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On The Metric Dimension for The Line Graphs of Hammer and Triangular Benzene Structures

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Abstract The metric dimension of a chemical graph is a fundamental parameter in the study of molecular structures and their properties. This metric dimension is a numerical measure of the smallest set of atoms required to uniquely determine the location of all other atoms within the molecule. In this abstract, we explore the concept of metric dimension in chemical graphs, discussing its theoretical foundations and its applications in various fields such as navigation, network theory, drug design, optimization, pattern recognition, and other related fields computational chemistry, and material science. Understanding the metric dimension of chemical graphs enables the identification of crucial atoms or bonds that significantly impact the properties and behavior of molecules, aiding in the design of more effective drugs, catalysts, and materials. Finding the metric dimension of any given graph poses a computational challenge classified within the NP-complete problem category. A group of nodes, denoted as T, is regarded as a locating set if, every pair of nodes p and q within the graph G, there is a minimum of one node w in W such a way that the separation between p and w is not the same as the separation between q and w. The G's metric dimension is represented by $dim(G)$ and corresponds to the minimum size of a locating set for G. The primary objective of this effort is to establish the proof that, for $n \geq 2$, the metric dimensions of the line network for the Hammer and triangular benzene structures are 2 and 3, respectively. We also established the existence of a constant metric dimension for this class of line graphs, which includes Hammer and triangular benzene structures.

Keywords Metric Basis, Metric Dimension, Hammer Graph, Triangular Benzenoid Structure

1 Introduction

To deal with a chemical complex's chemical structure, chemists need a mathematical representation of that compound. A group of chosen atoms in a chemical structure were mathematically represented in a way that supplied unique representations to unique atoms in the structure. The vertices of the chemical structure which mention the element atom, and the edges which show the different kinds of bonds, can be used to define it. Thus, a graph-theoretic study of this concept produces representations for every vertex in a structure that is distinct from one another with respect to particular atoms in that structure.

Slater [1] first presented the idea of a locating set in 1975, referring to it as the lowest cardinality of a resolving set of a graph resolving number. Sonar or loran stations were assigned to members of the metric base set. After Slater's concepts, Metric generators were described as resolving sets in 1976 by Harary and Melter [2], who expanded the idea of metric dimension. Metric dimension is used in many different domains, including communications [3], Protocols for geographical routing [4], navigating a robot [5], connected joints in networks, and chemistry [6], among others. Metric dimension theory is frequently applied to resolve many challenging issues because of its huge range of applications. More details about the resolving parameters in certain chemical structures are found in [7 - 9].

Indra et al. [10] investigated the honeycomb network's minimal metric dimension which is 3 in 2008. Various groups of graphs have been extensively studied to determine their metric dimension, including the graphs for Johnson and Kneser graphs and Grassmann graph by Bailey et al. [11, 12]. Fehr et al. [13] studied Cayley digraphs and Cartesian products of graphs by Caceres et al. [14]. In 2014, Siddiqui et al. [15] investigated the metric dimension of infinite families of graphs (including wheels), and Kratica et al. [16] studied the convex polytope metric dimension problem. Imran et al. [17] investigated the metric dimensions of convex polytopes obtained using graphs related to wheels. Imran et al. [18] investigated the Cayley graph's metric dimension for several finite graphs, while Ahmad et al. [19] studied the resolving parameters for benzenoid Hammer graphs. Additionally, Xiujun et al. [20] explored the metric dimension of Aztec diamond networks and honeycomb networks with one subdivision. Veninstine et al. [21] investigated the tensor product of two graphs and the coloring of similar paths with wheel and helm, cycle with sunlet, and closed helm graphs, and then structured their nature. Kupan et al. [22] studied double duplication of special classes of cycle-related graph.

In this paper, we demonstrated the metric dimension for the line graph of the Hammer, and the triangular structure is the same compared with Ahmad et al. [18,19] results.

2 Preliminaries

The metric dimensions of a line network made up of a few benzenoid structures are determined in this work. The remaining portion of the paper is divided into the following sections: Section 2 covers background material and basic concepts, and Sections 3 and 4 present the findings of the main results. The concluding observations are found in Section 5.

In this study, a unidirectional, finite, connected, and simple graph is taken into consideration, Let $G = (V, E)$ together G has a set of nodes called V, and lines called E. The distance between any two vertices is separated from one another by the shortest $u - v$ path's length, which is the same as the total of their edges. A resolving or locating set W is a finite subset $W \in V(G)$ of the node set G. When each pair $p, q \in V(G)$, a vertex emerges there $w \in W$ so that p to w's shortest path's length differs from q to w's. Alternatively put, we say $r(p \setminus w) \neq r(q \setminus w)$, where $r(p \setminus W)$ is an accurate depiction of a node $p \in V$ with regard to of W, as described $r(p \setminus W) = (d(p, w_1), d(p, w_2), d(p, w_3), \ldots, d(p, w_k))$. The cardinality of a basis of G, which is a minimal resolving or locating set, is known as the metric dimension of G and is denoted by $dim(G)$.

Definition 2.1. *A network G is represented by the line network $L(G)$ that represents the lines of a given graph as nodes and two of its nodes of the line network $L(G)$ are adjacent if and only if their corresponding lines in the given graph G share a common node. Figure 1 illustrates the network G and its corresponding line network $L(G)$.*

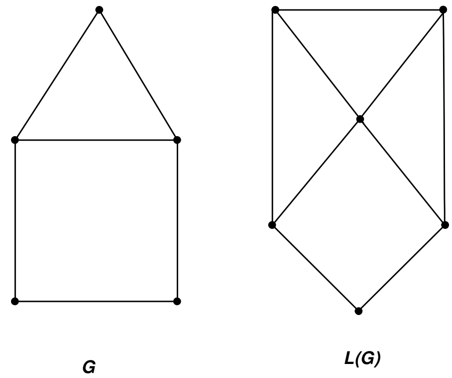

Figure 1. A network G and its corresponding line network $L(G)$.

Theorem 2.1. *[5] Let $\{l, m\} \subset V(G)$ be a metric basis of G and let $G = (V, E)$ be a finite, simple graph with metric dimension 2. Consequently, the following claims are accurate.*

(i) *There exists one particular shortest path, denoted as P, between vertices l and m.*

(ii) *The maximum degree of vertices l and m is 3.*

(iii) *On the path P, each vertex can have a degree of at most 5.*

Theorem 2.2. *[5] Let G be a connected, simple, and finite network with n vertices where $n \geq 2$. The following claims are accurate.*

(i) *G is an n - vertex path if and only if the metric dimension of the path is* 1.

(ii) *G is a complete graph K_n if and only if G's $n - 1$ metric dimension.*

3 Line graph of Hammer benzenoid structure

The Hammer graph is used in chemical graph theory to model molecular structures. In particular, it is used to model the molecular structure of adamantane, which is a highly symmetrical hydrocarbon molecule. The Hammer structure represents the central tetrahedral carbon atom in adamantane, which is connected to four other carbon atoms by single bonds. The line graph of the Hammer benzenoid graph's metric dimension is obtained in this section. The subsequent findings are required to support the primary findings.

The benzenoid hydrocarbon family includes the Hammer structure, which is essentially a benzenoid structure. Hammer benzenoid structure consists of $n + 8$ hexagons in a systematic way. An n dimensional Hammer benzenoid structure H_n and its line graph $L(H_n)$ are depicted in Figures 2 and 3. According to the following theorem, we establish the metric dimension of the line network by utilizing the Hammer benzenoid structure.

Theorem 3.1. *The line graph of the benzene Hammer network H_n has a metric dimension 2, $n \geq 1$.*

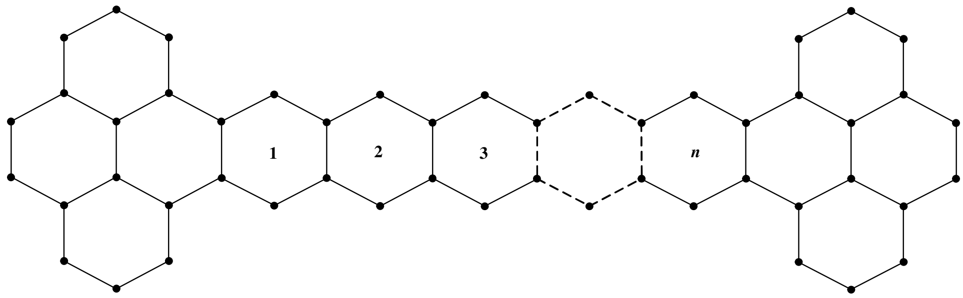

Figure 2. Hammer graph of dimension n

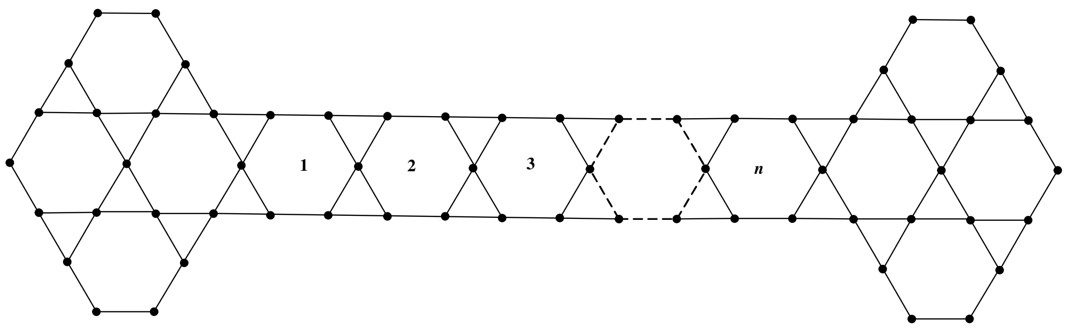

Figure 3. The line graph of Hammer graph of dimension n

Proof. Since the left and right hexagonal contains only 19 vertices in $L(H_n)$ and the bridge contains $5n-1$ vertices in $L(H_n)$. Label the left and right hexagonal as $l_1, l_2, \ldots, l_{19}$ starting with the top of the left most vertex and $r_1, r_2, \ldots, r_{19}$ starting with the top of the right most vertex respectively. Since the bridge contains three layers, say the top, centre, and bottom, and label them as $t_1, t_2, \ldots, t_{2n}$; $m_1, m_2, \ldots, m_{n-1}$ and $b_1, b_2, \ldots, b_{2n}$ respectively. Figure 4 provides the labeling of $L(H_n)$.

Since the graph is not a path, then according to Theorem 2.2, $dim(L(G)) > 1$. In order to prove the equality, consider $W = \{l_1, r_1\} \in V(L(H_n))$. For $k = 1, 2, 3, \ldots, 19$, the representation of each vertex in the left hexagonal of $L(H_n)$ with respect to W is as follows.

$$r(l_k|W) = \begin{cases} (k-1, 2n+7) & \text{if } 1 \leq k \leq 3 \\ (k-1, 2n+8) & \text{if } 4 \leq k \leq 7 \\ (k-2, 2n+7) & \text{if } k = 8 \\ (k-4, 2n+6) & \text{if } k = 9 \\ (15-k, 2n+15-k) & \text{if } k = 10, 11 \\ (15-k, 2n+k-8) & \text{if } 12 \leq k \leq 14 \\ (k-13, 2n+21-k) & \text{if } k = 15, 16 \\ (k-14, 2n+6) & \text{if } k = 17 \\ (4, 2n+25-k) & \text{if } k = 18, 19. \end{cases}$$

We can represent each vertex on the top of the bridge of $L(H_n)$ with respect to W for $k = 1, 2, 3, \ldots, 2n$ as $r(t_k|W) = (k+3, 2n+4-k)$.

For $k = 1, 2, 3, \ldots, n-1$, the representation of each vertex in the middle of the bridge of $L(H_n)$ with respect to W can be written as $r(m_k|W) = (2k+4, 2(n+2-k))$.

For $k = 1, 2, 3, \ldots, 2n$ the representation of each vertex in the bottom of the bridge of $L(H_n)$ with respect to W as $r(b_k|W) = (k+4, 2n+5-k)$.

For $k = 1, 2, 3, \ldots, 19$ the representation of each vertex in the right hexagonal of $L(H_n)$ with respect to W can be written as follows.

$$r(r_k|W) = \begin{cases} (2n+7, k-1) & \text{if } 1 \leq k \leq 3 \\ (2n+8, k-1) & \text{if } 4 \leq k \leq 7 \\ (2n+7, k-2) & \text{if } k = 8 \\ (2n+6, k-4) & \text{if } k = 9 \\ (2n+15-k, 15-k) & \text{if } k = 10, 11 \\ (2n+k-8, 15-k) & \text{if } 12 \leq k \leq 14 \\ (2n+21-k, k-13) & \text{if } k = 15, 16 \\ (2n+6, k-14) & \text{if } k = 17 \\ (2n+25-k, 4) & \text{if } k = 18, 19. \end{cases}$$

From the aforementioned depiction of each vertex in relation to W, we get, $r(a|W) \neq r(b|W)$, for any $a, b \in V(L(H_n))$. Hence the proof. □

4 Metric dimension of the line network of triangular benzene

Triangular benzene is highly helpful in synthesizing aromatic compounds using the benzene molecule. The

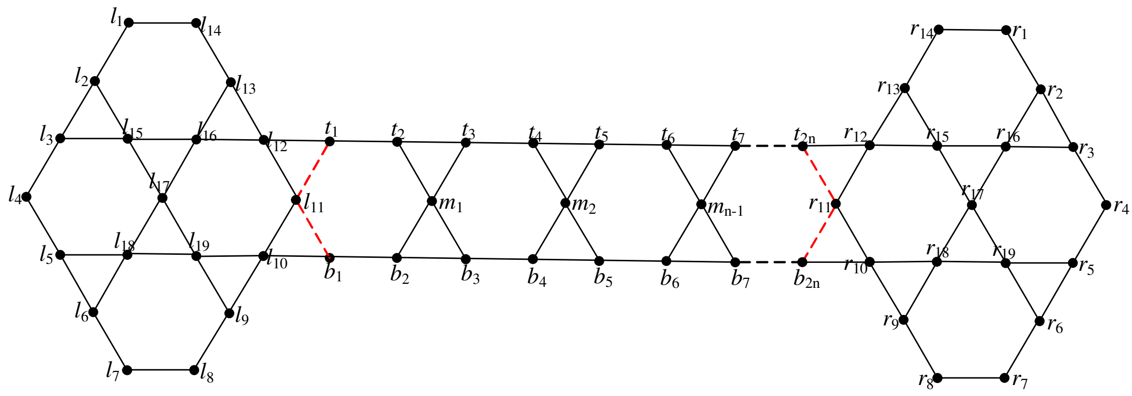

Figure 4. Labeling of the line graph of Hammer graph with dimension n

triangular benzenoids, denoted by $T(n)$, are a family of benzenoid molecular graphs that can be seen as a generalization of the benzene molecule C_6H_6. In triangular benzenoids, the benzene rings have a triangular shape. Hexagons are stacked in rows in a triangular benzenoid, and one hexagon grows in each row. For more structural analysis refer to [23]. We use T_n and $L(T_n)$ to denote the n - dimensional triangular benzenoid and its corresponding line graph, respectively. For example, Figure 5 shows a triangular benzenoid and its line graph of dimension 4.

The metric dimension of the line network of the triangular benzenoid structure is determined in the following theorem.

Theorem 4.1. *If G is a triangular benzenoid with dimension $n \geq 2$, then the metric dimension of its line graph $L(G)$ is greater than* 2.

Proof. Since $M_{l,m}$ denotes the vertex in the l^{th} level and m^{th} position from top to bottom and left to right respectively, $1 \leq l \leq 2n+1$, $1 \leq m \leq 2n$. For illustration, the labeling of $L(T_n)$ is shown in Figure 6.

We will prove this result by contradiction. Suppose that $dim(L(G)) = 2$. Let $A = \{x|deg_{L(G)}(x) = 2\}$ and $B = \{x|deg_{L(G)}(x) = 3\}$. The following cases are present after that.

Case 1: Let $x, y \in A$, next, we have the subsequent sub cases.

Subcase 1a: Consider $W = \{x, y\} = \{M_{1,1}, M_{1,2}\}$ is a $L(G)$ locating set then $r(M_{2n+1,2n-1}|W) = r(M_{2n+1,2n}|W)$. It would eliminate the resolving property.

Subcase 1b; Consider $W = \{x, y\} = \{M_{1,1}, M_{2n,1}\}$ is a $L(G)$ locating set then $r(M_{2n,n}|W) = r(M_{2n-1,2n-1}|W)$, and it would eliminate the resolving property.

Subcase 1c; Consider $W = \{x, y\} = \{M_{1,1}, M_{2n+1,1}\}$ is a $L(G)$ locating set then $r(M_{2n-1,2}|W) = r(M_{2n-1,3}|W)$. It would destroy the resolving property.

Subcase 1d: Consider $T = \{x, y\} = \{M_{1,1}, M_{2n+1,2n}\}$ is a $L(G)$ locating set then $r(M_{2n+1,2n-1}|T) = r(M_{2n,n+1}|T)$, and it would eliminate the resolving property.

Subcase 1e: Consider $W = \{x, y\} = \{M_{1,1}, M_{2n,n+1}\}$ is a $L(G)$ locating set then $r(M_{3,3}|W) = r(M_{4,2}|W)$. It would destroy the resolving property.

By the nature of the rotational symmetric, we prove the remaining subcases.

Case 2: Let $x \in A$ an $y \in B$, next, we have the subsequent sub cases.

Subcase 2a: Consider $W = \{x, y\} = \{M_{1,1}, M_{p,1}\}$, $2 \leq p \leq 2n-1$ is a $L(G)$ locating set then $r(M_{2n+1,3}|W) = r(M_{2n+1,4}|W)$. It would eliminate the resolving property.

Subcase 2b: Consider $W = \{x, y\} = \{M_{1,1}, M_{2n+1,p}\}$, $2 \leq p \leq 2n-1$ is a $L(G)$ metric basis then $r(M_{2n-1,2}|W) = r(M_{2n-1,3}|W)$. It would eliminate the resolving property.

Subcase 2c: Consider $W = \{x, y\} = \{M_{1,1}, M_{2p-2,p}\}$, $2 \leq p \leq n$ is a $L(G)$ metric basis then $r(M_{2n-1,p}|W) = r(M_{2n+1,p+2}|W)$, and it would eliminate the resolving property.

Subcase 2d: Consider $W = \{x, y\} = \{M_{1,1}, M_{2p-1,2p}\}$, $3 \leq p \leq n$ is a $L(G)$ metric basis then $r(M_{2n+1,p}|W) = r(M_{2n+1,p+1}|W)$. It would destroy the resolving property.

By the nature of the rotational symmetry, we prove the remaining possibilities.

Case 3: Let $x, y \in B$ then we have the following subcases.

Subcase 3a Consider $W = \{x, y\} = \{M_{2,1}, M_{p,1}\}$, $3 \leq p \leq 2n-3$ is a $L(G)$ locating set then $r(M_{2n+1,3}|W) = r(M_{2n+1,4}|W)$.

Consider $W = \{x, y\} = \{M_{2,1}, M_{p,1}\}$, $2n-2 \leq p \leq 2n-1$ is a $L(G)$ metric basis then $r(M_{2n+1,2}|W) = r(M_{2n+1,3}|W)$. It would eliminate the resolving property.

Subcase 3b: Consider $W = \{x, y\} = \{M_{2,1}, M_{2n+1,p}\}$, $2 \leq p \leq 2n-1$ is a $L(G)$ metric basis then $r(M_{2n+1,p \text{ or } p-1}|W) = r(M_{2n+1,p+1 \text{ or } p}|W)$. It would eliminate the resolving property.

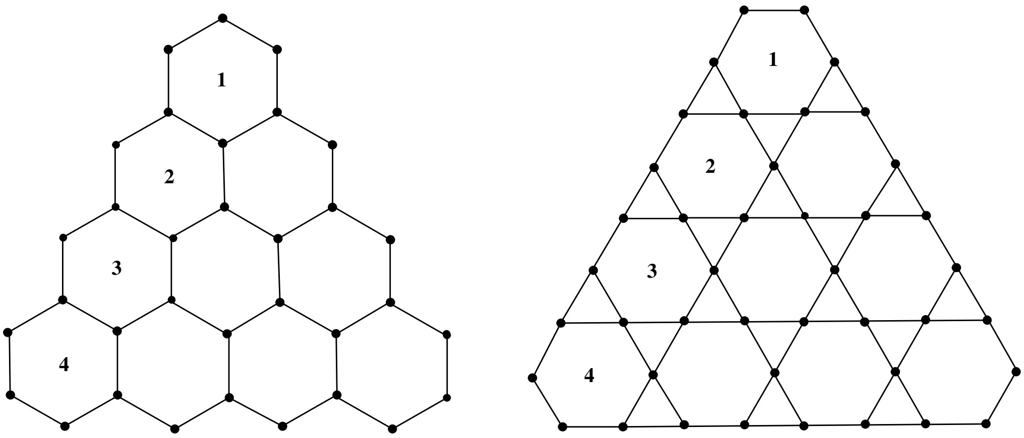

Figure 5. Triangular benzenoid and its corresponding line graph of dimension 4

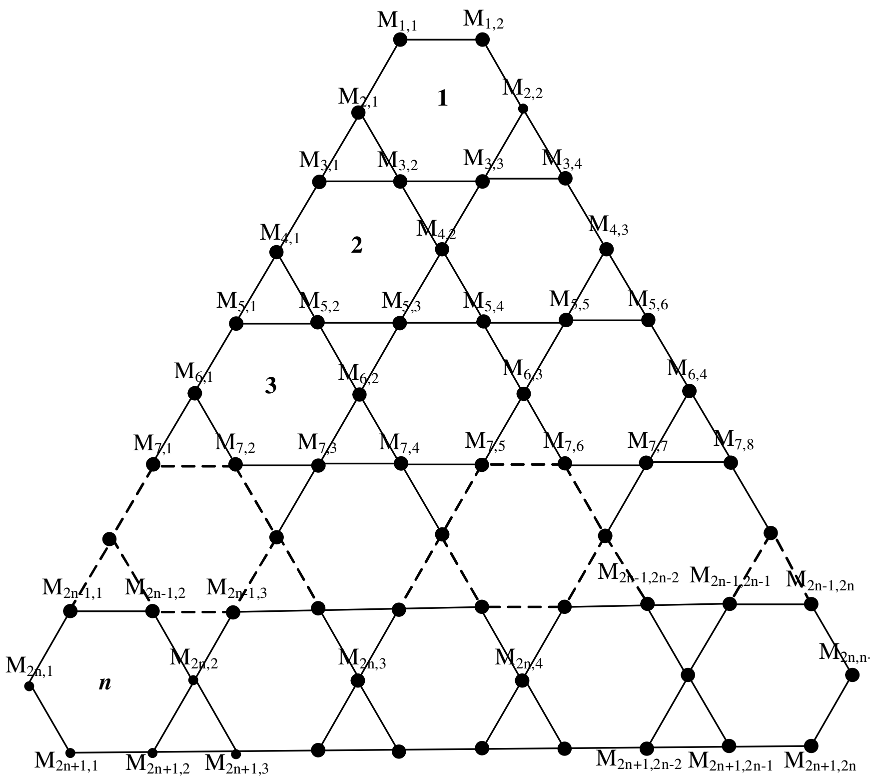

Figure 6. Labeling of the line graph of triangular benzene of dimension n

Subcase 3c: Consider $W = \{x, y\} = \{M_{2,1}, M_{2p-2,p}\}$, $2 \leq p \leq n-2$, is a $L(G)$ metric basis then $r(M_{2n+1,p+1}|W) = r(M_{2n+1,p+2}|W)$.

Consider $W = \{x, y\} = \{M_{2,1}, M_{2n-2,n}\}$, is a $L(G)$ metric basis then $r(M_{2n+1,p}|W) = r(M_{2n+1,p+1}|W)$. It will destroy the resolving property.

Subcase 3d: Consider $W = \{x, y\} = \{M_{2,1}, M_{2p-1,2p}\}$, $3 \leq p \leq n-1$, is a $L(G)$ locating set then $r(M_{2n+1,p}|W) = r(M_{2n+1,p+1}|W)$.

Consider $W = \{x, y\} = \{M_{2,1}, M_{2n-1,2n}\}$, is a $L(G)$ metric basis then $r(M_{2n+1,p-1}|W) = r(M_{2n+1,p}|W)$. It would eliminate the resolving property.

In a similar argument, we prove other possibilities. Hence, the triangular benzenoid structure's line graph has a metric dimension greater than 2. □

Theorem 4.2. *The metric dimension for the line graph of triangular benzene structure T_n is 3, for $n > 2$.*

Proof. Since we have $dim(L(G)) \geq 3$ according to Theorem 4.1. In order to prove the equality, consider $W = \{M_{1,1}, M_{2n+1,1}, M_{2n+1,2n}\}$ is metric basis for $L(G)$. To show W is a metric basis, it is enough to show all the horizontal l^{th} level and diagonal m^{th} level Vertices are represented differently with respect to W. The representation of each vertex in horizontal and diagonal vertices is as follows.

For $2 \leq l \leq 2n$ the representation of $M_{l,1}$ of $L(G)$ as

$$r(M_{l,1}|W) = (l-1, 2n-l+1, 2n).$$

For l is odd and $1 \leq l \leq 2n+1$, the representation of $M_{l,2}$ of $L(G)$ as

$$r(M_{l,2}|W) = \begin{cases} (1, 2n+1, 2n), & l = 1 \\ (l-1, 2n-l+2, 2n-1), & 3 \leq l \leq 2n-1. \end{cases}$$

For m is odd and $3 \leq m \leq 2n-1$, $m-1 \leq l \leq 2n+1$ the representation of $M_{l,m}$ of $L(G)$ as

$$r(M_{l,m}|W) = \begin{cases} (l, 2n-l+m-1, 2n-m+2), & l = m-1, m \\ (l-1, 2n-l+m-1, 2n-m+1), & m+1 \leq l \leq 2n+1. \end{cases}$$

For m is even, l is odd and $4 \leq m \leq 2n$, $m-1 \leq l \leq 2n+1$ the representation of $M_{l,m}$ of $L(G)$ as

$$r(M_{l,m}|W) = \begin{cases} (l, 2n, 2n-m+2), & l = m-1, \\ (l-1, 2n-l+m-1, 2n-m+1), & m+1 \leq l \leq 2n+1. \end{cases}$$

For $m = 2n+1$, $l = 2n$ then representation of $M_{l,m}$ of $L(G)$ as

$$r(M_{l,m}|W = (2n, 2n, 1).$$

From the above representation of each vertex of $L(G)$ with respect to W, we get, $r(p|W) \neq r(q|W)$, for any $p, q \in V(L(G))$. Hence the proof. □

5 Conclusions

In the present investigation, we determined the metric dimension for the line graph of Hammer and triangular benzene structures. For the line graph of the Hammer structure, the metric dimension is 2, meaning that at least two locating vertices are required to uniquely identify all vertices in the graph. For the triangular benzene structure, the metric dimension is 3, indicating that at least three locating vertices are needed to identify all vertices in the graph. Studies are carried out to establish the metric dimension of various line graphs of benzenoid structures.

Acknowledgement

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