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The Impact of Deletion of Vertex or Edge on Mostar Index

B. Gautham Shenoy, Vishu Kumar M., Suhas

ABSTRACT: The Mostar index, is a novel bond additive structural invariant which measures the degree of peripherality of an edge. The Mostar index is defined by T. Došlić et al. We figure out effect of vertex or edge removal on Mostar index. This is done for generalized wheel graph, wheel graph, cycle, star graph, complete graph and complete bipartite graph. Also, the Mostar index of generalized wheel is computed and analysis of Mostar index of hetero atom with π electron energy is done.

Keywords: Mostar index, generalized wheel graph, edge deletion, vertex deletion.

Contents

1. Introduction

In Graph theory, graph invariant is trait of graph that remains unchanged under isomorphism. Large number of real-valued graph invariants called topological indices are defined to collect and study the information regarding the connectivity pattern of components in graph. It is possible to correlate these numerical quantities of graph with various physico-chemical values of corresponding molecular compound. Weiner in 1947 defined a distance based topological indices named has path number, called Weiner index now, to investigate the nature of acyclic saturated hydrocarbons. Overtime many topological indices are defined. Depending on various parameter of graph such as distance the distance based topological indices emerged, based on degree the degree based topological indices emerged. Also, there turn up another type of indices which mainly based on contribution of induvial vertices and / or edges. These indices are called vertex and bond additive indices.

The graph consider in this paper are undirected graph without self-loop and multiple edges. Let $G = (V, E)$ with vertex set $V(G)$ and edge set $E(G)$ of order n and m respectively. A peripheral edge is an edge whose one end vertex has extra vertices closer compared to the other. The peripheral position of an edge uv in G can be expressed by absolute value of difference between the number of vertices closer to u than to v and the number of vertices closer to u than to v. A Bond additive structural invariant, the Mostar index was defined on basis of this peripheral property of an edge, by T. Došlić et al. in [1]. The Mostar index of a graph G is defined as,

$$M_o(G) = \sum_{uv \in E(G)} |n_u - n_v|$$

where n_u denote the number of vertices closer to u than v.

In [1] T. Došlić et al. characterised extremal trees and unicyclic graphs based on Mostar index. Also, derived explicit formulae for Benzenoid graphs and cartesian product of graphs using cut method. Along with this study various other researchers examined the properties of Mostar index of graphs. In [2] upper bound for the Mostar index of cacti of order n with k cycle is studied. In [3] minimum and / or

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maximum Mostar index among the families of tree of order n are obtained. In [5] the conjecture of Došlić et al. is proved. In [7] sharp lower bound on the Mostar index of trees based on their order is identified. In [8] with respect to vertex orbits the Mostar index is calculated under the action of automorphism. In [10] some results on bounds and extremal of Mostar index are collected. In [12] the difference of Mostar index and irregularity of graph are studied. In [13] the Mostar index of trees and graph products are studied. In [14] extremal Mostar index of chemical trees is found. In [14] the Mostar index of graph obtained by generalised hierarchical product, lexicographic product, cartesian product, corona product, join, subdivision vertex edge join, and Indu Bala product of graphs are calculated. Also, the by applying these results the Mostar index of some types of nanostructures and chemical graphs are determined. In [17] the Mostar index of bridge graphs of path, star, cycle and complete graphs are calculated. In [18] Mostar index of probabilistic neural network and convolutional neural network are computed. In [20] the greatest Mostar index for extremal hexagonal system of cacti-condensed hexagonal system containing p hexagon is computed. In [24] Mostar index of certain classes of bicyclic graphs are computed. In [27] the Mostar index of Tribonacci cubes is derived. Later, modified version of Mostar index were defined and studied in [5], [9], [11], [16], [19], [22]. Now will discuss some known results that will be used in the rest of the paper.

Proposition 1.1 *[1]* $M_o(G)(K_n) = M_o(C_n) = M_o(K_{n,n}) = 0$ *and also* $M_o(P_n) = \lfloor \frac{(n-1)^2}{2} \rfloor$.

Proposition 1.2 *[1]* $M_o(T_n) \leq (n-1)(n-2) = M_o(S_n)$.

Proposition 1.3 *[6]* $M_o(W_n) = n(n-3)$.

In this paper, the Mostar index of generalized wheel is computed. Also, we study the effect of vertex or edge removal on Mostar index. This is done for generalized wheel graph, wheel graph, cycle, star graph, complete graph and complete bipartite graph. The analysis of Mostar index of hetero atom with π electron energy is done.

2. Main Results

In this section we compute Mostar index of generalized wheel graph. Also, we compute Mostar index of generalized wheel graph, wheel graph, cycle, star graph, complete graph and complete bipartite graph by deletion of vertex or edge.

Proposition 2.1 *For generalized wheel graph* $W_{m,n}$*. The Mostar index is given by:*

$$M_o(W_{m,n}) = mn \cdot |m - n + 2|.$$

Proof: Let us consider a generalized wheel graph $W_{m,n}$. We partition the vertex set of $W_{m,n}$ into V_1 and V_2. Where V_1 is set of all rim vertices of $W_{m,n}$ and V_2 is set of all central vertices of $W_{m,n}$.
For each edge between vertices of V_1 in $W_{m,n}$, say u and v, the value $|n_u - n_v| = 0$
For each edge between vertex of V_1 in $W_{m,n}$, say u and vertex of V_2 say v, the value $|n_u - n_v| = |(m-1) - (n-3)| = |m - n + 2|$
Applying the definition of Mostar index we get,

$$M_o(W_{m,n}) = \sum_{uv \in E(G)} |n_u - n_v| = \sum_{\substack{uv \in E(G) \\ u,v \in V_1}} |n_u - n_v| + \sum_{\substack{uv \in E(G) \\ u \in V_1, v \in V_2}} |n_u - n_v|$$
$$= 0 + mn|m - n + 2| = mn|m - n + 2|.$$

□

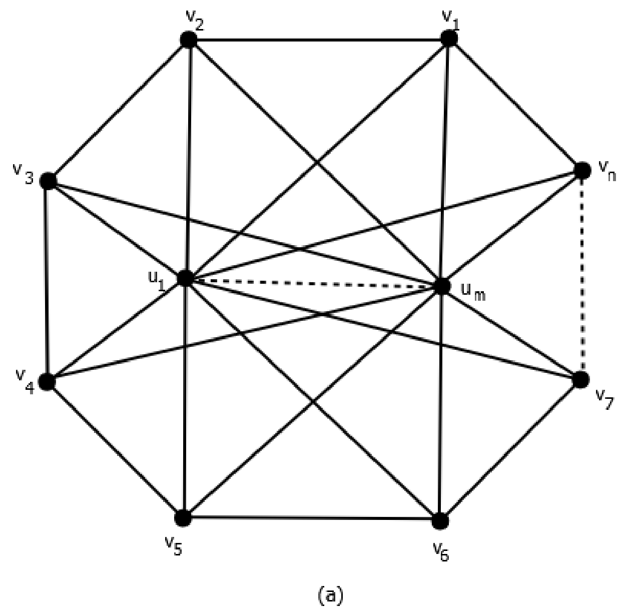


Figure 1: The graph $W_{m,n}$

Example 2.1 *To find Mostar index of $W_{2,8}$(Figure 2). We partition the vertex set of $W_{2,8}$ into V_1 and V_2. Where V_1 is set of all rim vertices of $W_{2,8}$,i.e., $V_1 = \{v_1, v_2, v_3, v_4, v_5, v_6, v_7, v_8\}$ and V_2 is set of all central vertices of $W_{2,8}$,i.e., $V_1 = \{u_1, u_2\}$.*
For each edge between vertices of V_1 in $W_{2,8}$, say u and v, the value $|n_u - n_v| = 0$
For each edge between vertex of V_1 in $W_{2,8}$, say u and vertex of V_2 say v, the value $|n_u - n_v| = |(2-1)-(8-3)| = |2-8+2| = |-4| = 4$
Applying the definition of Mostar index we get,

$$M_o(W_{2,8}) = \sum_{uv \in E(G)} |n_u - n_v| = \sum_{\substack{uv \in E(G) \\ u,v \in V_1}} |n_u - n_v| + \sum_{\substack{uv \in E(G) \\ u \in V_1, v \in V_2}} |n_u - n_v|$$
$$= 0 + 2 \times 8 \times 4 = 64.$$

Proposition 2.2 *Let $W_{m,n}$ generalized wheel graph, $m \geq 2$ and e be an edge of $W_{m,n}$. The Mostar index of $W_{m,n} - \{e\}$ is given by:*

$$M_o(W_{m,n} - \{e\}) = \begin{cases} 2m|m-n+1| + (n-2)m|m-n+2| + 2 & \text{if } e \text{ is rim edge} \\ (m-1)(n-1)|m-n+2| + (m-1)|m-n+1| & \text{if } e \text{ is spoke edge} \\ +(n-1)|m-n+3| + 2 & \end{cases}$$

Proof: Let us consider a generalized wheel graph $W_{m,n}$, $m \geq 2$. Deletion of an edge e from $W_{m,n}$, results in graph $W_{m,n} - \{e\}$.
If $e = xy$ is a rim edge. We partition the vertex set of $W_{n,m} - \{e\}$ into $V_1 = \{x, y\}$, V_2 is a set of all rim vertices of $W_{m,n}$ except x and y, and V_3 is set of all central vertices of $W_{m,n}$.
For each edge between the vertex of V_1, say u and the vertex of V_2, say v, the value $|n_u - n_v| = 1$.
For each edge between the vertex of V_1, say u and the vertex of V_3, say v, the value $|n_u - n_v| = |m-n+1|$.
For each edge between the vertex of V_2, say u and the vertex of V_3, say v, the value $|n_u - n_v| = |m-n+2|$.
For each edge between the vertices of V_2, say u and v, the value $|n_u - n_v| = 0$.

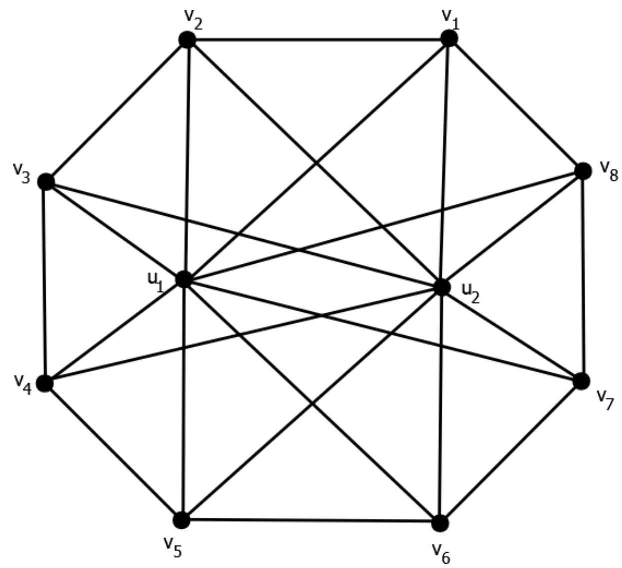


Figure 2: The graph $W_{2,8}$

Applying the definition of Mostar index we get,

$$\begin{aligned} M_o(W_{m,n}-\{e\}) &= \sum_{uv\in E(G)} |n_u-n_v| \\ &= \sum_{\substack{uv\in E(G)\\ u\in V_1, v\in V_2}} |n_u-n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_1, v\in V_3}} |n_u-n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_2, v\in V_3}} |n_u-n_v| \\ &+ \sum_{\substack{uv\in E(G)\\ u,v\in V_2}} |n_u-n_v| \\ &= 2+2m|m-n+1|+(n-2)m|m-n+2|. \end{aligned}$$

If $e=cx$ is a spoke edge, where c is central vertex and x is a rim vertex of $W_{m,n}-\{e\}$. We partition the vertex set of $W_{n,m}-\{e\}$ into $V_1=\{x\}$, $V_2=\{c\}$, V_3 is a set of all rim vertices of $W_{m,n}-\{e\}$ at distance one from x, V_4 is set of all rim vertices of $W_{m,n}-\{e\}$ at distance greater than 1 from x, V_5 is set all central vertices of $W_{m,n}-\{e\}$ except c.

For each edge between the vertex x and the vertex of V_3, say v, the value $|n_x-n_v|=1$.

For each edge between the vertex x and the vertex of V_5, say v, the value $|n_x-n_v|=|m-n+1|$.

For each edge between the vertex c and the vertex of V_3, say v, the value $|n_c-n_v|=|m-n+3|$.

For each edge between the vertex c and the vertex of V_4, say v, the value $|n_c-n_v|=|m-n+3|$.

For each edge between the vertex of V_3, say u and the vertex of V_5, say v, the value $|n_u-n_v|=|m-n+2|$.

For each edge between the vertex of V_4, say u and the vertex of V_5, say v, the value $|n_u-n_v|=|m-n+2|$.

For each edge between the vertices of V_5, say u and v, the value $|n_u-n_v|=0$.

Applying the definition of Mostar index we get,

$$\begin{aligned}
M_o(W_{m,n}-\{e\}) &= \sum_{uv\in E(G)} |n_u-n_v| \\
&= \sum_{\substack{uv\in E(G)\\ u\in V_1, v\in V_3}} |n_u-n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_1, v\in V_5}} |n_u-n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_2, v\in V_3}} |n_u-n_v| \\
&+ \sum_{\substack{uv\in E(G)\\ u\in V_2, v\in V_4}} |n_u-n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_3, v\in V_5}} |n_u-n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_4, v\in V_5}} |n_u-n_v| \\
&+ \sum_{\substack{uv\in E(G)\\ u,v\in V_4}} |n_u-n_v| \\
&= 2+(m-1)|m-n+1|+2|m-n+3|+(n-3)|m-n+3|+2(m-1)|m-n+2| \\
&+ (m-1)(n-3)|m-n+2|+0 \\
&= (m-1)(n-1)|m-n+2|+(m-1)|m-n+1|+(n-1)|m-n+3|+2.
\end{aligned}$$

□

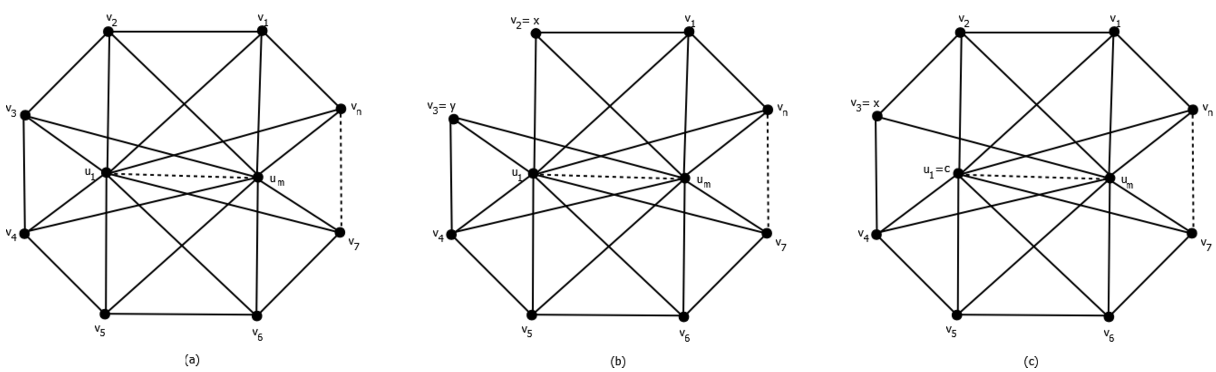


Figure 3: (a) The graph $W_{m,n}$, (b) The graph $W_{m,n}-\{e\}$ where $e=xy$ is rim edge, (c) The graph $W_{m,n}-\{e\}$ where $e=cx$ is spoke edge

Example 2.2 *To find Mostar index of $W_{2,8}-\{e\}$(Figure 4).*
The removal of rim edge $e=xy$. We partition the vertex set of $W_{2,8}-\{e\}$ into $V_1=\{v_2=x, v_3=y\}$, V_2 is a set of all rim vertices of $W_{m,n}$ except x and y,i.e., $V_2=\{v_1,v_4,v_5,v_6,v_7,v_8\}$ and V_3 is set of all central vertices of $W_{m,n}$, i.e., $V_3=\{u_1,u_2\}$.
For each edge between the vertex of V_1, say u and the vertex of V_2, say v, the value $|n_u-n_v|=1$.
For each edge between the vertex of V_1, say u and the vertex of V_3, say v, the value $|n_u-n_v|=|2-8+1|=|-5|=5$.
For each edge between the vertex of V_2, say u and the vertex of V_3, say v, the value $|n_u-n_v|=|2-8+2|=|-4|=4$.
For each edge between the vertices of V_2, say u and v, the value $|n_u-n_v|=0$.
Applying the definition of Mostar index we get,

$$\begin{aligned}
M_o(W_{2,8}-\{e\}) &= \sum_{uv\in E(G)} |n_u - n_v| \\
&= \sum_{\substack{uv\in E(G)\\ u\in V_1, v\in V_2}} |n_u - n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_1, v\in V_3}} |n_u - n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_2, v\in V_3}} |n_u - n_v| \\
&+ \sum_{\substack{uv\in E(G)\\ u,v\in V_2}} |n_u - n_v| \\
&= 2\times 1 + 2\times 2\times 5 + (8-2)\times 2\times 4 = 70.
\end{aligned}$$

The removal of spoke edge $e = cx$, where c is central vertex and x is a rim vertex of $W_{2,8}-\{e\}$. We partition the vertex set of $W_{2,8}-\{e\}$ into $V_1=\{v_3=x\}$, $V_2=\{u_1=c\}$, V_3 is a set of all rim vertices of $W_{2,8}-\{e\}$ at distance one from x, V_4 is set of all rim vertices of $W_{2,8}-\{e\}$ at distance greater than 1 from x, V_5 is set all central vertices of $W_{2,8}-\{e\}$, i.e., $V_5=\{u_2\}$.
For each edge between the vertex x and the vertex of V_3, say v, the value $|n_x - n_v| = 1$.
For each edge between the vertex x and the vertex of V_5, say v, the value $|n_x - n_v| = |2-8+1| = |-5| = 5$.
For each edge between the vertex c and the vertex of V_3, say v, the value $|n_c - n_v| = |2-8+3| = |-3| = 3$.
For each edge between the vertex c and the vertex of V_4, say v, the value $|n_c - n_v| = |2-8+3| = |-3| = 3$.
For each edge between the vertex of V_3, say u and the vertex of V_5, say v, the value $|n_u - n_v| = |2-8+2| = |-4| = 4$.
For each edge between the vertex of V_4, say u and the vertex of V_5, say v, the value $|n_u - n_v| = |2-8+2| = |-4| = 4$.
For each edge between the vertices of V_5, say u and v, the value $|n_u - n_v| = 0$.
Applying the definition of Mostar index we get,

$$\begin{aligned}
M_o(W_{2,8}-\{e\}) &= \sum_{uv\in E(G)} |n_u - n_v| \\
&= \sum_{\substack{uv\in E(G)\\ u\in V_1, v\in V_3}} |n_u - n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_1, v\in V_5}} |n_u - n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_2, v\in V_3}} |n_u - n_v| \\
&+ \sum_{\substack{uv\in E(G)\\ u\in V_2, v\in V_4}} |n_u - n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_3, v\in V_5}} |n_u - n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_4, v\in V_5}} |n_u - n_v| \\
&+ \sum_{\substack{uv\in E(G)\\ u,v\in V_4}} |n_u - n_v| \\
&= 2\times 1 + (2-1)\times 5 + 2\times 3 + (8-3)\times 3 + 2(2-1)\times 4 \\
&+ (2-1)(8-3)\times 4 + 0 \\
&= 56.
\end{aligned}$$

Proposition 2.3 *Let $W_{m,n}$ generalized wheel graph, $m \geq 2$ and v be a vertex of $W_{m,n}$. The Mostar index of $W_{m,n}-\{v\}$ is given by:*

$$M_o(W_{m,n}-\{v\}) = \begin{cases} 2m|m-n+2| + (n-3)m|m-n+3| + 2 & \text{if } v \text{ is rim vertex} \\ (m-1)n|m-n+1| & \text{if } v \text{ is central vertex} \end{cases}$$

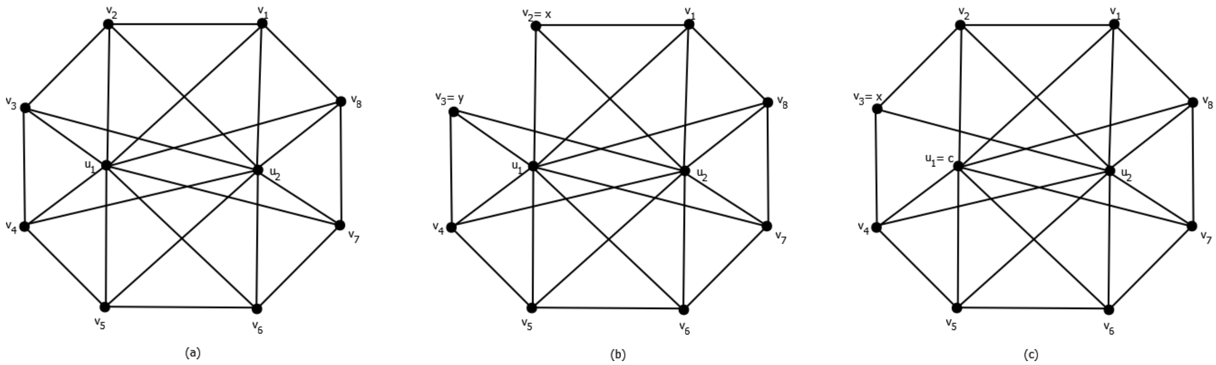


Figure 4: (a) The graph $W_{2,8}$, (b) The graph $W_{2,8} - \{e\}$ where $e = xy$ is rim edge, (c) The graph $W_{2,8} - \{e\}$ where $e = cx$ is spoke edge

Proof: Let us consider a generalized wheel graph $W_{m,n}$, $m \geq 2$. Deletion of a vertex v from $W_{m,n}$, results in graph $W_{m,n} - \{v\}$.
If v is a central vertex. Then the graph $W_{m,n} - \{v\}$ is isomorphic to $W_{m-1,n}$. Since the Mostar index of a graph depends only on its structure, it follows that:

$$M_o(W_{m,n} - \{v\}) = M_o(W_{m-1,n}) = (m-1)n|m-n+1|.$$

If v is a rim vertex. Then the graph $W_{m,n} - \{v\}$ is isomorphic to $W_{m,n-1} - \{e\}$, for some rim edge e. Since the Mostar index of a graph depends only on its structure, it follows that:

$$M_o(W_{m,n} - \{v\}) = M_0(W_{m,n-1} - \{e\}) = 2m|m-n+2| + (n-3)m|m-n+3| + 2.$$

□

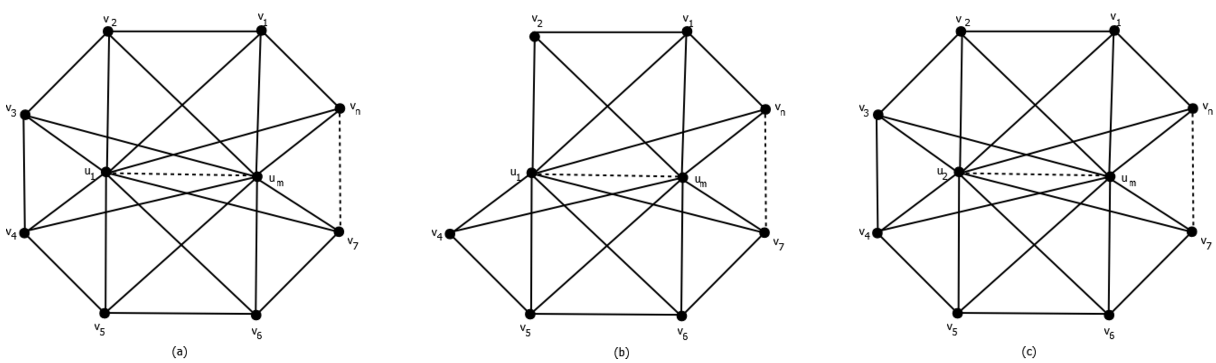


Figure 5: (a) The graph $W_{m,n}$, (b) The graph $W_{m,n} - \{v\}$ where v is rim vertex, (c) The graph $W_{m,n} - \{v\}$ where v is central vertex

Example 2.3 *To find Mostar index of $W_{3,8} - \{v\}$(Figure 6).*
The removal of central vertex u_1. Then the graph $W_{3,8} - \{u_1\}$ is isomorphic to $W_{2,8}$. Since the Mostar index of a graph depends only on its structure, it follows that:

$$M_o(W_{3,8} - \{u_1\}) = M_o(W_{2,8}) = 2 \times 8|3-8+1| = 64.$$

The removal of rim vertex v_3. Then the graph $W_{3,8} - \{v_3\}$ is isomorphic to $W_{3,7} - \{e\}$, for some rim edge e. Since the Mostar index of a graph depends only on its structure, it follows that:

$$M_o(W_{3,8} - \{v_3\}) = M_0(W_{3,7} - \{e\}) = 2 \times 3|3 - 8 + 2| + (8 - 3) \times 3|3 - 8 + 3| + 2 = 50.$$

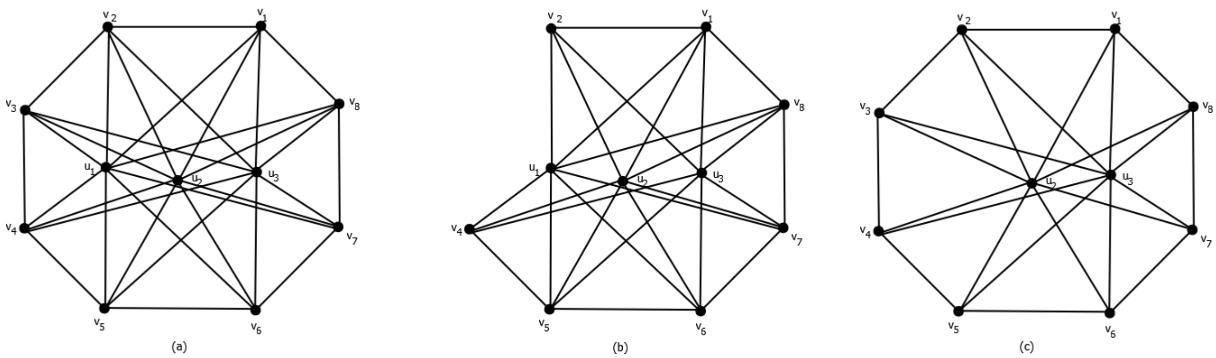


Figure 6: (a) The graph $W_{3,8}$, (b) The graph $W_{3,8} - \{v\}$ where v is rim vertex, (c) The graph $W_{3,8} - \{v\}$ where v is central vertex

Proposition 2.4 *Let W_n wheel graph, $n \geq 7$ and e be an edge of W_n. The Mostar index of $W_n - \{e\}$ is given by:*

$$M_o(W_n - \{e\}) = \begin{cases} n^2 - 5n + 8 & \text{if } e \text{ is rim edge} \\ n^2 - 5n + 4 & \text{if } e \text{ is spoke edge} \end{cases}$$

Proof: Let us consider the wheel graph W_n, $n \geq 7$. Deletion of an edge e from W_n, results in graph $W_n - \{e\}$.
If $e = xy$ is a rim edge. We partition the vertex set of $W_n - \{e\}$ into $V_1 = \{x, y\}$, V_2 is a set of all rim vertices of $W_n - \{e\}$ except x and y, and V_3 is a singleton set containing central vertex of $W_n - \{e\}$.
For each edge between the vertex of V_1, say u and the vertex of V_2, say v, the value $|n_u - n_v| = 1$.
For each edge between the vertex of V_1, say u and the vertex c, the value $|n_u - n_c| = (n - 3)$.
For each edge between the vertex of V_2, say u and the vertex c, the value $|n_u - n_c| = (n - 4)$.
For each edge between the vertices of V_2, say u and v, the value $|n_u - n_v| = 0$.
Applying the definition of Mostar index we get,

$$\begin{aligned} M_o(W_n - \{e\}) &= \sum_{uv \in E(G)} |n_u - n_v| \\ &= \sum_{\substack{uv \in E(G) \\ u \in V_1, v \in V_2}} |n_u - n_v| + \sum_{\substack{uv \in E(G) \\ u \in V_1, v \in V_3}} |n_u - n_v| + \sum_{\substack{uv \in E(G) \\ u \in V_2, v \in V_3}} |n_u - n_v| \\ &+ \sum_{\substack{uv \in E(G) \\ u, v \in V_2}} |n_u - n_v| \\ &= 2 + 2(n - 3) + (n - 3)(n - 4) + 0 = n^2 - 5n + 8. \end{aligned}$$

If $e = cx$ is a spoke edge. We partition the vertex set of $W_n - \{e\}$ into V_1 is a singleton set containing rim vertex x of $W_n - \{e\}$, V_2 is a set of all rim vertices of $W_n - \{e\}$ and at distance 1 from x,V_3 is a set of all rim vertices of $W_n - \{e\}$ and at distance 2 from x, V_4 is a set of all rim vertices of $W_n - \{e\}$ and

at distance > 2 from x and V_5 is a singleton set containing central vertex C of $W_n - \{e\}$.
For each edge between the vertex x and the vertex of V_2, say v, the value $|n_x - n_v| = 1$.
For each edge between the vertex of V_2, say u and the vertex of V_3, say v, the value $|n_u - n_v| = 0$.
For each edge between the vertex of V_2, say u and the vertex c, the value $|n_u - n_c| = (n-5)$.
For each edge between the vertex of V_3, say u and the vertex c, the value $|n_u - n_c| = (n-5)$.
For each edge between the vertex of V_4, say u and the vertex c, the value $|n_u - n_c| = (n-4)$.
For each edge between the vertices of V_4, say u and v, the value $|n_u - n_v| = 0$.
Applying the definition of Mostar index we get,

$$\begin{aligned} M_o(W_n - \{e\}) &= \sum_{uv \in E(G)} |n_u - n_v| \\ &= \sum_{\substack{uv\in E(G)\\ u\in V_1, v\in V_2}} |n_u - n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_2, v\in V_3}} |n_u - n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_2, v\in V_5}} |n_u - n_v| \sum_{\substack{uv\in E(G)\\ u\in V_3, v\in V_5}} |n_u - n_v| \\ &+ \sum_{\substack{uv\in E(G)\\ u\in V_4, v\in V_5}} |n_u - n_v| + \sum_{\substack{uv\in E(G)\\ u,v\in V_4}} |n_u - n_v| \\ &= 2 + 0 + 2(n-5) + 2(n-5) + (n-5)(n-4) + 0 = n^2 - 5n + 4. \end{aligned}$$

□

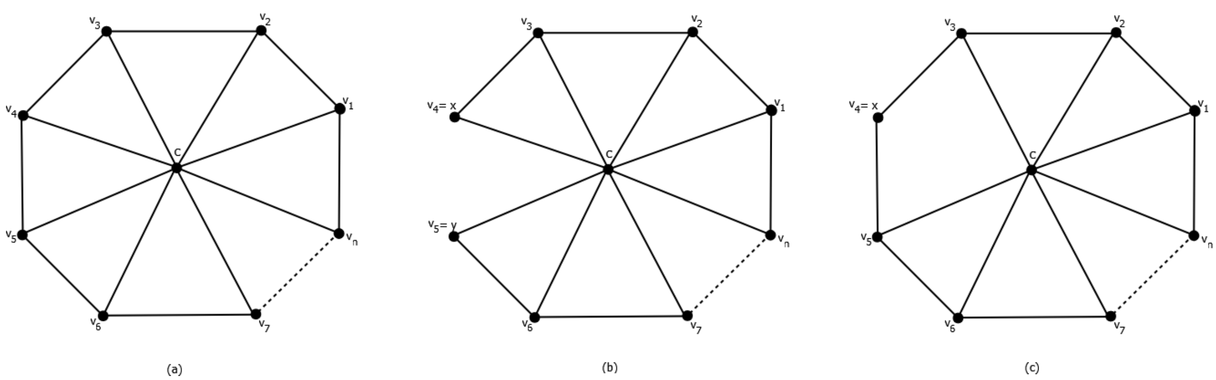


Figure 7: (a) The graph W_n, (b) The graph $W_n - \{e\}$ where $e = xy$ is rim edge, (c) The graph $W_n - \{e\}$ where e is spoke edge

Example 2.4 *To find Mostar index of $W_9 - \{e\}$(Figure 8).*
The removal of rim edge $e = xy$. We partition the vertex set of $W_9 - \{e\}$ into $V_1 = \{v_4 = x, v_5 = y\}$, V_2 is a set of all rim vertices of $W_9 - \{e\}$ except x and y, i.e., $V_2 = \{v_1, v_2, v_3, v_6, v_7, v_8\}$, and V_3 is a singleton set containing central vertex of $W_9 - \{e\}$, i.e., $V_3 = \{c\}$.
For each edge between the vertex of V_1, say u and the vertex of V_2, say v, the value $|n_u - n_v| = 1$.
For each edge between the vertex of V_1, say u and the vertex c, the value $|n_u - n_c| = (9-3) = 6$.
For each edge between the vertex of V_2, say u and the vertex c, the value $|n_u - n_c| = (9-4) = 5$.
For each edge between the vertices of V_2, say u and v, the value $|n_u - n_v| = 0$.
Applying the definition of Mostar index we get,

$$
\begin{aligned}
M_o(W_9-\{e\}) &= \sum_{uv\in E(G)} |n_u-n_v| \\
&= \sum_{\substack{uv\in E(G)\\ u\in V_1, v\in V_2}} |n_u-n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_1, v\in V_3}} |n_u-n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_2, v\in V_3}} |n_u-n_v| \\
&+ \sum_{\substack{uv\in E(G)\\ u,v\in V_2}} |n_u-n_v| \\
&= 2\times 1 + 2\times 6 + (9-3)\times 5 + 0 = 44.
\end{aligned}
$$

The removal of spoke edge $e = cx$. We partition the vertex set of $W_9-\{e\}$ into V_1 is a singleton set containing rim vertex $v_4 = x$ of $W_9-\{e\}$, i.e., $V_1 = \{v_4\}$, V_2 is a set of all rim vertices of $W_9-\{e\}$ and at distance 1 from x, i.e., $V_2 = \{v_3, v_5\}$,V_3 is a set of all rim vertices of $W_9-\{e\}$ except and at distance 2 from x, i.e., $V_3 = \{v_2, v_6\}$, V_4 is a set of all rim vertices of $W_9-\{e\}$ and at distance > 2 from x, i.e., $V_4 = \{v_1, v_7, v_8\}$ and V_5 is a singleton set containing central vertex c of $W_9-\{e\}$, i.e., $V_5 = \{c\}$.
For each edge between the vertex v_4 and the vertex of V_2, say v, the value $|n_{v_4} - n_v| = 1$.
For each edge between the vertex of V_2, say u and the vertex of V_3, say v, the value $|n_u - n_v| = 0$.
For each edge between the vertex of V_2, say u and the vertex c, the value $|n_u - n_c| = (9-5) = 4$.
For each edge between the vertex of V_3, say u and the vertex c, the value $|n_u - n_c| = (9-5) = 4$.
For each edge between the vertex of V_4, say u and the vertex c, the value $|n_u - n_c| = (9-4) = 5$.
For each edge between the vertices of V_4, say u and v, the value $|n_u - n_v| = 0$.
Applying the definition of Mostar index we get,

$$
\begin{aligned}
M_o(W_9-\{e\}) &= \sum_{uv\in E(G)} |n_u-n_v| \\
&= \sum_{\substack{uv\in E(G)\\ u\in V_1, v\in V_2}} |n_u-n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_2, v\in V_3}} |n_u-n_v| + \sum_{\substack{uv\in E(G)\\ u\in V_2, v\in V_5}} |n_u-n_v| \sum_{\substack{uv\in E(G)\\ u\in V_3, v\in V_5}} |n_u-n_v| \\
&+ \sum_{\substack{uv\in E(G)\\ u\in V_4, v\in V_5}} |n_u-n_v| + \sum_{\substack{uv\in E(G)\\ u,v\in V_4}} |n_u-n_v| \\
&= 2\times 1 + 0 + 2\times 5 + 2\times 4 + (9-5)\times 5 + 0 = 40.
\end{aligned}
$$

Proposition 2.5 *Let W_n wheel graph, $n \geq 7$ and v be a vertex of W_n. The Mostar index of $W_n - \{v\}$ is given by:*

$$
M_o(W_n-\{v\}) = \begin{cases} 0 & \text{if } v \text{ is central vertex} \\ n^2 - 7n + 14 & \text{if } v \text{ is rim vertex} \end{cases}
$$

Proof: Let us consider the wheel graph W_n, $n \geq 7$. Deletion of a vertex v from W_n, results in graph $W_n - \{v\}$.
If v is a central vertex. Then the graph $W_n - \{v\}$ is isomorphic to C_{n-1}. Since the Mostar index of a graph depends only on its structure, it follows that:

$$M_o(W_n - \{v\}) = M_o(C_{n-1}) = 0.$$

If v is a rim vertex. Then the graph $W_n - \{v\}$ is isomorphic to $W_{n-1} - \{e\}$, for some rim edge e. Since the Mostar index of a graph depends only on its structure, it follows that:

$$M_o(W_n - \{v\}) = M_0(W_{n-1} - \{e\}) = (n-1)^2 - 5(n-1) + 8 = n^2 - 7n + 14.$$

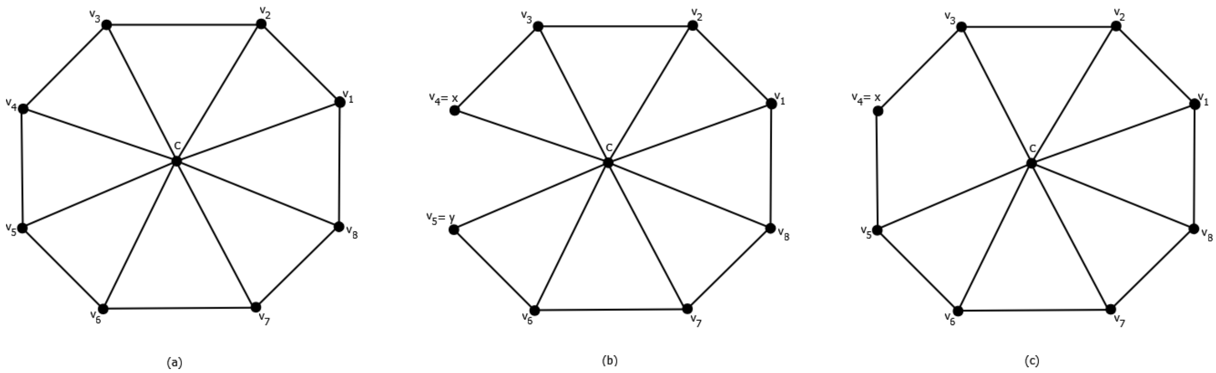


Figure 8: (a) The graph W_9, (b) The graph $W_9 - \{e\}$ where $e = xy$ is rim edge, (c) The graph $W_9 - \{e\}$ where $e = cx$ is spoke edge

□

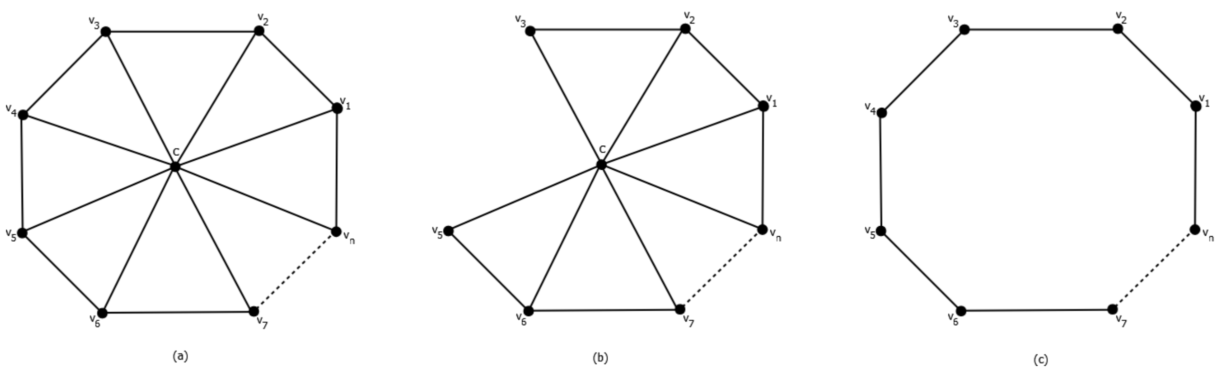


Figure 9: (a) The graph W_n, (b) The graph $W_n - \{v\}$ where v is rim vertex, (c) The graph $W_n - \{v\}$ where v is central vertex

Example 2.5 *To find Mostar index of* $W_9 - \{v\}$*(Figure 10).*
The removal of central vertex $v = c$*. Then the graph* $W_9 - \{v\}$ *is isomorphic to* C_8*. Since the Mostar index of a graph depends only on its structure, it follows that:*

$$M_o(W_9 - \{v\}) = M_o(C_8) = 0.$$

The removal of rim vertex $v = v_4$*. Then the graph* $W_9 - \{v\}$ *is isomorphic to* $W_8 - \{e\}$*, for some rim edge* e*. Since the Mostar index of a graph depends only on its structure, it follows that:*

$$M_o(W_9 - \{v\}) = M_0(W_8 - \{e\}) = (9-1)^2 - 5(9-1) + 8 = 32.$$

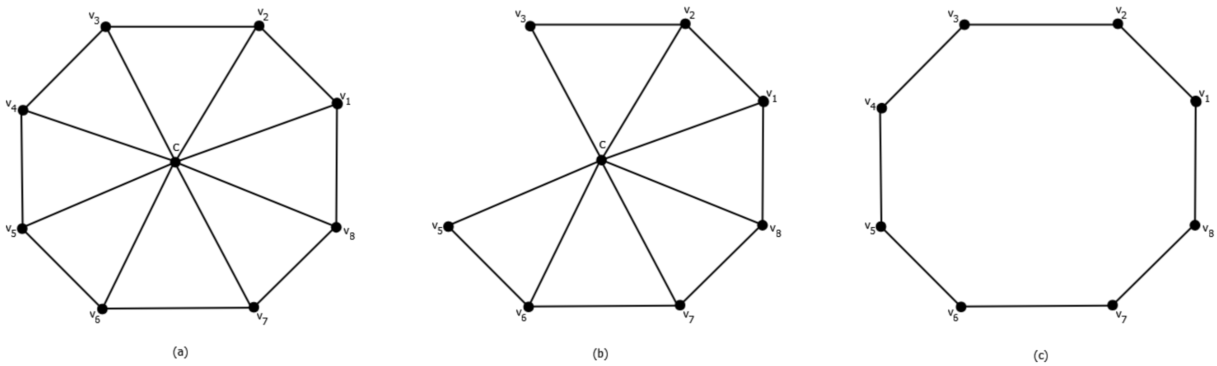


Figure 10: (a) The graph W_9, (b) The graph $W_9 - \{v\}$ where v is rim vertex, (c) The graph $W_9 - \{v\}$ where v is central vertex

Proposition 2.6 *Let $K_{m,n}$ complete bipartite graph and e be an edge of $K_{m,n}$. The Mostar index of $K_{m,n} - \{e\}$ is given by:*

$$M_o(K_{m,n} - \{e\}) = \begin{cases} (mn - m - n - 1)|m - n| + (n - 1)|n - m + 1| + (m - 1)|m - n - 1| & \text{if } m \neq n \\ 2(n - 1) & \text{if } m = n \end{cases}$$

Proof: Let us consider complete bipartite graph $K_{m,n}$. We can partition vertex set of $K_{m,n}$ into $U = \{u_1, u_2, \ldots, u_m\}$ and $V = \{v_1, v_2, \ldots, v_n\}$. Deletion of an edge e from $K_{m,n}$, results in graph $K_{m,n} - \{e\}$. Let us partition vertex set of $K_{m,n} - \{e\}$ into V_1 is a set containing end vertex of e in U of $K_{m,n} - \{e\}$, V_2 is a set containing end vertex of e in V of $K_{m,n} - \{e\}$, V_3 is a set of vertices in U of $K_{m,n} - \{e\}$ except end vertex of e, containing $m - 1$ vertices and V_4 is a set of all vertices in V of $K_{m,n} - \{e\}$ except end vertex of e, containing $n - 1$ vertices.
For each edge between vertex of V_1, say u and vertex of V_4 say v, the value
$|n_u - n_v| == |n - (m - 1)| = |n - m + 1|$
For each edge between vertex of V_2, say u and vertex of V_3 say v, the value
$|n_u - n_v| = |(m - 1) - n| = |m - n - 1|$
For each edge between vertex of V_3, say u and vertex of V_4 say v, the value
$|n_u - n_v| = |m - n|$
Applying the definition of Mostar index we get,

$$\begin{aligned} M_o(K_{m,n} - \{e\}) &= \sum_{uv \in E(G)} |n_u - n_v| \\ &= \sum_{\substack{uv \in E(G) \\ u \in V_1, v \in V_4}} |n_u - n_v| + \sum_{\substack{uv \in E(G) \\ u \in V_2, v \in V_3}} |n_u - n_v| + \sum_{\substack{uv \in E(G) \\ u \in V_3, v \in V_4}} |n_u - n_v| \\ &= (n - 1)|n - m + 1| + (m - 1)|m - n - 1| + (mn - m - n - 1)|m - n| \end{aligned}$$

If m=n,
$M_o(K_{n,n} - \{e\}) = 2(n - 1)$

□

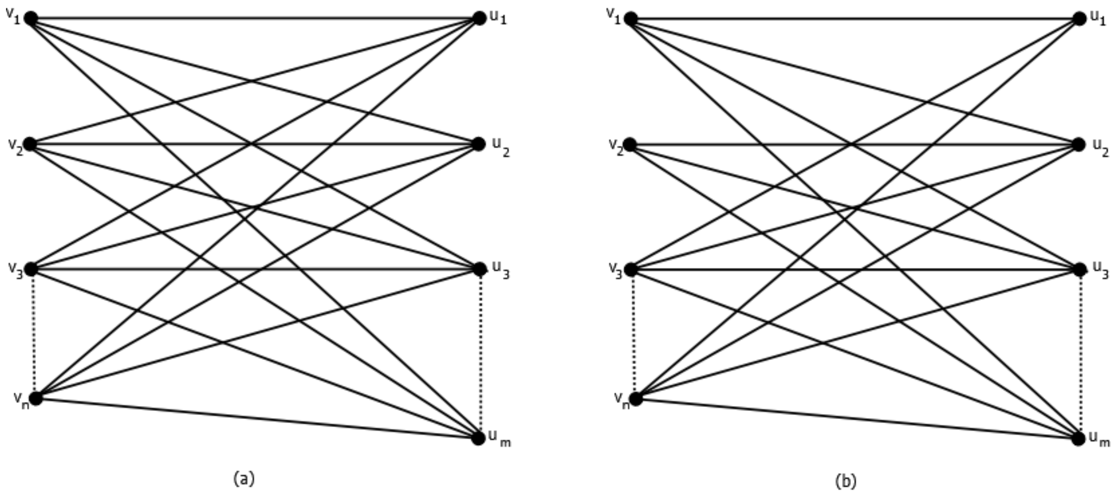


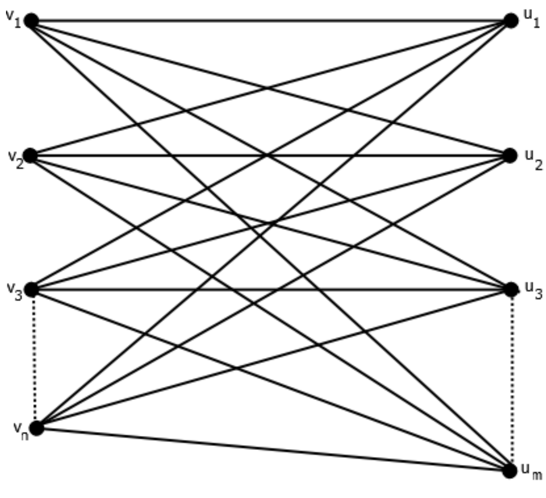
Figure 11: (a) The graph $K_{m,n}$, (b) The graph $K_{m,n} - \{e\}$

Proposition 2.7 *Let $K_{m,n}$ complete bipartite graph and v be a vertex of $K_{m,n}$. The Mostar index of $K_{m,n} - \{v\}$ is given by:*

$$M_o(K_{m,n} - \{v\}) = \begin{cases} (m-1)n|n-m+1| & \text{if } m \neq n \\ n(n-1) & \text{if } m = n \end{cases}$$

Proof: Let us consider a complete bipartite graph $K_{m,n}$. We can partition vertex set of $K_{m,n}$ into $U = \{u_1, u_2, \ldots, u_m\}$ and $V = \{v_1, v_2, \ldots, v_n\}$. Deletion of a vertex v from $K_{m,n}$, results in graph $K_{m,n} - \{v\}$ which is isomorphic to $K_{m-1,n}$, if the vertex is removed from U. We can be partition the vertex set of $K_{m-1,n}$ into V_1 and V_2. Where V_1 is set of all vertices in U of $K_{m-1,n}$, containing $m-1$ vertices and V_2 is set of all vertices in V of $K_{m-1,n}$, containing n vertices .
For each edge between vertex of V_1, say u and vertex of V_2 say v, the value $|n_u - n_v| = |n - (m-1)| = |n - m + 1|$.
Applying the definition of Mostar index we get,
$$M_o(K_{m-1,n}) = \sum_{uv \in E(G)} |n_u - n_v| = \sum_{\substack{uv \in E(G) \\ u \in V_1, v \in V_2}} |n_u - n_v| = (m-1)n|n-m+1|.$$
If m=n,
$M_o(K_{n-1,n}) = n(n-1)$.

□



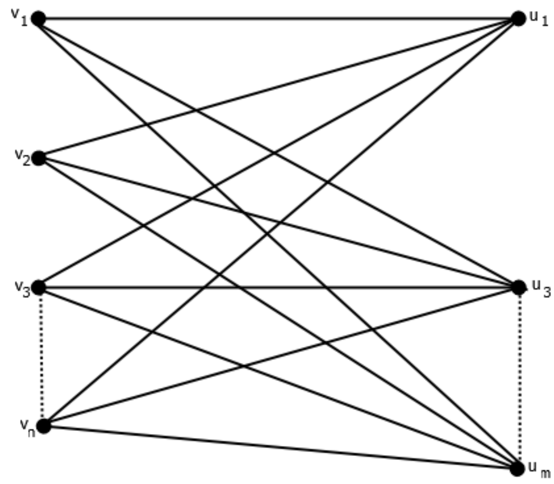


Figure 12: (a) The graph $K_{m,n}$, (b) The graph $K_{m,n} - \{v\}$

Example 2.6 *To find $K4,3 - \{e\}$ and $K_{4,3} - \{v\}$(Figure 13).*
We can partition vertex set of $K_{4,3}$ into $U = \{u_1, u_2, u_3, u_4\}$ and $V = \{v_1, v_2, v_3\}$. Deletion of an edge $e = u_1v_2$ from $K_{4,3}$, results in graph $K_{4,3} - \{e\}$. Let us partition vertex set of $K_{4,3} - \{e\}$ into $V_1 = \{u_1\}$, $V_2 = \{v_2\}$, $V_3 = \{u_2, u_3, u_4\}$ and $V_4 = \{v_1, v_3\}$
For each edge between vertex of V_1, say u and vertex of V_4 say v, the value
$|n_u - n_v| = |3 - (4 - 1)| = 0$
For each edge between vertex of V_2, say u and vertex of V_3 say v, the value
$|n_u - n_v| = |(4 - 1) - 3| = 0$
For each edge between vertex of V_3, say u and vertex of V_4 say v, the value
$|n_u - n_v| = |4 - 3| = 1$
Applying the definition of Mostar index we get,

$$\begin{aligned} M_o(K_{4,3} - \{e\}) &= \sum_{uv \in E(G)} |n_u - n_v| \\ &= \sum_{\substack{uv \in E(G) \\ u \in V_1, v \in V_4}} |n_u - n_v| + \sum_{\substack{uv \in E(G) \\ u \in V_2, v \in V_3}} |n_u - n_v| + \sum_{\substack{uv \in E(G) \\ u \in V_3, v \in V_4}} |n_u - n_v| \\ &= (3 - 1) \times 0 + (4 - 1) \times 0 + (4 \times 3 - 4 - 3 - 1) \times 1 = 4. \end{aligned}$$

To find $K4,3 - \{e\}$ and $K_{4,3} - \{v\}$. We can partition vertex set of $K_{4,3}$ into $U = \{u_1, u_2, u_3, u_4\}$ and $V = \{v_1, v_2, v_3\}$. Deletion of a vertex v_2 from $K_{4,3}$, results in graph $K_{4,3} - \{v_3\}$ which is isomorphic to $K_{4,2}$, if the vertex is removed from V. We can be partition the vertex set of $K_{4,2}$ into $V_1 = \{v_1, v_3\}$ and $V_2 = \{u_1, u_2, u_3, u_4\}$.
For each edge between vertex of V_1, say u and vertex of V_2 say v, the value $|n_u - n_v| = |4 - 3 + 1| = 2$.
Applying the definition of Mostar index we get,
$M_o(K_{4,2}) = \sum_{uv \in E(G)} |n_u - n_v| = \sum_{\substack{uv \in E(G) \\ u \in V_1, v \in V_2}} |n_u - n_v| = 4 \times 2 \times 2 = 16.$

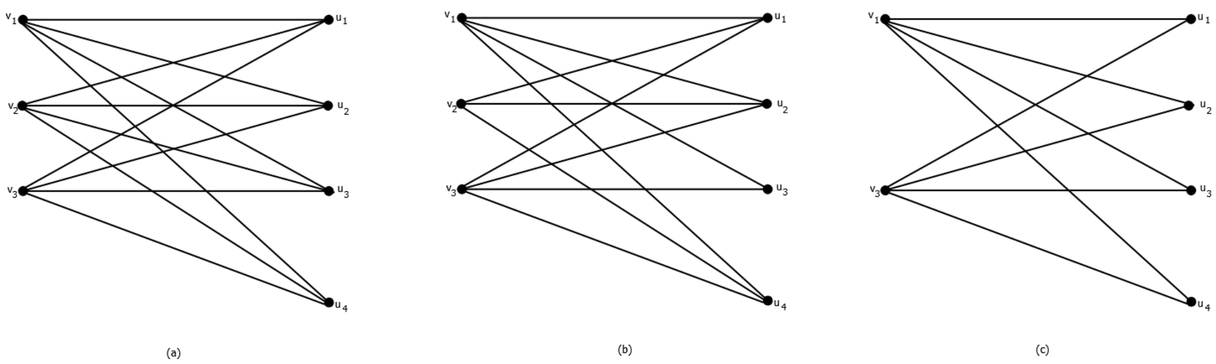


Figure 13: (a) The graph $K_{4,3}$, (b) The graph $K_{4,3} - \{e\}$, (c) The graph $K_{4,3} - \{v\}$

Observation 2.1 *Let C_n cycle graph and e be any edge of C_n. The Mostar index of $C_n - \{e\}$ is given by:*

$$M_o(C_n - \{e\}) = \begin{cases} \frac{n(n-2)}{2} & \text{if } n \text{ is even} \\ \frac{(n-1)^2}{2} & \text{if } n \text{ is odd} \end{cases}$$

Proof: Deletion of any edge e from the cycle graph C_n, results in a graph $C_n - \{e\}$ which is isomorphic to a path graph P_n. Since the Mostar index of a graph depends only on its structure, it follows that:

$$M_o(C_n - \{e\}) = M_o(P_n).$$

Applying the known result for the Mostar index of P_n in proposition 1.1 completes the proof. □

Observation 2.2 *Let C_n cycle graph and v be any vertex of C_n. The Mostar index of $C_n - \{v\}$ is given by:*

$$M_o(C_n - \{v\}) = \begin{cases} \frac{(n-1)(n-3)}{2} & \text{if } n \text{ is even} \\ \frac{(n-2)^2}{2} & \text{if } n \text{ is odd} \end{cases}$$

Proof: Deletion of any vertex v from the cycle graph C_n, results in a graph $C_n - \{v\}$ which is isomorphic to a path graph P_{n-1}. Since the Mostar index of a graph depends only on its structure, it follows that:

$$M_o(C_n - \{v\}) = M_o(P_{n-1}).$$

Applying the known result for the Mostar index of P_{n-1} in proposition 1.1 completes the proof. □

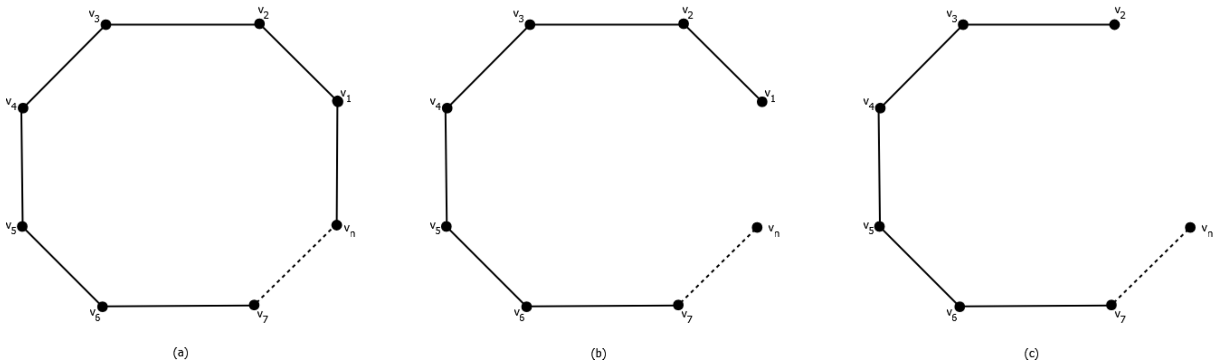


Figure 14: (a) The graph C_n, (b) The graph $C_n - \{e\}$, (c) The graph $C_n - \{v\}$

Observation 2.3 *Let K_n complete graph and e be any edge of K_n. The Mostar index of $K_n - \{e\}$ is given by:*

$$M_o(K_n - \{e\}) = 2n - 4.$$

Proof: Let us consider a complete graph K_n. Deletion of an edge $e = xy$ from the complete graph K_n, results in a graph $K_n - \{e\}$. Let us partition the vertex set of $K_n - \{e\}$ into $V_1 = \{x, y\}$ and $V_2 = \{v \in V(K_n)|\ v \text{ is not } x \text{ and } y\}$
For each edge between vertex of V_1, say u and vertex of V_2, say v, the value $|n_u - n_v| = 1$.
For each edge between vertices of V_2, say in between two distinct vertices u and v, the value $|n_u - n_v| = 0$.
Applying the definition of Mostar index we get,

$$M_o(K_n - \{e\}) = \sum_{uv \in E(G)} |n_u - n_v| = \sum_{\substack{uv \in E(G) \\ u,v \in V_2}} |n_u - n_v| + \sum_{\substack{uv \in E(G) \\ u \in V_1, v \in V_2}} |n_u - n_v| = 0 + 2(n-2) = 2n - 4$$

□

Observation 2.4 *Let K_n complete graph and v be any vertex of K_n. The Mostar index of $K_n - \{v\}$ is given by:*

$$M_o(K_n - \{v\}) = 0.$$

Proof: Let us consider a complete graph K_n. Deletion of any vertex v from the complete graph K_n, results in a graph $K_n - \{v\}$ which is isomorphic to a complete graph K_{n-1}. Since the Mostar index of a graph depends only on its structure, it follows that:

$$M_o(K_n - \{v\}) = M_o(K_{n-1}).$$

Applying the known result for the Mostar index of K_n in proposition 1.1 completes the proof. □

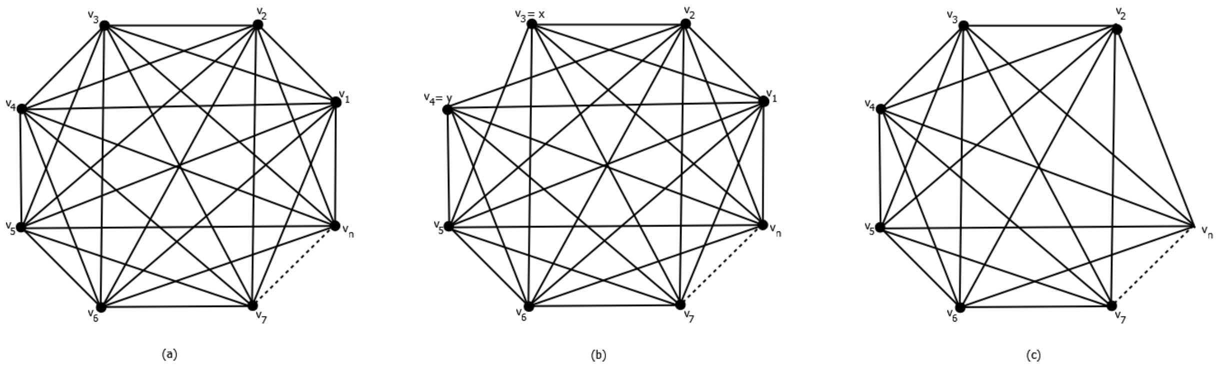


Figure 15: (a) The graph K_n, (b) The graph $K_n - \{e\}$, (c) The graph $K_n - \{v\}$

Observation 2.5 *Let S_n star graph and e be any edge of S_n. The Mostar index of $S_n - \{e\}$ is given by:*

$$M_o(S_n - \{e\}) = (n-2)(n-3).$$

Proof: Let us consider a star graph S_n. Deletion of any edge e from the star graph S_n, results in a graph $S_n - \{e\}$, which is isomorphic to a star graph S_{n-1} union a singleton vertex v of S_n. Since the Mostar index of a graph depends only on its structure, it follows that:

$$M_o(S_n - \{e\}) = M_o(S_{n-1} \cup \{v\}) = M_o(S_{n-1}) + M_o(\{v\}) = M_o(S_{n-1})$$

Applying the known result for the Mostar index of S_{n-1} in proposition 1.2 completes the proof. □

Observation 2.6 *Let S_n star graph and v be a vertex of S_n. The Mostar index of $S_n - \{v\}$ is given by:*

$$M_o(S_n - \{v\}) = \begin{cases} 0 & \textit{if } v \textit{ is central vertex} \\ (n-2)(n-3) & \textit{if } v \textit{ is leaf vertex} \end{cases}$$

Proof: Let us consider a star graph S_n. Deletion of a vertex v from the star graph S_n, results in a graph $S_n - \{v\}$.

If v is leaf vertex, the graph $S_n - \{v\}$ is isomorphic to a star graph S_{n-1}. If v is central vertex, the graph $S_n - \{v\}$ is isomorphic to totally disconnected graph with $n-1$ vertices. Since the Mostar index of a graph depends only on its structure, it follows that:

$$M_o(S_n - \{v\}) = \begin{cases} 0 & \text{if } v \text{ is central vertex} \\ M_o(S_{n-1}) & \text{if } v \text{ is leaf vertex} \end{cases}$$

Applying the known result for the Mostar index of S_{n-1} in proposition 1.2 completes the pf. □

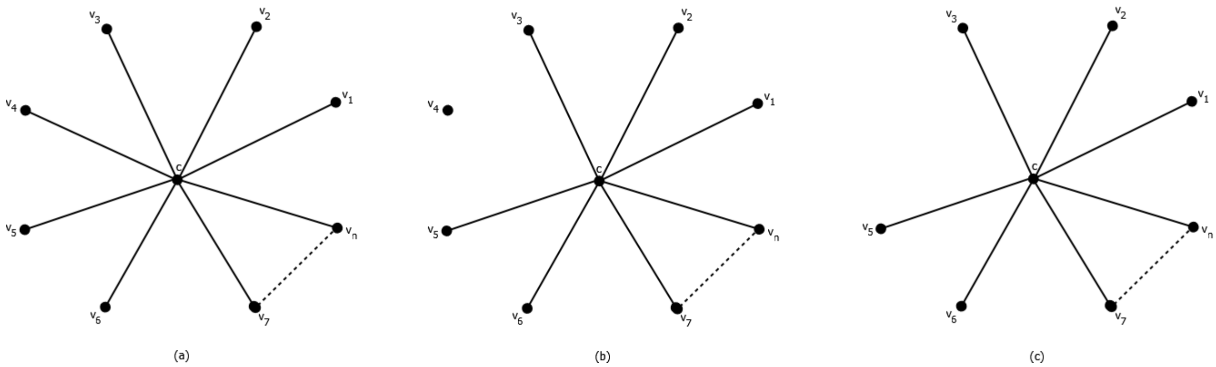


Figure 16: (a) The graph S_n, (b) The graph $S_n - \{e\}$, (c) The graph $S_n - \{v\}$

3. Chemical Significance of $M_o(G)$

In this section, we have conducted correlation analysis of $M_o(G)$ with π-electron energy of some hetero atoms.

3.1. Correlation analysis of $M_o(G)$ with π-electron energy of hetero atoms

We calculate $M_o(G)$ and tabulate in table 3.1 with a data set of total π-electron energy value of hetero atoms, derived from [21] . Further, we have found that $M_o(G)$ has a strong correlation with π electron energy of hetero atoms, with correlation coefficient $r = 0.95227$ and $r^2 = 0.95508$(Figure)

Molecule	Total π-electron energy	Mostar index
Butadiene perturbed at C_2	5.66	4
Acrolein like systems	5.76	4
1, 1-Dichloro-ethylene like systems	6.96	6
Glyoxal-like and 1, 2-Dichloro-ethylene systems	6.82	4
Aniline like systems	8.19	8
O-Phenylene-diamine like systems	12.21	20
m-Phenylene-diamine like systems	12.22	16
p-Phenylene-diamine like systems	12.21	20
Benzaldehyde like systems	11	22
Quinoline like systems	14.23	32
Iso-quinoline like systems	14.23	32
1-Naphthalein like systems	16.15	48
2-Naphthalein like systems	16.12	44
Iso-indole like systems	13.46	24
Indole like systems	13.59	24
Acridine like systems	20.56	64
Phenazine like systems	21.62	64
9, 10-Anthraquinoline like structures	24.23	80

Table 1: π-electron energy [21] , Mostar index of molecules containing hetero atoms.

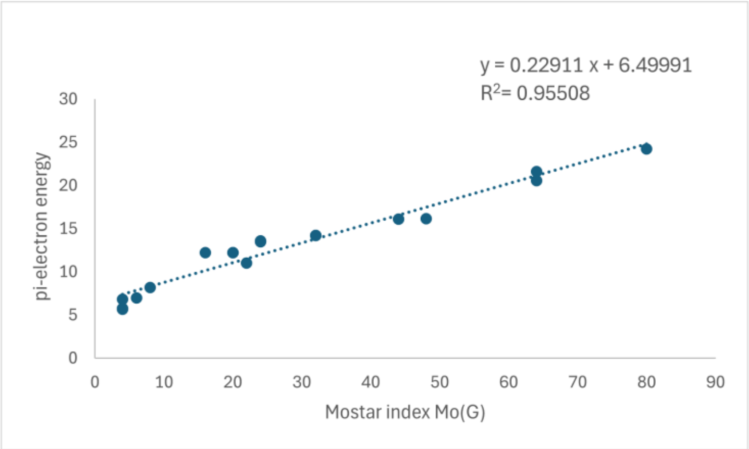


Figure 17: Correlation of $M_o(G)$ with the total π-electron energy of molecules

4. Conclusions

In this article, we have given the results for the Mostar index of generalized wheel. Also, we studied the effect of vertex or edge removal on Mostar index. This is done for generalized wheel graph, wheel graph, cycle, star graph, complete graph and complete bipartite graph. These can be applied to apply these outcomes to design and study how molecular properties changes when atoms or bonds are removed.

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B. Gautham Shenoy,
Department of Mathematics,
School of Applied Science, REVA University, Bengaluru,
India.
E-mail address: gautham.shenoy1996@gmail.com

and

B. Gautham Shenoy,
Department of Mathematics,
Poornaprajna College, Udupi, Karnataka,
India.
E-mail address: gautham.shenoy1996@gmail.com

and

Vishu Kumar M,
Department of Mathematics,
School of Applied Science, REVA University, Bengaluru,
India.
E-mail address: vishukumarm@reva.edu.in

and

Suhas,
Department of Mathematics,
Poornaprajna College, Udupi, Karnataka,
India.
E-mail address: suhaspoojary03@gmail.com