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Optimal Bounds for the Mostar Index of Chemical Trees

*Hafiza Sana Sattar
Faculty of Sciences,
The Superior University Lahore, Pakistan

Saima Mushtaq
Faculty of Sciences,
The Superior University Lahore, Pakistan

Zunera Shoukat
Faculty of Sciences,
The Superior University Lahore, Pakistan

*Corresponding Author
sanasattaramz@gmail.com

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Abstract. Topological indices are the numerical values of a chemical graph which are uniquely defined for that graph. Topological indices play a pivotal role in Quantitative Structure-Property/Activity Relationship in-vestigations, offering a robust framework for elucidating intricate corre-lations between molecular architecture and physicochemical properties. They used to predict the bio-chemical activities of graphs. Topological in-dices constitute a specialized domain within chemical graph theory, hav-ing garnered significant attention in scholarly literature. Essentially, topo-logical indices provide a quantitative representation of molecular graphs, which can be visualized through various mathematical constructs, such as polynomials, numerical sequences, matrices, or singular values. Mostar index is one of the last distance based topological index. In this article, we discuss the Mostar index for chemical trees. Also we compute some upper bounds of chemical trees using Mostar index.

AMS (MOS) Subject Classification Codes: 05C12, 05C90
Keywords: Topological indices, Mostar index, Chemical trees.

1. INTRODUCTION

Graph theory originate in 1736 when Euler tried to solve the problem of Königsberg bridge [1]. That problem is the hardest problem of that time. Euler tried his best to overcome the problem by converting the 7 bridges of Königsberg with lines and the lands with dots and represented it as a graph, but he didn't succeed his goal. The work of Euler started a new area of research. In the 19^{th} century, mathematicians called this field as graph theory and Euler became the father of graph theory.
The subdivision of mathematics that is developing and rapidly growing is graph theory. That contributes in many fields like electrical networks, chemistry, computer science and bioinformatics, etc., which is appreciable. Our research area is chemical graph theory. Mathematical chemistry's subset, chemical graph theory, provides a theoretical framework for representing and analyzing molecular structures, bridging the gap between chemistry and mathematics. It is combination of chemistry and graph theory. In it vertices of graph are atoms and edges represents bond between these atoms [5].
This research focuses on finite, undirected graphs, which consist of two distinct sets: a set of vertices (V) and a set of edges (E), collectively denoted as $G(V, E)$. Notably, each graph can be uniquely represented through various mathematical constructs, including numerical values, polynomials, matrices, relation tables, or topological indices. A topological index is a function Top : $\Sigma \to \mathbb{R}$, where $\mathbb{R}$ represent the real numbers and Σ represents simple graph which containing a characteristic that, if G_1 and G_2 are isomorphic then $\text{Top}(G_1) = \text{Top}(G_2)$ [9].
Topological indices constitute a specialized domain within chemical graph theory, having garnered significant attention in scholarly literature. Essentially, topological indices provide a quantitative representation of molecular graphs, which can be visualized through various mathematical constructs, such as polynomials, numerical sequences, matrices, or singular values. These indices remain invariant under graph isomorphism, ensuring uniqueness. Molecular graphs offer a concise and intuitive visualization of molecules and their compounds, facilitating deeper understanding and analysis.

Topological descriptors play a pivotal role in Quantitative Structure-Activity/Property Relationships (QSAR/QSPR) [14], as they facilitate the translation of complex molecular graphs into concise numerical values. In addition to topological descriptors, beyond topological descriptors, researchers also examine various other physicochemical attributes of carbon-based materials, encompassing structures such as nanotubes, hydrocarbons, nanocones, and fullerenes, to glean a deeper understanding of their properties and behavior. The unique characteristics of topological descriptors underpin their diverse applications in organic chemistry, biotechnology, and nanotechnology, enabling researchers to elucidate intricate relationships between molecular structure and properties.

Cheminformatics represents the convergence of mathematics, chemistry, and computer science, facilitating the analysis and interpretation of chemical data. A molecular descriptor is a quantitative representation of a chemical structure's topological features, encapsulated in a numerical value. These descriptors draw on a range of theoretical frameworks, including graph theory, information theory, and quantum mechanics. By leveraging molecular

descriptors, researchers can design and optimize chemical compounds for various applications in pharmaceuticals, analytical chemistry, and medicinal chemistry [16]. Figure 1, explains the tabular representation of molecular descriptor. The theory of topological in-

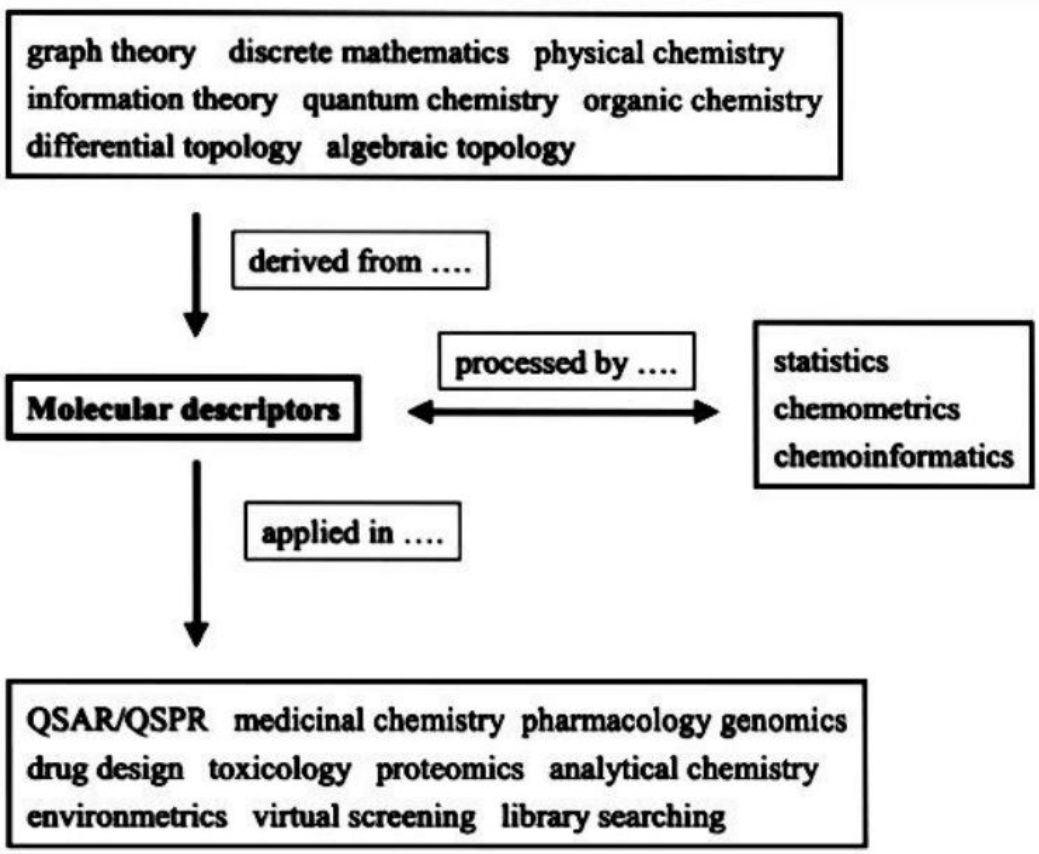

FIGURE 1. Tabular Representation of Molecular Descriptor

dices started in 1947 when Harry Wiener published his paper named as "Structural Determination of Paraffins Boiling Points" and the theory of topological indices started. Initially "path number" is the name of this index and denoted by W. After that, it is recalled as Wiener index [18]. Wiener index is written as,

$$W(G) = \sum_{(u,v)\subseteq V(G)} d(u,v),$$

where $d(u,v)$ denote the shortest-path distance between vertices u and v, where $u, v \in V(G)$. Due to the success of the Wiener index, numerous related indices have been developed based on it [15].

In case of trees, the Wiener index is defined as;

$$W(T) = \sum_{u,v \in E(T)} n_u n_v.$$

Szeged index was first studied by Gutman [7], in 1994. The Szeged index is the altered form of Wiener index. The Szeged index is defined as,

$$Sz(G) = \sum_{u,v \in E(G)} n_u n_v,$$

here n_u denote the number of vertices closer to u than to v, and let n_v be defined analogously for v. The Szeged index shares similarities with the Wiener index; however, it often provides more refined results. For instance, in trees, $W(T) = Sz(T)$ [8].

The Mostar index of a graph G is defined by summing the absolute differences between the partitions of vertices induced by each edge, i.e., $|n_u - n_v|$ for every edge $uv \in E(G)$. Previous studies include Arockiaraj et al. [4], who investigated the Mostar indices of carbon nanostructures; Hayat et al. [10], who derived extremal Mostar indices for cacti; and Hu et al. [11], who computed the Mostar index of chemical interconnection networks. Formally, the Mostar index is defined as:

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

For the convenience of our work we represent $|n_u - n_v|$ as $\phi(e)$.

2. Main Results

The main goal of this article is to compute the mostar index of chemical trees. Also we compute some of the upper bounds for the mostar index by using the diameter and path of chemical trees. The theory of trees was started by Kirchhoff [13], in 1847. Kirchhoff is physicist by profession, but he thought like a mathematician. He converted the whole electric network consisted on resistance and inductance etc., into its corresponding structure of points and lines. By the matrix tree theorem of the Kirchhoff, Kirchhoff provided the idea of number of spanning trees. In order to solve the simultaneous linear equations, he developed the theory of trees which gives the current in each circuit of an electric network. After that, Cayley extend his work in 1857 [6, 12]. A tree is said to be chemical tree if its maximum degree is 4. Zolfi et al. [20], computed the extremal properties of chemical trees for NK index. Zhang et al. [19] computed the topological indices for molecular graphs. For study more about topological indices, see [2, 3]. All the notations used in this paper are taken from the book of West [17].

2.1. **Results for Chemical Trees.**

Theorem 2.2. *For any graph G with n vertices its Mostar index is even.*

Proof. If G be any graph of n vertices then there arise two cases.
Case 1 If G is a graph with n number of vertices and n is even then G has $n-1$ number of edges which is odd. Here each edge gives even value of Mostar index because n is even. So, the sum of even numbers odd times will give the value of Mostar index even.
Case 2 If G is a graph with n number of vertices and n is odd then G has $n-1$ number of

edges which is even. Here each edge gives odd value of Mostar index because n is odd and we know that the sum of odd numbers even time is even. So, the sum of odd numbers even times will give the value of Mostar index even.
Which is required. □

Theorem 2.3. *For a graph G with n vertices, if $e \in E(G)$ of G is a leaf then $\phi(e)$ attain the value $(n-2)$.*

Proof. For a graph G with n vertices and $e = uv$ be any edge also e is a leaf of G then $n_u = 1$ because u is pendent vertex, so $n_v = n - 1$. Therefore we have,

$$\begin{aligned}
\phi(e) &= |n_u - n_v|,\\
\phi(e) &= |1 - (n-1)|,\\
\phi(e) &= |1 - n + 1|,\\
\phi(e) &= |-n + 2|,\\
\phi(e) &= |-(n-2)|,\\
\phi(e) &= n - 2,
\end{aligned}$$

which is required. □

Theorem 2.4. *Let T_n be a chemical tree with n number of vertices and $e = uv$ be an edge then maximum value that an edge can obtain is $n - 4$.*

Proof. Let T_n is chemical tree of order n and uv be an edge which is not a leaf then maximum value of n_u and n_v is 2 and $n - 2$ respectively. So by the definition of Mostar index we have,

$$\begin{aligned}
\phi(e) &= |n_u - n_v|,\\
\phi(e) &= |2 - (n-2)|,\\
\phi(e) &= |2 - n + 2|,\\
\phi(e) &= |-n + 4|,\\
\phi(e) &= |-(n-4)|,\\
\phi(e) &= n - 4,
\end{aligned}$$

which is required. □

Theorem 2.5. *For a chemical tree T_n, where l is the leaf and e is the edge of T_n then $Mo(e) \leq Mo(l)$.*

Proof. Let T_n be the chemical tree where l is the leaf of T_n and e be the edge of T_n then by using the Theorem 2.3 and 2.4 we can conclude that $Mo(e) \leq Mo(l)$ with the equality only holds if $e = l$. □

Theorem 2.6. *For a linear tree P_n. The Mostar index of P_n is $\lfloor \frac{(n-1)^2}{2} \rfloor$.*

Proof. The linear tree P_n is also known as path graph where all the vertices has degree 2 except end vertices which are leafs as shown in Figure 2. The Mostar index of linear tree is shown in Table 1, with the alternate second difference of 2 and 0.
There arises two cases.

FIGURE 2. Linear Tree

n	1	2	3	4	5	6	7	8
$Mo(P_n)$	0	0	2	4	8	12	18	24
Δ^2	-	2	0	2	0	2	0	-

TABLE 1. Second difference table for P_n

When n is even. Then

n	2	4	6	8
Mo	0	4	12	24
Δ^2	-	4	4	-

TABLE 2. Second difference n is even

$$\Rightarrow Mo(P_n) = \frac{n^2}{2} - n. \tag{2. 1}$$

When n is odd. Then

n	1	3	5	7
Mo	0	2	8	18
Δ^2	-	4	4	-

TABLE 3. Second difference n is odd

$$\Rightarrow Mo(P_n) = \frac{n^2 - 2n + 1}{2}, \tag{2. 2}$$

by combining the Mostar index of equations 2. 1 , 2. 2 , also Tables 2, 3 and using the floor function. We get,

$$\Rightarrow Mo(P_n) = \lfloor \frac{(n-1)^2}{2} \rfloor,$$

which is required. □

Theorem 2.7. *For a chemical tree T_n of order n with 3^{rd} leaf at second vertex. Then* $Mo(T_n) = \lfloor \frac{(n-1)^2+4}{2} \rfloor$.

Proof. For a chemical tree T_n of order n where $n \geq 4$. T_n has three number of leafs where 3^{rd} leaf is at second vertex as shown in Figure 3. The Mostar index of linear tree is shown in Table 4, with the alternate second difference of 0 and 2.
There arises two cases.

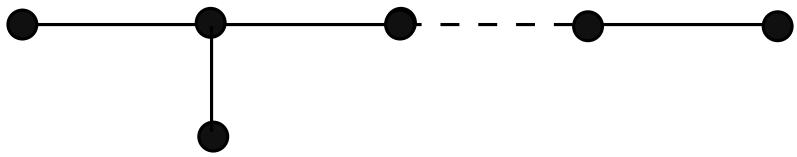

FIGURE 3. Chemical Tree with 3 leafs

n	4	5	6	7	8	9	10	11
$Mo(T_n)$	6	10	14	20	26	34	42	52
Δ^2	-	0	2	0	2	0	2	-

TABLE 4. Second difference table for T_n

When n is even. Then

n	4	6	8	10
Mo	6	14	26	42
Δ^2	-	4	4	-

TABLE 5. Second difference n is even

$$\Rightarrow Mo(T_n) = \frac{n^2 - 2n + 4}{2}. \tag{2. 3}$$

When n is odd. Then

$$\Rightarrow Mo(T_n) = \frac{n^2 - 2n + 5}{2}, \tag{2. 4}$$

by combining the Mostar index of equations 2. 3 , 2. 4 , also Tables 5, 6 and using the floor function. We get,

$$\Rightarrow Mo(T_n) = \lfloor \frac{(n-1)^2 + 4}{2} \rfloor,$$

n	5	7	9	11
Mo	10	20	34	52
Δ^2	-	4	4	-

TABLE 6. Second difference n is odd

which is required. □

Theorem 2.8. *For a chemical tree T_n with n vertices having maximum path $n-2$ with diameter d and 3^{rd} leaf at $\lceil \frac{d}{2} \rceil$, then its Mostar index is maximum which is $\lceil \frac{n^2-5}{2} \rceil$.*

Proof. Let T_n be chemical tree of order n, $n \geq 4$ with maximum path $n-2$ and having leaf at the $(\frac{n}{2})^{th}$ vertex in case of even and $(\frac{n+1}{2})^{th}$ vertex as shown if Figure 4. In case of odd then two edges will have the same value of Mostar index and contribute $2\phi(e_i)$ in the Mostar index.
In case of even the contribution of edges is,

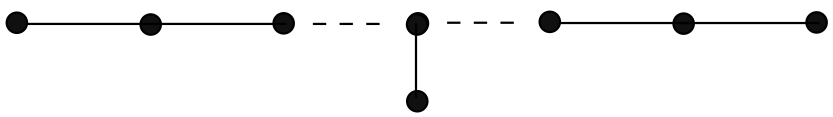

FIGURE 4. Tree with 3 Leafs

$$\begin{aligned} Mo(T_n) &= 3(n-2) + 2(n-4) + 2(n-6) + ... + 2(n-(n-2)), \\ Mo(T_n) &= \frac{n^2-4}{2}. \end{aligned}$$

In case of odd the contribution of edges is,

$$\begin{aligned} Mo(T_n) &= 3(n-2) + 2(n-4) + 2(n-6) + ... + (n-(n-1)), \\ Mo(T_n) &= \frac{n^2-5}{2}. \end{aligned}$$

By combining the Mostar index of both cases and using the ceiling function. We get, $Mo(T_n) = \lceil \frac{n^2-5}{2} \rceil$. □

Theorem 2.9. *For a chemical tree T_n with n vertices having maximum path $n-3$ with diameter d and 3^{rd}, 4^{th} leaf at $\lceil \frac{d}{2} \rceil$, then its Mostar index is maximum which is $\lfloor \frac{(n+1)^2-12}{2} \rfloor$.*

Proof. Let T_n be chemical tree of order n, $n \geq 5$ with maximum path $n-3$ and having the 3^{rd} and 4^{th} leaf at the $(\frac{n}{2})^{th}$ vertex as shown in Figure 5. In case of even and $(\frac{n-1}{2})^{th}$ vertex in case of odd then two edges will have the same value of Mostar index and contribute $2\phi(e_i)$ in the Mostar index.

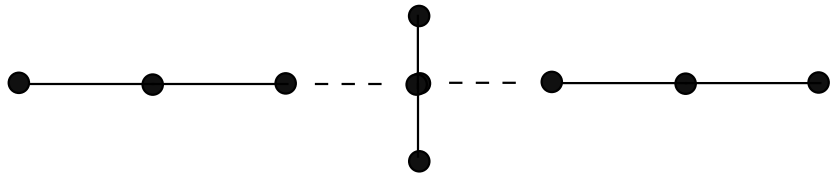

FIGURE 5. Tree with 4 Leafs

In case of even the contribution of edges is,

$$\begin{aligned} Mo(T_n) &= 4(n-2)+2(n-4)+2(n-6)+...+(n-(n-2)), \\ Mo(T_n) &= \frac{n^2+2n-12}{2}. \end{aligned}$$

In case of odd the contribution of edges is,

$$\begin{aligned} Mo(T_n) &= 4(n-2)+2(n-4)+2(n-6)+...+2(n-(n-3)), \\ Mo(T_n) &= \frac{n^2+2n-11}{2}. \end{aligned}$$

By combining the Mostar index of both cases and using the floor function. We get, $Mo(T_n) = \lfloor \frac{(n+1)^2-12}{2} \rfloor$. □

Theorem 2.10. *For a chemical tree T_n with n vertices having maximum path $n-4$. T_n has diameter d with 3^{rd}, 4^{th} leaf at $\lceil \frac{d}{2} \rceil$ and 5^{th} leaf at $\lceil \frac{d}{2}+1 \rceil$, then its Mostar index is maximum which is $\lceil \frac{(n+2)^2-29}{2} \rceil$.*

Proof. Let T_n be chemical tree of order n, $n \geq 7$ with maximum path $n-4$ and having the 3^{rd}, 4^{th} leaf at $\lceil \frac{d}{2} \rceil$ with 5^{th} leaf at $\lceil \frac{d}{2}+1 \rceil$ as shown in Figure 6. Then two edges will have the same value of Mostar index and contribute $2\phi(e_i)$ in the Mostar index.
In case of even the contribution of edges is,

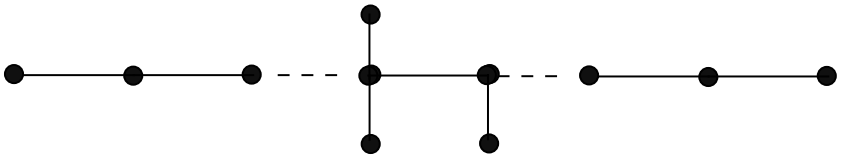

FIGURE 6. Tree with 5 Leafs

$$\begin{aligned} Mo(T_n) &= 5(n-2)+2(n-4)+2(n-6)+...+(n-(n-4))+(n-(n-2)), \\ Mo(T_n) &= \frac{n^2+4n-24}{2}. \end{aligned}$$

In case of odd the contribution of edges is,

$$\begin{aligned} Mo(T_n) &= 5(n-2)+2(n-4)+2(n-6)+...+(n-(n-1)), \\ Mo(T_n) &= \frac{n^2+4n-25}{2}. \end{aligned}$$

By combining the Mostar index of both cases and using the ceiling function. We get, $\lceil \frac{(n+2)^2-29}{2} \rceil$. □

Theorem 2.11. *For a chemical tree T_n with n vertices having maximum path $n-5$. T_n has diameter d with 3^{rd}, 4^{th} leaf at $\lceil \frac{d}{2} \rceil$ and 5^{th}, 6^{th} leaf at $\lceil \frac{d}{2}+1 \rceil$, then its Mostar index is maximum which is $\lfloor \frac{(n+3)^2-48}{2} \rfloor$.*

Proof. Let T_n be chemical tree of order n, $n \geq 8$ with maximum path $n-5$ and having the 3^{rd}, 4^{th} leaf at $\lceil \frac{d}{2} \rceil$ with 5^{th}, 6^{th} leaf at $\lceil \frac{d}{2}+1 \rceil$ as shown in Figure 7. Then two edges will have the same value of Mostar index and contribute $2\phi(e_i)$ in the Mostar index.
In case of even the contribution of edges is,

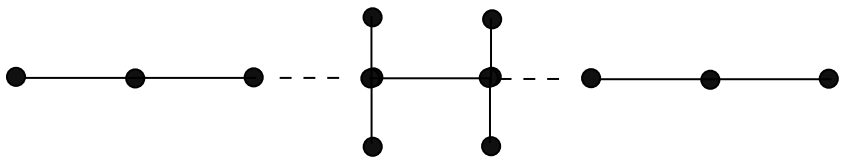

FIGURE 7. Tree with 6 Leafs

$$\begin{aligned} Mo(T_n) &= 6(n-2)+2(n-4)+2(n-6)+...+2(n-(n-4))+2(n-(n-2)), \\ Mo(T_n) &= \frac{n^2+6n-40}{2}. \end{aligned}$$

In case of odd the contribution of edges is,

$$\begin{aligned} Mo(T_n) &= 6(n-2)+2(n-4)+2(n-6)+...+(n-(n-1)), \\ Mo(T_n) &= \frac{n^2+6n-39}{2}. \end{aligned}$$

By combining the Mostar index of both cases and using the floor function. We get, $\lfloor \frac{(n+3)^2-48}{2} \rfloor$.
□

Theorem 2.12. *For a chemical tree T_n with n vertices having maximum path $n-6$. T_n has diameter d with 3^{rd}, 4^{th} leaf at $\lceil \frac{d}{2} \rceil$, 5^{th}, 6^{th} leaf at $\lceil \frac{d}{2}+1 \rceil$ and 7^{th} leaf at $\lceil \frac{d}{2}-1 \rceil$, then its Mostar index is maximum which is $\lfloor \frac{(n+4)^2-72}{2} \rfloor$.*

Proof. Let T_n be chemical tree of order n, $n \geq 10$ with maximum path $n-6$ and having the 3^{rd}, 4^{th} leaf at $\lceil \frac{d}{2} \rceil$ with 5^{th}, 6^{th} leaf at $\lceil \frac{d}{2}+1 \rceil$ and 7^{th} leaf at $\lceil \frac{d}{2}-1 \rceil$ as shown in Figure 8. Then two edges will have the same value of Mostar index and contribute $2\phi(e_i)$ in the Mostar index.
In case of even the contribution of edges is,

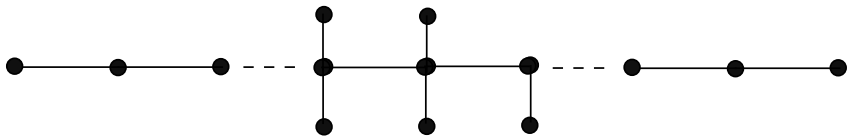

FIGURE 8. Tree with 7 Leafs

$$\begin{aligned} Mo(T_n) &= 7(n-2)+2(n-4)+2(n-6)+...+(n-(n-4))+(n-(n-2)), \\ Mo(T_n) &= \frac{n^2+8n-56}{2}. \end{aligned}$$

In case of odd the contribution of edges is,

$$\begin{aligned} Mo(T_n) &= 7(n-2)+2(n-4)+2(n-6)+...+(n-(n-1)), \\ Mo(T_n) &= \frac{n^2+8n-57}{2}. \end{aligned}$$

By combining the Mostar index of both cases and using the floor function. We get, $\lfloor \frac{(n+4)^2-72}{2} \rfloor$.
□

Theorem 2.13. *For a chemical tree T_n with n vertices having maximum path $n-7$. T_n has diameter d with 3^{rd}, 4^{th} leaf at $\lceil \frac{d}{2} \rceil$, 5^{th}, 6^{th} leaf at $\lceil \frac{d}{2}+1 \rceil$ and 7^{th},8^{th} leaf at $\lceil \frac{d}{2}-1 \rceil$, then its Mostar index is maximum which is $\lfloor \frac{(n+5)^2-100}{2} \rfloor$.*

Proof. Let T_n be chemical tree of order n, $n \geq 10$ with maximum path $n-6$ and having the 3^{rd}, 4^{th} leaf at $\lceil \frac{d}{2} \rceil$ with 5^{th}, 6^{th} leaf at $\lceil \frac{d}{2}+1 \rceil$ and 7^{th},8^{th} leaf at $\lceil \frac{d}{2}-1 \rceil$ as shown in Figure 9. Then two edges will have the same value of Mostar index and contribute $2\phi(e_i)$ in the Mostar index.
In case of even the contribution of edges is,

$$\begin{aligned} Mo(T_n) &= 8(n-2)+2(n-4)+2(n-6)+...+(n-(n-4))+(n-(n-2)), \\ Mo(T_n) &= \frac{n^2+10n-76}{2}. \end{aligned}$$

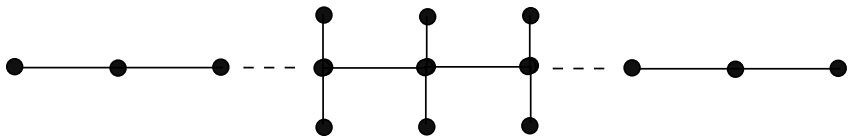

FIGURE 9. Tree with 8 Leafs

In case of odd the contribution of edges is,

$$\begin{aligned} Mo(T_n) &= 7(n-2)+2(n-4)+2(n-6)+...+2(n-(n-3)), \\ Mo(T_n) &= \frac{n^2+10n-75}{2}. \end{aligned}$$

By combining the Mostar index of both cases and using the floor function. We get, $\lfloor \frac{(n+5)^2-100}{2} \rfloor$. □

n	Linear Tree	Tree with 3 Leafs	Tree with 4 Leafs	Tree with 5 Leafs	Tree with 6 Leafs	Tree with 7 Leafs	Tree with 8 Leafs
10	40	48	54	58	60	62	62
11	50	58	66	70	74	76	78
12	60	70	78	84	88	92	94
13	72	82	92	98	104	108	112
14	84	96	106	114	120	126	130
15	98	110	122	130	138	144	150
16	112	126	138	148	156	164	170
17	128	142	156	166	176	184	192
18	144	160	174	186	196	206	214
19	162	178	194	206	218	228	238

TABLE 7. Comparison Table

For the comparison of Mostar index of different chemical trees, we computed it for different values of n. As we can see from Table 7 for each increasing value of n the value of mostar index increases for each case of chemical tree.

The above Figure 10 shows the comparison of the values of the mostar index for different values of n taken from the Table 7 and we can clearly say that by each addition of leaf in a chemical tree increases the value of mostar index.

3. CONFLICT OF INTEREST

The authors declare no conflict of interest.

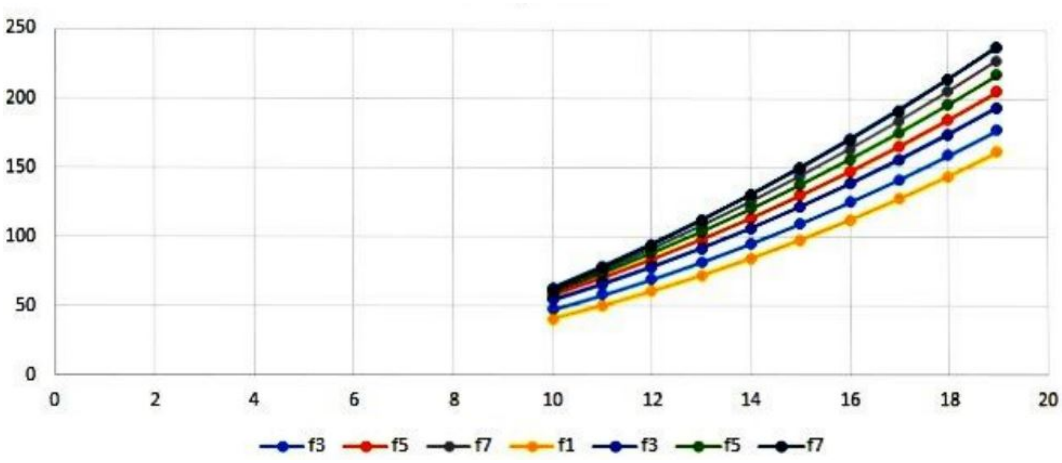

FIGURE 10. Graph Comparison

4. CONCLUSION

In this study, we have investigated several key properties of the Mostar index and derived closed-form expressions for its computation in chemical trees. Additionally, we established upper bounds for the Mostar index in specific cases by considering structural parameters such as diameter and path length. Our findings contribute to a deeper understanding of the Mostar indexs behavior in chemical graphs, which is essential for applications in quantitative structure-activity relationships (QSAR) and molecular descriptor analysis.

The results obtained have significant implications beyond theoretical chemistry, particularly in fields such as data science, where graph-based indices are used for pattern recognition and predictive modeling; electrical circuit design, where topological indices help optimize network stability and efficiency; and computer science, particularly in algorithm design for graph traversal and network analysis. Future research could explore the Mostar index in more complex graph structures, dynamic networks, or its potential in machine learning for molecular property prediction.

By refining the mathematical bounds and extending the applicability of the Mostar index, this work opens new avenues for interdisciplinary research, bridging graph theory with practical computational and engineering challenges.

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