ABSTRACT Due to its superlative physical qualities and its beauty, the diamond is a renowned structure. While the green-colored perimantanes diamondoid is one of a higher diamond structure. Motivated by the structure’s applications and usage, we look into the metric-based parameters of this structure. In this draft, we have discussed metric dimension and their generalizations for the generalized perimantanes diamondoid structure and proved that each parameter depends on the copies of original or base perimantanes diamondoid structure and changes with the parameter \(n\) or its number of copies.

INDEX TERMS Vertex metric dimension, generalized perimantanes diamondoids, diamond structure, resolving set.

I. INTRODUCTION
Due to its superlative physical qualities and its beauty, the diamond is a renowned structure. Polishing, drilling, cutting, and heatsink in electronics are numerous practical and industrial applications of diamond. Its hardness, exceptional thermal conductivity determines by its rigor of composition. A single molecule with macroscopic size makes it into a diamond crystal. The model depicting fundamental atomic groupings undergoes alterations while going from molecules to materials, both in terms of idea and actual manifestation, as well as insignificant computational processing [1].

There are four types of higher diamondoids and each have been assigned with four different colors and name. The assigned colors are yellow, red, blue, and green, while the names are, nonbranched rodlike zigzag catamantanes associated with yellow. The regularly branched catamantanes are linked with blue diamondoids, chiral diamondoids are red-colored and the green-colored are perimantanes diamondoids. All these series have been isolated and found from petroleum [2].

A chemical/molecular graph is a hydrogen-depleted molecular structure in which the edges represent bonds and the vertices represent atoms in the underlying organic chemical compounds. The chemical graph theory is the study of these chemical graphs [3], [4]. There are enough data available on this assumption and transformation from a chemical structure to a graph (vertex-edge-based structure). More detail can be found in the recent literature such as [5]–[10].

The notion of resolving set was proposed by the researcher in [11]. It is the first study to look at the notion of finding a graph’s metric dimension using the definition of a resolving set. The least cardinality of a resolving set is the metric dimension. The impetus for inventing the notion of finding the set came from LORAN and sonar stations. After that, several academics took this concept and labeled it in a variety of ways. The idea of a resolving set is dubbed as a metric dimension in [12]’s study. While the researchers in [13], [14] renamed the same notion with metric foundation or resolving set in a purely theoretical fashion. A more advanced definition of a resolving set was developed in the last decade. Researchers of [15] in which the idea of one node faultiness from the resolving set is explained. The notion is referred to as a fault-tolerant resolving set, and it is a generalized form of the resolving set.

Many concepts and implementations sprang from the generalized approach of resolving set. In electronics, [16], a recent innovation reveals the implementation of locating set (and its extensions). A method for studying diverse polyphenyl structures, especially for the polymer industry [17]. In the broader view, this idea is used in combinatorial optimization [18], some complex games or robotic roving [19], image processing [11], pharmaceutical chemistry [20].

The job of determining a graph’s resolving set is a non-deterministic polynomial-time hard problem (NP), with an
unknown algorithmic difficulty [20]–[23]. Metric dimension or resolving set has a large literature because of its many variations and applications in various disciplines. Only the most current and broad results will be discussed here. The Internet graph and its fault-tolerant structure are discussed in [24]. Quartz structure is studied with the concept of fault-tolerant locating number in [25]. Computer-related interconnection networks are studied in [26]. On the topic of fault-tolerant locating set, [27] discussed convex polytopes and found their exact fault-tolerant locating numbers. There is extensive literature available on this topic, we refer to see some recent research work on this definition [28]–[32]. A general graph of a kayak paddle and some other cycle-related graphs are dealt with in [33]. A cellulose network is studied in [34], they computed some upper bounds for the structure. A corona structure is reestablished in the form of a metric of a graph in [35]. A hydrocarbon-based class of structure was studied in [36] with the concept of locating numbers and also determined some other variants. The generalized class of the Harary family is studied with the definition of locating set [37]. Generalized Peterson graphs and multi-graphs are discussed in [3], with the concept of metric basis. The researchers in [38] studied this definition on the Cayley graph and find out the locating number for such a generalized class. Moreover, some recent studies and literature are available at [39]–[41]. On the topic of partition dimension we refer to the extensive study and some bounds on this topic, the literature is [42]–[45].

Given below are some basic concepts elaborated for further use in our main results.

Definition 1 [46]: “Let \( G \) be a connected graph with vertex set \( V(G) \), the distance between two vertices \( v_1, v_2 \in V(G) \) is the length of a shortest \( v_1 - v_2 \) path between them. It is denoted by \( d(v_1, v_2) \).”

Definition 2: Let \( B \) be an ordered simple subset from the vertex set of a graph, say \( B(G) = \{v_1, v_2, \ldots, v_n\} \), consider \( v \in V(G) \). The location (position, representation) \( r(\{v\} | B) \) of \( v \) according to the subset \( B \) is the \( i \)-tuple distances \( d(v, v_1), d(v, v_2), \ldots, d(v, v_i) \). Taking any two vertices of a graph \( G \), if these vertices have different locations \( r(\{v\} | B) \) according to chosen subset \( B \), then \( B \) is considered as a locating set for the graph. The minimum possible members (or the cardinality) of locating set is the metric dimension of the graph and we will defined this with the symbol \( dim(G) \).

Definition 3: A pertinent chosen subset \( B \) which is locating set becomes fault-tolerant locating set \( B_f \), if it fulfills the condition \( B_f \backslash \{v\} \) for each vertex \( v \in I_s \) and it remains locating set. The minimum possible members (or the cardinality) of fault-tolerant locating set is the fault-tolerant metric dimension of the graph and we will defined this with the symbol \( dim_f(G) \).

Definition 4: Let \( B_p = \{B_{p_1}, B_{p_2}, \ldots, B_{p_k}\} \) be the partition of a connected graph. Now for a vertex \( j \in V(G) \) the partition dimension with respect to \( B_p \) is \( r(\{j\} | B_p) = \{d(j, B_{p_1}), d(j, B_{p_2}), \ldots, d(j, B_{p_k})\} \), where \( d(j, B_w) = \min\{d(j, y) : y \in B_w\} \) for \( 1 \leq w \leq \ell \). The distinct codes of the two vertices \( i, j \in V(G) \) with respect to \( B_p \), that is \( r(\{i\} | B_p) \neq r(\{j\} | B_p) \), such a partition \( B_p \) is known as distinguishing partition of \( G \) and denoted by \( pd(G) \) [47].

In this draft, we have discussed metric dimension and their generalizations for the generalized perimantas diamondoid structure and proved that each parameter depends on the copies of original or base perimantas diamondoid structure and changes with the parameter \( n \) or its number of copies. The next section will present some main results, conclusions are drawn and at the end, references are given for more and deep insight into this topic and structure.

II. GENERALIZED PERIMANTANES DIAMONDOID STRUCTURE AND MAIN RESULTS

The structure shown in Figure 1, is a green-colored perimantas diamondoid and one of a higher diamond structure. Its topological version is found in [1], [2] and motivated by the structures applications and usage, we look into the metric-based parameters of this structure. The perimantas diamondoid structure has total \( |V(D_n)| = 22n + 3 \), number of vertices and total edges are \( |E(D_n)| = 38n + 2 \). The labelling of vertices and edges is described in the Figure 1 and is utilized in the major results. Furthermore, vertex and edge are stated given below.

\[
V(D_n) = \{d_1^i : i = 1, 2, \ldots, 19, j = 1, 2, \ldots, n\}
\]
\[
\cup \{b_i : i = 1, 2, \ldots, 3(n + 1)\},
\]
\[
E(D_n) = \{d_1^j \cup d_2^j : i = 1, 2, 4, 5, 7, 9, 10, 12, 14, 15, 17, 18, j = 1, 2, \ldots, n\} \cup \{b_i b_{i+1} : i = 1, 4, 7, \ldots, 3n + 1, j = 2, 5, \ldots, 3n + 1\} \cup \{b_{i+1} b_{i+2} : i = 1, 4, 7, \ldots, 3n - 2, j = 1, 2, \ldots, n\} \cup \{b_i d_2^j, b_i d_1^j : i = 2, 5, 8, \ldots, 3n - 1, j = 1, 2, \ldots, n\} \cup \{b_i d_1^j : i = 3, 6, 9, \ldots, 3n, j = 1, 2, \ldots, n\} \cup \{b_{i+1} d_1^j : i = 4, 7, 10, \ldots, 3n + 1, j = 1, 2, \ldots, n\} \cup \{b_{i+1} d_1^j, b_{i+1} d_2^j : i = 5, 8, 11, \ldots, 3n + 2, j = 1, 2, \ldots, n\} \cup \{b_i d_1^j : i = 6, 9, 12, \ldots, 3n + 3, j = 1, 2, \ldots, n\}.
\]

Presented below are the main results of this novel structure.

Lemma 1: Let \( D_n \) is a structure of perimantas diamondoid with \( n \geq 1 \), and \( B \) is the vertex resolving set of \( D_n \) for \( n = 1 \). Then one of the possible resolving set is stated by

\[
B = \{b_1, b_4, a_1^2\}.
\]

Proof: To demonstrate that the resolving set for the structure of perimantas diamondoid, shown in the Figure 1 and labeled as \( D_1 \), for its particular value of \( n = 1 \). Let \( B \) be a resolving set and stated by, \( B = \{b_1, b_4, a_1^2\} \). Moreover its resolving set shown in the Figure 2. The unique locations of
the full vertex set of $D_1$, with regard to the elements of $B$ are as follows.

\[ r(a'_1)|B| = \begin{cases} 
(3 - i, 5 - i, i), & \text{if } i = 1, 2; \\
(2, 4, i), & \text{if } i = 3; \\
(2, i, i + 1), & \text{if } i = 4; \\
(i - 2, i, i + 1), & \text{if } i = 5, 6; \\
(10 - i, 10 - i, i - 7), & \text{if } i = 7, 8; \\
(i - 7, i - 7, i - 7), & \text{if } i = 9, 10, 11; \\
(i - 8, i - 8, i - 5), & \text{if } i = 12, 13; \\
(18 - i, 16 - i, i - 13), & \text{if } i = 14, 15; \\
(4, 2, i - 13), & \text{if } i = 16; \\
(i - 13, i - 15, i - 12), & \text{if } i = 17, 18, 19. 
\end{cases} \]

\[ r(b_1)|B| = \begin{cases} 
(i - 1, 3 + i, i + 2), & \text{if } i = 1, 2, 3; \\
(i, i - 4, i - 1), & \text{if } i = 4, 5, 6. 
\end{cases} \]  

We also observe that each vertex has a different representation and satisfy the concept of resolving set based on the arguments given above in the form of identifications of the whole vertex set of $D_1$, which leads to the conclusion that defined $B$ is one of a possible resolving set with $|B| = 3$.

**Lemma 2:** Let $D_n$ be a structure of perimantanes diamondoid with $n = 1$. Then

\[ \dim(D_1) = 3. \]

**Proof:** We employ the double inequality method and refer to Lemma 1 to establish that the metric dimension of $D_1$ is 3. This plainly demonstrates that the resolving set has cardinality 3, which is described by $B = \{b_1, b_4, a'_1\}$.

Now on contrary we have $\dim(D_1) = 2$. from the assertion $\dim(D_1) \geq 3$. Consider the resolving set $B'$ with cardinality 2. This assumption is discussed in the following cases.

**Case 1:** Let a chosen subset $B'$ having two distinct elements, say $B' = \{b_1, b_2\}$. The contradiction will be arise due the vertices which have two distance to any of the chosen element of $B'$. Mathematically, it can be written as $r(a'_1|B') = r(a'_1|b') = d(a'_1, b_1) = 2$.

**Case 2:** Let a chosen subset $B'$ having two distinct elements, say $B' = \{b_1, b_3\}$. The contradiction will be arise due the vertices which have two distance to any of the chosen element of $B'$. Mathematically, it can be written as $r(a'_1|B') = r(a'_1|b') = d(a'_1, b_1) = 2$.

**Case 3:** Let a chosen subset $B'$ having two distinct elements, say $B' = \{b_1, b_3\}$, with distinct $i, j$. The contradiction will be arise due the vertices which have two distance to any of the chosen element of $B'$. Mathematically, it can be written as $r(a'_1|B') = r(a'_1|b') = d(a'_1, b_1) = 2$.

Similarly, there is not just one option among the available combinations $\binom{|V|}{2} = \binom{|V(D_1)|}{2} = \binom{25}{2} = 300$ of the entire vertex set of $D_1$. This indicate that two metric dimension of $D_1$ is not possible. Hence; $\dim(D_1) \geq 3$.

Hence,

\[ \dim(D_1) = 3. \]  

**Theorem 1:** Let $D_n$ be a structure of perimantanes diamondoid with $n \geq 2$. Then

\[ \dim(D_n) = n + 2. \]

**Proof:** To show that $\dim(D_n) = n + 2$, we will applying the induction method on $n$ showing the number of copies of base perimantanes diamondoid graph. The base case for $n = 1$ proved in the Lemmas 1 and 2, now assume that the assertion is true for $n = \alpha$.

\[ \dim(D_\alpha) = \alpha + 2. \]

We will show that it is true for $n = \alpha + 1$. Suppose

\[ \dim(D_{\alpha + 1}) = \dim(D_\alpha) + \dim(D_1) - 2. \]

Using Equations 3 and 5 in Equation 6, we have

\[ \dim(D_{\alpha + 1}) = \alpha + 2 + 3 - 2, = \alpha + 3. \]
As a result, the conclusion holds for all positive integers \( n \geq 1 \).

Moreover, the generalize resolving set for the generalized structure of perimantanes diamondoid, shown in the Figure 3 and stated by in the set form \( B = \{b_1, b_3n+1, a_1^l, a_2^l, a_3^l, \ldots, a^l_2\} \).

This concludes. \( \square \)

**Lemma 3:** Let \( D_n \) is a structure of perimantanes diamondoid with \( n \geq 1 \), and \( B_f \) is the vertex fault-tolerant resolving set of \( D_n \) for \( n = 1 \). Then one of the possible vertex fault-tolerant resolving set is stated by

\[
B_f = \{b_1, b_3, b_4, b_6, a_1^l, a_1^{13}\}.
\]

**Proof:** To demonstrate that the fault-tolerant resolving set for the structure of perimantanes diamondoid, shown in the Figure 1 and labeled as \( D_1 \), for its particular value of \( n = 1 \). Let \( B_f \) be the fault-tolerant resolving set and stated by, \( B_f = \{b_1, b_3, b_4, b_6, a_1^l, a_1^{13}\} \). Moreover its resolving set shown in the Figure 4. The locations of the full vertex set of \( D_1 \), in regard to the elements of \( B_f \) are described as (8) and (9), as shown at the bottom of the page.

\[
r(b_i|B_f) = \begin{cases} 
(3-i, 5-i, 5-i, 7-i, i, 8-i), & \text{if } i = 1, 2; \\
(2, 5-i, 4, 7-i, i, 8-i), & \text{if } i = 3; \\
(2, 6-i, 8-i, i+1, 7-i), & \text{if } i = 4; \\
(i-2, 6-i, i, 8-i, i+1, 7-i), & \text{if } i = 5; \\
(i-2, 2, i, i-2, i+1, 7-i), & \text{if } i = 6; \\
(10-i, 12-i, 10-i, 2, 7-i, 15-i), & \text{if } i = 7; \\
(10-i, 12-i, 10-i, 4, 7-i, 15-i), & \text{if } i = 8; \\
(i-7, 12-i, i-7, 13-i, i-7, 14-i), & \text{if } i = 9; \\
(i-7, 13-i, i-7, 14-i, 7-i, 14-i), & \text{if } i = 10, 11; \\
(i-8, i-10, i-8, i-14, i-5, 13-i), & \text{if } i = 12, 13; \\
(18-i, 20-i, 16-i, i-14, i-13, 20-i), & \text{if } i = 14; \\
(18-i, 20-i, 16-i, 18-i, i-13, 20-i), & \text{if } i = 15; \\
(4, 20-i, 2, 18-i, i-13, 20-i), & \text{if } i = 16; \\
(i-13, 21-i, i-15, 19-i, i-12, 20-i), & \text{if } i = 17, 18; \\
(i-13, 4, i-15, 2, i-12, 20-i), & \text{if } i = 19. 
\end{cases}
\]

\[
r(a_i|B_f) = \begin{cases} 
(i-1, 3-i, 3+i, 7-i, i+2, 6-i), & \text{if } i = 1, 2, 3; \\
(i, 10-i, i-4, 6-i, i-1, 9-i), & \text{if } i = 4, 5, 6.
\end{cases}
\]

We can look over the entire vertex set of perimantanes diamondoid structure \( D_1 \), have unique locations and fulfilling the idea of fault-tolerant resolving set, which leads to the conclusion that defined \( B_f \) is one of a possible resolving set with \( |B_f| = 6 \).

**Lemma 4:** Let \( D_n \) is a structure of perimantanes diamondoid with \( n = 1 \). Then

\[
dim_f(D_1) = 6.
\]

**Proof:** We employ the double inequality approach and refer to Lemma 3 to establish that the fault-tolerant metric dimension of \( D_1 \) is 6. This clearly demonstrates that the fault-tolerant resolving set defined as \( B_f = \{b_1, b_3, b_4, b_6, a_1^l, a_1^{13}\} \), has cardinality 6.

Now we need to prove that \( \dim_f(D_1) \geq 6 \). On contrary we suppose \( \dim_f(D_1) = 5 \). For this, consider the fault-tolerant...
resolving set $B'_i$ with cardinality 5. This assumption is discussed in the following sections.

Let a chosen subset $B'_j$ having five distinct elements, say $B'_j = \{a'_i, d'_i\}$, with distinct $i, j$. The contradiction will be arise due the vertices which have two distance to any of the chosen element of $B'_j$. Mathematically, it can be written as $r \left( a'_i | B'_j \right) = r \left( d'_i | B'_j \right) = d \left( a'_i, d'_i \right) = 2$.

Similarly, there is not a single case among the available combinations $|V|C_5 = \frac{\sqrt{\left| \left( D_{n} \right) \right|}}{5! \times 3 \times 2} = 53130$ of the entire vertex set of $D_1$. This indicate that five fault-tolerant metric dimension of $D_1$ is not possible. Hence, $\dim_f (D_1) \geq 5$.

Hence,

$$\dim_f (D_1) = 6.$$  

**Theorem 2:** Let $D_n$ is a structure of perimantanes diamondoid with $n \geq 2$. Then

$$\dim_f (D_n) = 2(n + 2). \quad (10)$$

**Proof:** To show that $\dim_f (D_n) = 2(n + 2)$, we will applying the induction method on $n$ showing the number of copies of base perimantanes diamondoid graph. The base case for $n = 1$ proved in the Lemmas 3 and 4, now assume that the assertion is true for $n = \alpha$.

$$\dim_f (D_\alpha) = 2(\alpha + 2). \quad (11)$$

We will show that it is true for $n = \alpha + 1$. Suppose

$$\dim_f (D_{\alpha+1}) = \dim_f (D_\alpha) + \dim_f (D_1) - 5. \quad (12)$$

Using Equations 10 and 11 in Equation 12, we have

$$\dim_f (D_{\alpha+1}) = 2(\alpha + 2) + 6 - 5 = 2(\alpha + 2) + 1. \quad (13)$$

As a result, the conclusion holds for all positive integers $n \geq 1$.

Moreover, the generalize fault-tolerant resolving set for the generalized structure of perimantanes diamondoid, shown in the Figure 5 and stated by in the set form $B'_j = \{b_1, b_3, b_{3n+1}, b_{3n+3}, a'_1, a'_2, \ldots, a'_3, a'_{13}, \ldots, a'_{13}\}$.

This concludes. □

**Lemma 5:** Let $D_n$ is a structure of perimantanes diamondoid with $n \geq 1$, and $B_p$ is the vertex partitioning resolving set of $D_n$ for $n = 1$. Then one of the possible vertex partitioning resolving set is stated by

$$B_p = \{b_{p1}, b_{p2}, b_{p3}, b_{p4}\}, \quad B_{p1} = \{b_1\}, \quad B_{p2} = \{b_4\}, \quad B_{p3} = \{a'_1\}, \quad B_{p4} = V (D_n) \setminus \{b_1, b_4, a'_1\}.$$  

**Proof:** To prove that the partitioning resolving set for the structure of perimantanes diamondoid, shown in the Figure 1 and labeled as $D_1$, for its particular value of $n = 1$. Let $B_p$ be the partitioning resolving set and stated by,

$$r \left( b_i | B_p \right) = \begin{cases} (3 - i, 5 - i, i, 0), & \text{if } i = 1, 2; \\ (2, 4, i, 0), & \text{if } i = 3; \\ (2, i, i + 1, 0), & \text{if } i = 4; \\ (i - 2, i, i + 1, 0), & \text{if } i = 5, 6; \\ (10 - i, i - 10, i - 10, 0), & \text{if } i = 7; \\ (i - 10, i - 10, i - 7, 0), & \text{if } i = 8; \\ (i - 7, i - 7, i - 7, 0), & \text{if } i = 9, 10, 11; \\ (i - 8, i - 8, i - 5, 0), & \text{if } i = 12, 13; \\ (18 - i, 16 - i, i - 13, 0), & \text{if } i = 14, 15; \\ (4, 2, i - 13, 0), & \text{if } i = 16; \\ (i - 13, i - 15, i - 12, 0), & \text{if } i = 17, 18, 19. \end{cases} \quad (14)$$

$$r \left( b_i | B_p \right) = \begin{cases} (i - 1, 3 + i, i + 2, z), & \text{if } i = 1, 2, 3; \\ (i, i - 4, i - 1, z), & \text{if } i = 4, 5, 6. \end{cases} \quad (15)$$

where

$$z = \begin{cases} 1, & \text{if } i = 1, 4; \\ 0, & \text{otherwise}. \end{cases} \quad (16)$$

We can observe that each vertex has a different representation and satisfy the concept of partition resolving set seen from presentation of the entire vertex set of $D_1$, in the form of representations which leads to the conclusion that defined $B_p$ is one of a possible resolving set with $|B_p| = 4$. □

**Lemma 6:** Let $D_n$ is a structure of perimantanes diamondoid with $n = 1$. Then

$$3 \leq \text{pd} (D_1) \leq 4.$$  

**Proof:** To show that the partition dimension of $D_1$ is either 3 or 4. We employ the method of twofold inequality and refer to Lemma 5. This clearly shows that the partition resolving set has the cardinality 4 and has been stated by,

$$B_p \setminus \{b_i \} = \{4, 5, 6\}.$$
\[ B_p = \{B_{p_1}, B_{p_2}, B_{p_3}, B_{p_4}\}, B_{p_1} = \{b_1\}, B_{p_2} = \{b_4\}, B_{p_3} = \{a_1\}, B_{p_4} = V(D_n) \setminus \{b_1, b_4, a_1\}. \]

This shows that the partition metric dimension of \(D_1\) is four or less. Two partition dimension is reserved for the path graph \(n\) or less. Two partition dimension is reserved for the path graph \(n\) or less. Two partition dimension is reserved for the path graph \(n\) or less. Two partition dimension is reserved for the path graph \(n\) or less.

\[ 3 \leq pd(D_1) \leq 4. \quad (17) \]

**Theorem 3:** Let \(D_n\) is a structure of perimantanes diamondoid with \(n \geq 2\). Then

\[ pd(D_n) \leq n + 3. \quad (18) \]

**Proof:** To show that \(pd(D_n) \leq n + 3\), we will applying the induction method on \(n\) showing the number of copies of base perimantanes diamondoid graph. The base case for \(n = 1\) proved in the Lemmas 5 and 6, now assume that the assertion is true for \(n = \alpha\).

\[ pd(D_\alpha) \leq \alpha + 3. \quad (19) \]

We will show that it is true for \(n = \alpha + 1\). Suppose

\[ pd(D_{\alpha+1}) \leq pd(D_\alpha) + pd(D_1) - 3. \quad (20) \]

Using Equations 17 and 19 in Equation 20, we have

\[ pd(D_{\alpha+1}) \leq \alpha + 3 + 4 - 3, \]

\[ = \alpha + 4. \quad (21) \]

As a result, the conclusion holds for all positive integers \(n \geq 1\). This concludes.

**III. CONCLUSION**

In this draft, we have discussed metric dimension and their generalizations for the generalized perimantanes diamondoid structure and proved that each parameter depends on the copies of original or base perimantanes diamondoid structure and changes with the parameter \(n\) or its number of copies. Future direction can be considered as to discussed its other parameters which are also based on the metric of structure.

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HAMDAN ALSHEHRI received the M.Sc. degree in computer and information science from Cleveland University, Cleveland, USA, in 2014, and the D.Sc. degree in information technology from Towson University, Towson, USA, in 2014. He is currently an Assistant Professor with the College of Computer Science and Information Technology, Jazan University, Saudi Arabia. His research interests include data analysis, data visualization, machine learning, and bioinformatics.

ALI AHMAD received the M.Sc. degree in mathematics from Punjab University, Lahore, Pakistan, in 2000, the M.Phil. degree in mathematics from Bahauddin Zakariya University, Multan, Pakistan, in 2005, and the Ph.D. degree in mathematics from the Abdus Salam School of Mathematical Sciences, GC University, Lahore, in 2010. He is currently an Assistant Professor with the College of Computer Science and Information Technology, Jazan University, Saudi Arabia. His research interests include graph labeling, metric dimension, minimal doubly resolving sets, distances in graphs, and topological indices of graphs.

YAHYA ALQAHTANI received the M.Sc. degree in information technology from Central Connecticut State University, New Britain, CT, USA, in 2012, and the Ph.D. degree in information technology from Towson University, Towson, MD, USA. He is currently an Assistant Professor with the College of Computer Science and Information Technology, Jazan University, Saudi Arabia. His research interests include health informatics, e-learning systems, and human–computer interaction.

MUHAMMAD AZEEM received the B.S. degree from COMSATS University Islamabad Lahore Campus, in 2018. He is a Research Associate with the Department of Mathematics, Riphah International University Lahore Campus. He has published research articles in reputed international journals of mathematics and informatics. His research interests include control theory, metric graph theory, graph labeling, spectral graph theory, and soliton theory. He is a Referee for several international mathematical journals.

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