 1| \\ &\quad + |l + m - n - 1| + |(m - 2)(l - n - m + 1)| + m^2 - 3m + 2. \end{aligned}$$

Case ii. When $i = \text{even}, k = \text{odd}$.

Using Lemmas 1.10-1.11 and Eq. (1), we have

$$\begin{aligned} \text{MoI}(\mathcal{B}^2(l, m, n)) &= \sum_{xy \in E_1(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_3(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| \\ &= 2ln + lm + mn - 2l - m - n + 1 + |l - n - m + 1| \\ &\quad + |l + m - n - 1| + |(m - 2)(l - n - m + 1)| + m^2 - 3m + 2. \end{aligned}$$

Case iii. When $i = \text{odd}, k = \text{odd}$.

In view of Lemmas 1.10-1.11 and Eq. (1), we have

$$\begin{aligned} \text{MoI}(\mathcal{B}^2(l, m, n)) &= \sum_{xy \in E_1(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_3(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| \\ &= 2ln + lm + mn - l - 2n - m + 1 + |l - n - m + 1| \\ &\quad + |l + m - n - 1| + |(m - 2)(l - n - m + 1)| + m^2 - 3m + 2. \end{aligned}$$

Case iv. When $i = \text{odd}, k = \text{even}$.

Using Lemmas 1.10-1.11 and Eq. (1), we have

$$\begin{aligned} \text{MoI}(\mathcal{B}^2(l, m, n)) &= \sum_{xy \in E_1(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_3(\mathcal{B}^2(l, m, n))} |\gamma_{xy} - \gamma_{yx}| \\ &= 2ln + lm + mn - 2l - 2n - 2m + 2 + |l - n - m + 1| \\ &\quad + |l + m - n - 1| + |(m - 2)(l - n - m + 1)| + m^2 - 3m + 2. \end{aligned}$$

□

1.3. Mostar index of bicyclic graph of class-III ($\mathcal{B}^3(l, m)$)

The bicyclic graph of class-III ($\mathcal{B}^3(l, m)$) has two cycles of length l and m with one vertex in common, where $l, m \geq 3$. The vertex set of $\mathcal{B}^3(l, m)$ is given by $\{u_a \mid 0 \leq a \leq l-1\} \cup \{v_b \mid 1 \leq b \leq m\}$ and $|V(\mathcal{B}^3(l, m))| = l+m$. The edge set of $\mathcal{B}^3(l, m)$ is defined as: $E(\mathcal{B}^3(l, m)) = \{u_a u_{(a+1)}, u_{l-1} u_0, \mid 0 \leq a \leq l-2\} \cup \{v_b v_{(b+1)}, v_{m-1} v_0, \mid 0 \leq b \leq m-2\}$ and $|E(\mathcal{B}^3(l, m))| = l+m+1$. The bicyclic graph of class-III $\mathcal{B}^3(9, 6)$ is shown in the Figure 3.

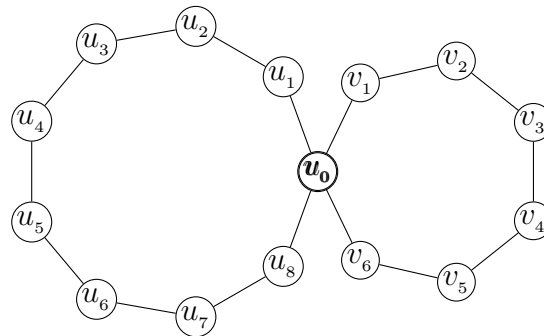


Fig. 3. Bicyclic graph of class-III ($\mathcal{B}^3(9, 6)$)

The following theorem computes Mostar index of bicyclic graph of class-III $\mathcal{B}^3(l, m)$.

Theorem 1.14. Let $(\mathcal{B}^3(l, m))$ be a bicyclic graph of class-III where $l, m \geq 3$ then

$$MoI(\mathcal{B}^3(l, m)) = \begin{cases} l(m-1) + m(l-1), & \text{if } l = \text{even}, m = \text{even} \\ l(m-1) + (m-1)(l-1), & \text{if } l = \text{even}, m = \text{odd} \\ (l-1)(m-1) + m(l-1), & \text{if } m = \text{even}, l = \text{odd} \\ (l-1)(m-1) + (m-1)(l-1), & \text{if } m = \text{odd}, l = \text{odd}. \end{cases}$$

Proof. Case i. When $l = \text{even}$, $m = \text{even}$.

In view of Lemmas 1.6-1.8 and Eq. (1), we have

$$\begin{aligned} MoI(\mathcal{B}^3(l, m)) &= \sum_{xy \in E_1(\mathcal{B}^3(l, m))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^3(l, m))} |\gamma_{xy} - \gamma_{yx}| \\ &= l(m-1) + m(l-1). \end{aligned}$$

Case ii. When $l = \text{even}$, $m = \text{odd}$.

With reference to Lemmas 1.6-1.8 and Eq. (1), we have

$$\begin{aligned} MoI(\mathcal{B}^3(l, m)) &= \sum_{xy \in E_1(\mathcal{B}^3(l, m))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^3(l, m))} |\gamma_{xy} - \gamma_{yx}| \\ &= l(m-1) + (m-1)(l-1). \end{aligned}$$

Case iii. When $l = \text{even}$, $m = \text{odd}$.

Using Lemmas 1.6-1.8 and Eq. (1), we have

$$\begin{aligned} MoI(\mathcal{B}^3(l, m)) &= \sum_{xy \in E_1(\mathcal{B}^3(l, m))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^3(l, m))} |\gamma_{xy} - \gamma_{yx}| \\ &= (l-1)(m-1) + m(l-1). \end{aligned}$$

Case iv. When $l = \text{odd}$, $m = \text{odd}$.

With reference to Lemmas 1.6-1.8 and Eq. (1), we have

$$\begin{aligned}\text{MoI}(\mathcal{B}^3(l, m)) &= \sum_{xy \in E_1(\mathcal{B}^3(l, m))} |\gamma_{xy} - \gamma_{yx}| + \sum_{xy \in E_2(\mathcal{B}^3(l, m))} |\gamma_{xy} - \gamma_{yx}| \\ &= (l-1)(m-1) + (m-1)(l-1).\end{aligned}$$

□

References

- [1] M. Arockiaraj, J. Clement, and N. Tratnik. Mostar indices of carbon nanostructures and circumscribed donut benzenoid systems. *International Journal of Quantum Chemistry*, 119(24):e26043, 2019. <https://doi.org/10.1002/qua.26043>.
- [2] F. Asif, A. Kashif, S. Zafar, A. Aljaedi, and U. Albalawi. Mostar index of neural networks and applications. *IEEE Access*, 11:21345–21353, 2023. [10.1109/ACCESS.2023.3246734](https://doi.org/10.1109/ACCESS.2023.3246734).
- [3] T. Došlić, I. Martinjak, R. Škrekovski, S. Tipurić Spužević, and I. Zubac. Mostar index. *Journal of Mathematical Chemistry*, 56:2995–3013, 2018. <https://doi.org/10.1007/s10910-018-0928-z>.
- [4] E. Estrada. *The Structure of Complex Networks: Theory and Applications*. American Chemical Society, 2012.
- [5] F. Gao, K. Xu, and T. Došlić. On the difference of mostar index and irregularity of graphs. *Bulletin of the Malaysian Mathematical Sciences Society*, 44:905–926, 2021. <https://doi.org/10.1007/s40840-020-00991-y>.
- [6] I. Gutman. A formula for the wiener number of trees and its extension to graphs containing cycles. *Graph Theory Notes NY*, 27(9):9–15, 1994.
- [7] F. Hayat and B. Zhou. On mostar index of trees with parameters. *Filomat*, 33(19):6453–6458, 2019. <https://doi.org/10.2298/FIL1919453H>.
- [8] S. Huang, S. Li, and M. Zhang. On the extremal mostar indices of hexagonal chains. *MATCH Communications in Mathematical and in Computer Chemistry*, 84(1):249–271, 2020.
- [9] J. Ma, Y. Shi, Z. Wang, and J. Yue. On wiener polarity index of bicyclic networks. *Scientific Reports*, 6(1):19066, 2016. <https://doi.org/10.1038/srep19066>.
- [10] B. Niu, S. Zhou, and H. Zhang. Extremal arithmetic–geometric index of bicyclic graphs. *Circuits, Systems, and Signal Processing*, 42(10):5739–5760, 2023. <https://doi.org/10.1007/s00034-023-02385-4>.
- [11] H. P. Schultz. Topological organic chemistry. 1. graph theory and topological indices of alkanes. *Journal of Chemical Information and Computer Sciences*, 29(3):227–228, 1989. <https://doi.org/10.1021/ci00063a012>.
- [12] A. Tepeh. Extremal bicyclic graphs with respect to mostar index. *Applied Mathematics and Computation*, 355:319–324, 2019. <https://doi.org/10.1016/j.amc.2019.03.014>.
- [13] R. Todeschini and V. Consonni. *Handbook of Molecular Descriptors*. John Wiley & Sons, 2008.
- [14] N. Trinajstić. *Chemical Graph Theory*. CRC press, 2018.
- [15] H. Wang and M. Liu. The upper bound of the edge mostar index with respect to bicyclic graphs. *Mathematics*, 11(11):2506, 2023. <https://doi.org/10.3390/math11112506>.

- [16] H. Wiener. Correlation of heats of isomerization, and differences in heats of vaporization of isomers, among the paraffin hydrocarbons. *Journal of the American Chemical Society*, 69(11):2636–2638, 1947. <https://doi.org/10.1021/ja01203a022>.
- [17] H. Wiener. Structural determination of paraffin boiling points. *Journal of the American Chemical Society*, 69(1):17–20, 1947. <https://doi.org/10.1021/ja01193a005>.