

On Strong Edge Metric Dimension of Crystal Cubic Carbon Structure

Ajay Kumar Sharma*, Malkesh Singh**

Submitted: 01/11/2023

Revised: 17/12/2023

Accepted: 26/12/2023

Abstract: The strong edge metric dimension of a carbon-based crystal structure is examined in this paper using the framework of chemical graph theory. The goal is to identify the smallest edge-resolving set that uniquely identifies each pair of edges based on their distance relationships. The crystal structures are treated as connected graphs. Exact formulations for the strong edge metric dimension of these carbon-based graph families are found by taking use of their underlying structural features. The results gained show how network topology affects edge distinguishability and offer closed-form mathematical characterizations for the graph classes under consideration. These results support the structural and mathematical analysis of crystalline materials based on carbon and advance the theoretical development of graph invariants in chemical graph theory.

MSC(2020): 05C10, 05C12, 68R10.

Keywords: Strong edge resolving set, Crystal structure of cubic carbon, Strong edge metric dimension.

1 Introduction

Chemical graph theory is a subfield of mathematical chemistry that models and analyzes chemical structures and processes mathematically using graph theory concepts and techniques [1]. It offers an effective theoretical framework for examining the topological and structural aspects of chemical compounds, allowing scientists to make significant connections between physicochemical traits and molecular structure. Computational chemistry, medicinal chemistry, drug discovery, nanotechnology, material science, and bioinformatics are just a few of the scientific fields that have come to rely heavily on this field over the years.

According to chemical graph theory, a molecular graph is used to depict a chemical compound, with the vertices standing in for atoms and the edges for the chemical bonds that bind them. The study of complex molecular structures is made

easier by this graphical depiction, which maintains the fundamental topological characteristics of the formations. Researchers can examine a variety of molecular features, including connectedness, cyclic structures, molecular symmetry, aromaticity, branching patterns, and reaction routes, by utilizing graph-theoretic principles, combinatorial techniques, and computer algorithms. Additionally, graph-based descriptors—also referred to as topological indices—have been widely employed to forecast molecules' physical, chemical, and biological characteristics without the need for expensive experimental techniques.

Chemical graph theory can be used for more than just analyzing individual molecules. It is essential for the development of sophisticated functional materials with desired qualities, the research of crystalline and nanostructured materials, the design and optimization of novel medicinal substances, and the analysis of molecular interactions. Because chemical graph theory offers effective mathematical models and computational methods for comprehending the structure, behavior, and usefulness of chemical systems, it continues to close the gap between mathematics and chemistry.

Throughout this article, let $G = G(V, E)$ denote a connected molecular graph with vertex set $V(G)$ and edge set $E(G)$. For any two vertices $p, q \in V(G)$, the distance between them, denoted by

Email: aksharmaju@gmail.com

Email: Malkeshsingh37@gmail.com

*Department of Mathematics, Government
College for Women, Udhampur-182101,
Jammu and Kashmir, India

**School of Mathematics, Shri Mata Vaishno Devi
University, Katra-182320, Jammu and Kashmir,
India

$d(p, q)$, is defined as the length of a shortest path connecting p and q in G . The concept of the metric dimension, introduced by Slater [2], has become an important graph invariant in graph theory due to its wide range of theoretical and practical applications. Let $R = r_1, r_2, \dots, r_k$ be an ordered subset of $V(G)$. The metric representation (or distance representation*) of a vertex $s \in V(G)$ with respect to the set R is defined as the ordered k -tuple $\zeta(s | R) = (d(s, r_1), d(s, r_2), \dots, d(s, r_k))$. If every pair of distinct vertices in G has different metric representations with respect to R , then the set R is called a resolving set (or locating set) of G [3]. In other words, for any two distinct vertices $u, v \in V(G)$, there exists at least one vertex $r \in R$ such that $d(u, r) \neq d(v, r)$.

Among all resolving sets of G , those having the smallest cardinality are of particular interest. The metric dimension of G , usually expressed by $\dim(G)$, is the cardinality of such a minimum resolving set, which is called a metric basis. Based on the distances between each vertex in the graph and the vertices of the resolving set, the metric dimension calculates the minimal number of reference vertices needed to uniquely identify each vertex. Because of its important applications in a variety of domains, such as network discovery, robot navigation, image processing, sensor networks, combinatorial optimization, chemistry, and pharmaceutical sciences, this graph invariant has garnered a lot of interest. Additionally, the metric dimension plays a significant role in the analysis of network topology, information distribution, and the unique identification of graph pieces, and it offers insightful information about the structural properties of graphs.

Since the metric dimension was first introduced, a great deal of research has been done to examine its many practical applications as well as its theoretical characteristics. The metric dimension has emerged as a key graph invariant with substantial significance in both mathematics and practical sciences due to its capacity to uniquely identify a graph's vertices through distance representations. Metric dimension is used in many theoretical and practical contexts. Melter and Tomescu [4] looked at applications in image analysis and pattern recognition, while Chartrand *et al.* [3] offered implications for chemical graph theory and molecular analysis. Furthermore, Seb"o and Tannier [5] investigated the issue in the context of combinatorial optimization,

supplementing Khuller *et al.* [6] on the use of landmark vertices to identify autonomous agents in network navigation. Further highlighting the importance of metric-based graph parameters in the research of complicated molecular structures, Al-Qudah *et al.* [7] recently investigated the metric basis and metric dimension of the molecular graph associated with a one-heptagonal carbon nancone.

Over the past ten years, a number of variations of the conventional resolving sets have been produced, driven by the increasing need to solve more complex theoretical and practical problems. Local resolving set [8], edge resolving set [10], mixed resolving set [9], fault-tolerant resolving set [11], and fault-tolerant edge resolving set (FTEMD) [12] are notable examples of these parameters. By adding more structural restrictions or taking into account other graph elements, each of these factors expands on the traditional idea of resolvability, resulting in more adaptable and effective models for a range of applications.

Numerous scientific and technical fields have made extensive use of these generalized metric dimensions. They have been used for drug discovery, chemical compound classification, and molecular characterization in chemistry and pharmaceutical sciences. They support network verification, source localization, sensor placement, and network motif identification in computer science and communication networks. Additionally, they are crucial for robot navigation, image processing, combinatorial optimization, pattern recognition, biological sequence data embedding, and the analysis of intricately linked networks. Thus, motivated by both theoretical interest and practical need, the ongoing development of new metric dimension variations continues to be an active and significant area of research in graph theory.

Elements of a metric basis are used as monitoring devices (sometimes known as "censors") in network surveillance applications [13] to detect threats such as fire or unauthorized access. Hernando *et al.* [11] developed fault-tolerant resolution sets to retain full network observability even during component outages because individual device failures can jeopardize the system's diagnostic capability. The strong edge metric dimension, which combines the ideas of edge resolving and strong resolving, is a more constrained variation. According to the graph's

shortest-path structure, a subset of vertices is selected in this context so that each pair of different edges is strongly resolved by at least one vertex. The strong edge metric dimension of the graph is the minimum cardinality of such a set. This parameter offers a better understanding of the structural characteristics of graphs due to its more stringent resolving criteria, and it frequently calls for alternative methods than the classical metric dimension or edge metric dimension. Because of its theoretical importance and practical use in network navigation, routing, optimization, and security, the research of the strong edge metric dimension has attracted more attention. This research examines the crystal cubic carbon structure's strong edge metric dimension.

1.1 Crystal Cubic Carbon Structure

Carbon is the main component of organic substances and an essential building block for all living things. Its unique electron structure permits substantial chemical bonding in addition to its natural abundance—it ranks sixth in the cosmos and fourth in the Earth's crust. Importantly, carbon easily forms a variety of allotropes with unique chemical and physical characteristics, making them useful in a wide range of industries [26, 27]. Among these structural forms, fullerenes, diamond, and graphite are prominent, each with distinct properties.

Diamond is the hardest material found in nature because its carbon atoms are organized in a strong three-dimensional network. In addition to its mechanical robustness, it has excellent thermal dissipation qualities and outstanding optical clarity over the majority of light wavelengths. Because of these qualities, diamonds are necessary for heavy-duty industrial cutting tools as well as gemological applications.

Graphite, on the other hand, is made up of hexagon-shaped layers of carbon sheets. The material's distinctive lubricity results from these planes shearing easily over one another due to The order of the graph $\Gamma(n)$ is given by

minimal interlayer interactions. These physical characteristics, when combined with its high electrical conductivity, allow for a wide range of applications in electrochemical electrodes, solid-state lubricants, and pencil leads [28].

Fullerenes, which are molecular structures that create hollow geometric shapes like spheres and tubes, are another important family of carbon allotropes. Buckminsterfullerene (C_{60}), the most extensively researched constituent, reflects a geodesic framework made up of 60 carbon vertices grouped in linked pentagons and hexagons. These molecules are essential components in materials science and nanoscale applications due to their special physical properties, such as high tensile strength [29].

Carbon's exceptional structural adaptability, as evidenced by its various allotropic forms, highlights its essential significance in a variety of multidisciplinary domains, from sophisticated materials production and biomedical applications to electronics and energy storage.

Primitive cubic carbon (PCC) is one of the potential allotropes of carbon. The molecular structure of primitive cubic carbon, represented by $\Gamma(n)$, is described in [30]. The following guidelines are used to design the network $\Gamma(n)$ inductively:

First Step ($n = 1$): $\Gamma(1)$ is the central core of the fundamental unit cube (Figure 1).

Second Step ($n = 2$): Each vertex of $\Gamma(1)$ is connected to a unique cube via a bridge edge to build the structure $\Gamma(2)$ (Figure 2).

Third Step ($n = 3$): All vertices of degree 3 in $\Gamma(2)$ are identified, and an extra cube is attached to each by a single edge to create $\Gamma(3)$.

General Step ($n \geq 2$): The graph $\Gamma(n)$ is built iteratively from $\Gamma(n - 1)$ by attaching a new unit cube to each degree 3 vertex in $\Gamma(n - 1)$ (Figure 3).

$$|V(\Gamma(n))| = 2 \left(24 \sum_{s=3}^n (2^3 - 1)^{s-3} + 31(2^3 - 1)^{n-2} + 2 \sum_{s=0}^{n-2} (2^3 - 1)^s + 3 \right).$$

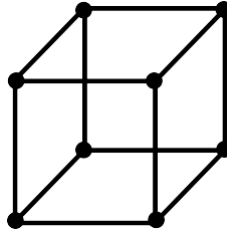


Figure 1: Central cube of $\Gamma(n)$

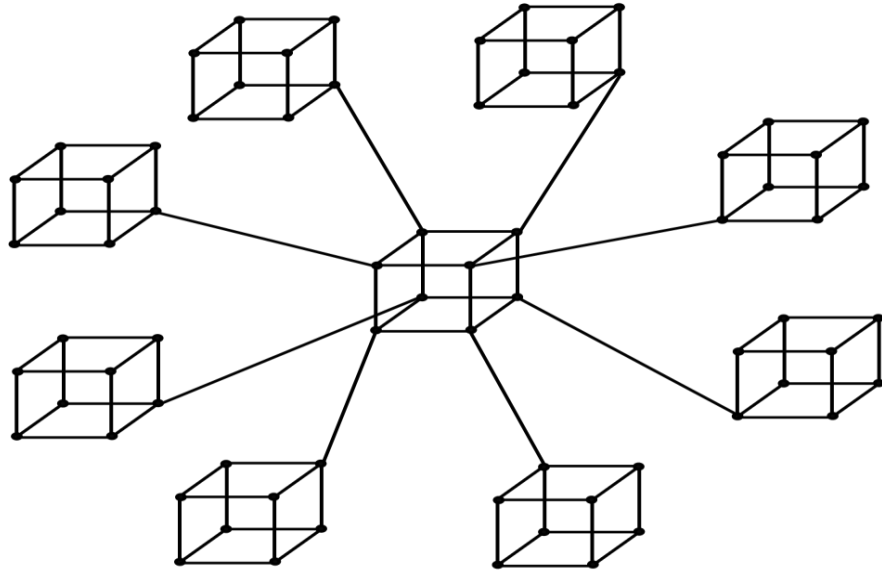


Figure 2: Second level of crystal cubic carbon

The size of the graph $\Gamma(n)$ is given by

$$|E(\Gamma(n))| = 4 \left(24 \sum_{s=3}^n 7^{s-3} + 24 \cdot 7^{n-2} + 2 \sum_{s=0}^{n-2} 7^s + 3 \right).$$

Each vertex in $\Gamma(n)$ has a degree of either 3 or 4. Specifically, the number of degree-3 vertices in $\Gamma(n)$ is

$$8 \cdot 7^{n-1},$$

while the number of degree-4 vertices is given by

$$2 \left(24 \sum_{s=3}^n 7^{s-3} + 3(7) + 1 \right) + 2 \sum_{s=0}^{n-2} 7^s + 3.$$

Primitive cubic carbon, denoted as $\Gamma(n)$, is a structurally significant carbon allotrope that has been well studied theoretically. Topological descriptors were the main focus of early computational research: While Baig *et al.* [27] obtained precise closed formulas for the first and second additive Zagreb indices, Gao *et al.* [26] assessed a variety of Zagreb polynomials and indices. Slater and Javaid [31] on connection-based Zagreb indices, Zahid *et al.* [33] on fifth M-Zagreb indices, and Yang *et al.* [32] on Forgotten,

Balaban, Augmented, and Zagreb-type indices carried out additional topological characterizations. Furthermore, Sharma *et al.* [35] investigated degree-based multiplicative invariants for $3 \leq n \leq 10$.

Imran *et al.* [28] and Yang *et al.* [34] investigated eccentricity-based invariants, such as the degree eccentric connectivity index, the connective eccentric index, and their underlying polynomials, in addition to

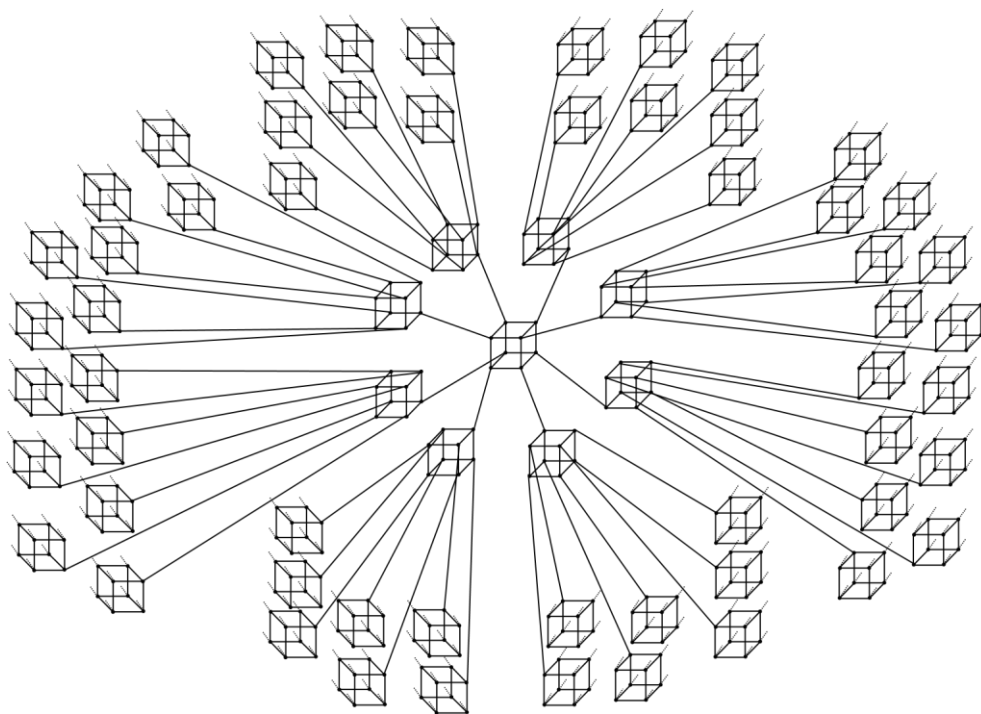


Figure 3: Molecular graph of $\Gamma(n)$

conventional degree-based descriptors. Yang *et al.* [29] examined distance-based metrics like the vertex Szeged, vertex PI, weighted vertex Szeged, and geometric-arithmetic indices. Structural resolvability has received more attention lately: The metric dimension (vertex resolvability) of $\Gamma(n)$ was examined by Zhang and Naeem [30], and its edge metric dimension was assessed by Sharma *et al.* [36]. This study examines the strong edge metric dimension of $\Gamma(n)$ and precisely characterizes its minimum strong edge resolving sets, motivated by these advances in graph-theoretic resolvability.

2 Preliminaries

This section provides essential definitions and foundational concepts necessary for the theoretical framework developed in this paper.

Definition 1. Strong Edge Metric Generator: [23]

Let $G = (V, E)$ be a connected graph. A vertex $w \in V(G)$ is said to *strongly resolve* two edges $e_1, e_2 \in E(G)$ if the distances from w to the endpoints of the edges satisfy the strong resolving condition. Equivalently, if one of the edges lies on a shortest path between w and the other edge (using the usual

edge-to-vertex distance), then w strongly distinguishes those two edges.

A set of vertices $S \subseteq V(G)$ is called a *strong edge metric generator* if each pair of distinct edges of G is strongly resolved by at least one vertex in S .

Definition 2. Strong Edge Metric Generator: [23]

The *strong edge metric dimension* of G , represented by $\text{sedim}(G)$, is the minimum cardinality of a strong edge metric generator.

In other words, $\text{sedim}(G) = \min\{|S| : S \subseteq V(G) \text{ and } S \text{ strongly resolves every pair of distinct edges of } G\}$.

3 Main Results

This section investigates the strong edge metric dimension and characterizes the corresponding metric bases for the primitive cubic carbon network $\Gamma(n)$. For the base structure ($n = 1$), the minimum strong edge resolving set has a cardinality of 3. For $n \geq 2$, the strong edge metric basis of $\Gamma(n)$ consists of exactly $24 \cdot 7^{n-2}$ vertices.

Theorem 1. The *sedim* of $\Gamma(1) \leq 3$, i.e., $\text{sedim}(\Gamma(1)) \leq 3$.

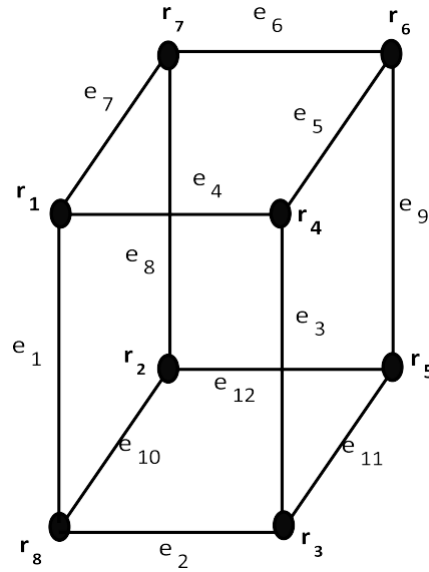


Figure 4: Molecular graph $\Gamma(1)$

Proof. Let $\{r_j \mid 1 \leq j \leq 8\}$ denote the vertex set of $\Gamma(1)$, as illustrated in Figure 4, and let $S_E = \{r_1, r_2, r_3\} \subset V(\Gamma(1))$. We demonstrate that S_E constitutes a strong edge resolving set for $\Gamma(1)$ of

minimal cardinality, thereby establishing that S_E is a minimum strong edge resolving set for $\Gamma(1)$. The distance between different vertices of $\Gamma(1)$ are shown in table 1.

$d(r_i, r_j)$	r_1	r_2	r_3	r_4	r_5	r_6	r_7	r_8
r_1	0	1	2	1	1	2	2	2
r_2	1	0	1	2	2	1	2	2
r_3	2	1	0	1	2	2	1	2
r_4	1	2	1	0	2	2	2	1
r_5	1	2	2	2	0	1	2	1
r_6	2	1	2	2	1	0	1	2
r_7	2	2	1	2	2	1	0	1
r_8	2	2	2	1	1	2	1	0

The distance between the edges e_i ; $i = 1,2,3,4,5,6,7,8,9,10,11,12$ and different elements from S_E is shown in table 2.

Edge	End vertices	$d(e_i, r_1)$	$d(e_i, r_2)$	$d(e_i, r_3)$
e_1	(r_1, r_2)	0	0	1
e_2	(r_2, r_3)	1	0	0
e_3	(r_3, r_4)	1	1	0
e_4	(r_1, r_4)	0	1	1
e_5	(r_5, r_6)	1	1	2
e_6	(r_6, r_7)	2	1	1
e_7	(r_7, r_8)	2	2	1
e_8	(r_5, r_8)	1	2	2
e_9	(r_1, r_5)	0	1	2
e_{10}	(r_2, r_6)	1	0	1
e_{11}	(r_3, r_7)	2	1	0
e_{12}	(r_4, r_8)	1	2	1

Now consider any two distinct edges e_i, e_j , we check the strong distinguishing condition: $|d(e_i, r_l) - d(e_j, r_l)| = d(e_i, e_j)$ for some $r_l \in S_E$. Table 3 and table 4 represents different pair of edges in $\Gamma(1)$ and corresponding vertex from S_E that strongly resolves that pair of distinct edges.

Pair of edges	$d(e_i, e_j)$	Strongly resolving vertex (r_l)	$d(e_i, r_l)$	$d(e_j, r_l)$	$\Delta = d(e_i, r_l) - d(e_j, r_l) $
(e_1, e_2)	0	r_2	0	0	0
(e_1, e_3)	1	r_1	0	1	1
(e_1, e_4)	0	r_1	0	0	0
(e_1, e_5)	1	r_1	0	1	1
(e_1, e_6)	1	r_2	0	1	1
(e_1, e_7)	2	r_1	0	2	2
(e_1, e_8)	1	r_1	0	1	1
(e_1, e_9)	0	r_1	0	0	0
(e_1, e_{10})	1	r_2	0	0	0
(e_1, e_{11})	1	r_1	0	1	1
(e_1, e_{12})	0	r_2	0	0	0
(e_2, e_3)	0	r_3	0	0	0
(e_2, e_4)	1	r_2	0	1	1
(e_2, e_5)	1	r_2	0	1	1

Pair of edges	$d(e_i, e_j)$	Strongly resolving vertex (r_i)	$d(e_i, r_i)$	$d(e_j, r_i)$	$\Delta = d(e_i, r_i) - d(e_j, r_i) $
(e_2, e_6)	1	r_2	0	1	1
(e_2, e_7)	2	r_2	0	2	2
(e_2, e_8)	2	r_3	0	2	2
(e_2, e_9)	1	r_2	0	1	1
(e_2, e_{10})	0	r_2	0	0	0
(e_2, e_{11})	0	r_3	0	0	0
(e_2, e_{12})	1	r_2	0	1	1
(e_3, e_4)	0	r_2	1	1	0
(e_3, e_5)	2	r_3	0	2	2
(e_3, e_6)	1	r_3	0	1	1
(e_3, e_7)	1	r_3	0	1	1
(e_3, e_8)	2	r_3	0	2	2
(e_3, e_9)	1	r_1	1	0	1
(e_3, e_{10})	1	r_3	0	1	1
(e_3, e_{11})	0	r_3	0	0	0
(e_3, e_{12})	0	r_1	1	1	0
(e_4, e_5)	1	r_1	0	1	1
(e_4, e_6)	2	r_1	0	2	2
(e_4, e_7)	2	r_1	0	2	2
(e_4, e_8)	1	r_1	0	1	1
(e_4, e_9)	0	r_1	0	0	0
(e_4, e_{10})	1	r_1	0	1	1
(e_4, e_{11})	1	r_3	1	0	1
(e_4, e_{12})	0	r_3	1	1	0
(e_5, e_6)	0	r_2	1	1	0
(e_5, e_7)	1	r_2	2	1	1
(e_5, e_8)	0	r_1	1	1	0
(e_5, e_9)	1	r_1	1	0	1
(e_5, e_{10})	0	r_1	1	1	0
(e_5, e_{11})	1	r_1	1	2	1
(e_5, e_{12})	1	r_2	1	2	1
(e_6, e_7)	0	r_3	1	1	0
(e_6, e_8)	1	r_3	1	2	1

(e_6, e_9)	1	r_3	1	2	1
(e_6, e_{10})	0	r_3	1	1	0
(e_6, e_{11})	0	r_2	1	1	0
(e_6, e_{12})	1	r_1	2	1	1
(e_7, e_8)	0	r_2	2	2	0
(e_7, e_9)	2	r_1	2	0	2
(e_7, e_{10})	2	r_2	2	0	2
(e_7, e_{11})	0	r_1	2	2	0
(e_7, e_{12})	0	r_3	1	1	0
(e_8, e_9)	0	r_3	2	2	0
(e_8, e_{10})	1	r_3	2	1	1
(e_8, e_{11})	1	r_1	1	2	1
(e_8, e_{12})	0	r_1	1	1	0
(e_9, e_{10})	1	r_1	0	1	1
(e_9, e_{11})	2	r_3	2	0	2
(e_9, e_{12})	1	r_1	0	1	1
(e_{10}, e_{11})	1	r_2	0	1	1
(e_{10}, e_{12})	2	r_2	0	2	2
(e_{11}, e_{12})	1	r_2	1	2	1

Since every pair of distinct edges is strongly resolved by some vertex from S_E , therefore the set S_E is a strong edge metric generator of $\Gamma(1)$. Thus $\text{sedim}(\Gamma(1)) \leq 3$.

Lemma 2 (Lower Bound)

No set of two vertices in $\Gamma(1)$ can be a strong edge metric generator. Consequently,

$$\text{sedim}(\Gamma(1)) \geq 3.$$

Proof. The automorphism group of $\Gamma(1)$ has order 48 and partitions the 28 two-vertex subsets into three orbits:

Orbit	Representative	Distance
I (Adjacent)	$\{v_1, v_2\}$	1
II (Distance 2)	$\{v_1, v_3\}$	2
III (Opposite)	$\{v_1, v_8\}$	3

It suffices to check one representative from each orbit. There are three cases:

Case I. Consider $S = \{v_1, v_2\}$.

Consider edges $e_2 = (v_2, v_3)$ and $e_{11} = (v_3, v_7)$. Since these edges share vertex v_3 , therefore, $d(e_2, e_{11}) = 0$. We have $d(e_2, v_1) = 1$, $d(e_{11}, v_1) = 2$

$$\Rightarrow |d(e_2, v_1) - d(e_{11}, v_1)| = |1 - 2| = 1 \neq 0 = d(e_2, e_{11})$$

$$\text{And } d(e_2, v_2) = 0,$$

$$d(e_{11}, v_2) = 1$$

$$\Rightarrow |d(e_2, v_2) - d(e_{11}, v_2)| = |0 - 1| = 1 \neq 0 = d(e_2, e_{11}) \text{ Thus, } S \text{ fails.}$$

Case II. Let $S = \{v_1, v_3\}$.

Consider edges $e_7 = (v_7, v_8)$ and $e_{10} = (v_2, v_6)$. Since these are opposite edges, therefore, $d(e_7, e_{10}) = 2$. We have $d(e_7, v_1) = 2$, $d(e_{10}, v_1) = 1$

$$\Rightarrow |d(e_7, v_1) - d(e_{10}, v_1)| = |2 - 1| = 1 \neq 2 = d(e_7, e_{10})$$

$$\text{And } d(e_7, v_3) = 1,$$

$$d(e_{10}, v_3) = 1$$

$$\Rightarrow |d(e_7, v_3) - d(e_{10}, v_3)| = |1 - 1| = 0 \neq 2 = d(e_7, e_{10}) \text{ Thus, } S \text{ fails.}$$

Case III. Let $S = \{v_1, v_8\}$.

Consider edges $e_2 = (v_2, v_3)$ and $e_{11} = (v_3, v_7)$. Since these edges share vertex v_3 , therefore, $d(e_2, e_{11}) = 0$. We have $d(e_2, v_1) = 1$, $d(e_{11}, v_1) = 2$

$$\Rightarrow |d(e_2, v_1) - d(e_{11}, v_1)| = |1 - 2| = 1 \neq 0 = d(e_2, e_{11})$$

$$\text{And } d(e_2, v_8) = 2,$$

$$d(e_{11}, v_8) = 1$$

$$\Rightarrow |d(e_2, v_8) - d(e_{11}, v_8)| = |2 - 1| = 1 \neq 0 = d(e_2, e_{11}) \text{ Thus, } S \text{ fails.}$$

Since all representatives fail, every two-vertex subset fails to be a strong edge metric generator. Therefore,

$$\text{sedim}(\Gamma(1)) \geq 3.$$

□

Theorem 2. The strong edge metric dimension of $\Gamma(1)$ is 3 i.e., $\text{sedim}(\Gamma(1)) = 3$.

Proof. From theorem 1, we have $\text{sedim}(\Gamma(1)) \leq 3$. From Lemma 2, we have $\text{sedim}(\Gamma(1)) \geq 3$. Therefore,

$$\text{sedim}(\Gamma(1)) = 3.$$

□

Theorem 3. For $n \geq 2$, the strong edge metric dimension of $\Gamma(n)$ is $7^{n-2} \times 24$.

Proof. Let S_E be the collection of vertices consisting of each of the outermost vertices of type r_1, r_2, r_3 from each branch of $\Gamma(n)$. Then number of elements in S_E is

$$|S_E| = 7^{n-2} \times 24.$$

We claim that $S_E \subset V(\Gamma(n))$ is a strong edge resolving set for $n \geq 2$.

For this, we need to show that for every pair of distinct edges, there exists a vertex in S_E which strongly resolves that pair of edges.

Consider any pair of distinct edges of $\Gamma(n)$. The selection of an arbitrary pair of distinct edges can be compared in the following ways:

Case I: If the pair of edges is such that both the edges lie in an outermost cube of $\Gamma(n)$.

In this case, the pair will be resolved by at least three vertices which are in S_E (by Theorem 1).

Case II: When two arbitrarily chosen edges belong to distinct cubes in a chain CH_C , where one such cube is an outer cube (as depicted in Figure 5).

Let e_L and e_M denote two distinct edges residing on separate cubes, L -cube and M -cube respectively, within the cube chain. Then the pair $\{e_L, e_M\}$ is strongly resolved by r_i , which is a vertex on the outermost cube and is an element of S_E .

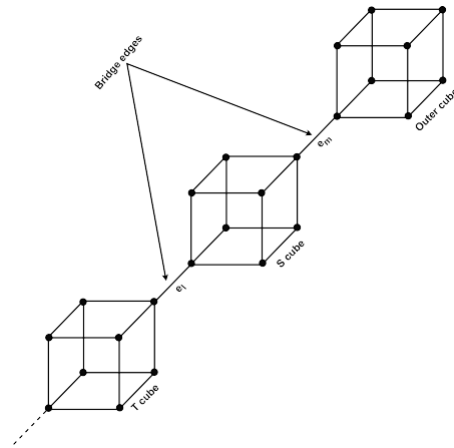


Figure 5: Chain CH_C of cubes

Case III: When both arbitrarily chosen edges act as bridge edges within the cube chain CH_C , with one edge terminated at an outermost-level cube (as depicted in Figure 5),

Let e_{b1} and e_{b2} be that pair of distinct edges. Then this pair of edges is strongly resolved by the vertex r_i , which is a vertex on the outermost cube and is an element of S_E .

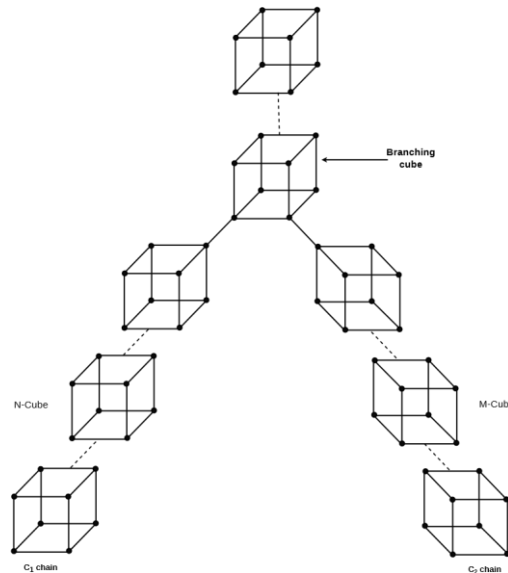


Figure 6: Two chain of cubes connected through a branching cube

Case IV: When two arbitrarily selected edges reside on distinct cube chains, denoted as C_1 and C_2 , both of which intersect at a shared cube known as the branching cube.

Assume that two selected edges, e_M and e_N , reside on distinct cubes designated as M -cube and N -cube, respectively. Furthermore, let these cubes belong to separate cube chains, denoted C_1 and C_2 , which join at a branching cube, as illustrated in Figure 6.

Then clearly, vertex r_j (a vertex from that outermost cube, from which the vertex e_N is at a shortest distance following through the edge e_M)

strongly resolves the pair of edges e_M and e_N as, moving from e_N to r_j , there exists a shortest path which includes e_M .

Case V: When two arbitrarily chosen bridge edges belong to distinct cube chains, denoted C_1 and C_2 , where both chains join at a mutual branching cube B .

Let e_{b1} and e_{b2} be the selected bridge edges. Then clearly, from the Case V, there exists a vertex r_k that will strongly resolve the pair $\{e_{b1}, e_{b2}\}$.

Case VI: When both arbitrarily chosen edges reside on the central cube, as illustrated in Figure 7.

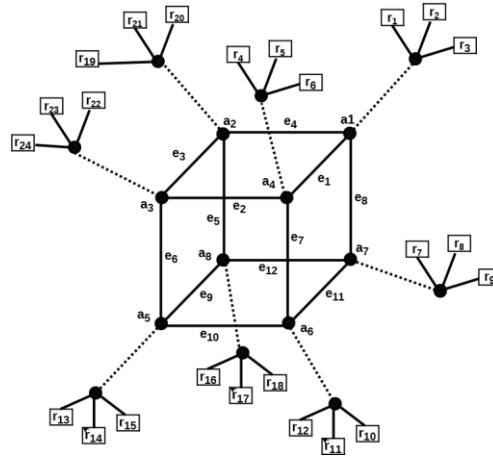


Figure 7: Central cube

The table below represents the various distinct pairs of edges from the central cube $\Gamma(n)$ and the corresponding vertex from the outermost cube that strongly resolves the pair of edges:

Edge Pair	Resolving Vertex	Edge Pair	Resolving Vertex
(e_1, e_2)	r_4	(e_2, e_6)	r_2
(e_1, e_3)	r_{19}	(e_3, e_4)	r_{19}
(e_1, e_4)	r_1	(e_3, e_5)	r_{19}
(e_1, e_5)	r_{19}	(e_3, e_6)	r_{22}
(e_1, e_6)	r_{22}	(e_4, e_5)	r_{19}
(e_2, e_3)	r_{22}	(e_4, e_6)	r_{22}
(e_2, e_4)	r_1	(e_5, e_6)	r_{13}
(e_2, e_5)	r_{19}	(e_{11}, e_{12})	r_7
(e_1, e_7)	r_4	(e_5, e_7)	r_4
(e_1, e_8)	r_1	(e_5, e_8)	r_1
(e_1, e_9)	r_{13}	(e_5, e_9)	r_{16}
(e_1, e_{10})	r_{10}	(e_5, e_{10})	r_{13}
(e_1, e_{11})	r_7	(e_5, e_{11})	r_7
(e_1, e_{12})	r_7	(e_5, e_{12})	r_{16}
(e_2, e_7)	r_4	(e_6, e_7)	r_4
(e_2, e_8)	r_1	(e_6, e_8)	r_1
(e_2, e_9)	r_{13}	(e_6, e_9)	r_{13}
(e_2, e_{10})	r_{13}	(e_6, e_{10})	r_{13}
(e_2, e_{11})	r_{10}	(e_6, e_{11})	r_{10}
(e_2, e_{12})	r_7	(e_6, e_{12})	r_{16}
(e_3, e_7)	r_4	(e_7, e_8)	r_1
(e_3, e_8)	r_1	(e_7, e_9)	r_{13}

(e_3, e_9)	r_{13}	(e_7, e_{10})	r_{10}
(e_3, e_{10})	r_{13}	(e_7, e_{11})	r_{10}
(e_3, e_{11})	r_{10}	(e_7, e_{12})	r_7
(e_3, e_{12})	r_{16}	(e_8, e_9)	r_{16}
(e_4, e_7)	r_4	(e_8, e_{10})	r_{10}
(e_4, e_8)	r_1	(e_8, e_{11})	r_7
(e_4, e_9)	r_{16}	(e_8, e_{12})	r_7
(e_4, e_{10})	r_{10}	(e_9, e_{10})	r_{13}
(e_4, e_{11})	r_7	(e_9, e_{11})	r_{10}
(e_4, e_{12})	r_7	(e_9, e_{12})	r_{16}
(e_{10}, e_{11})	r_{10}	(e_{10}, e_{12})	r_7

□

Case VII: When both the arbitrarily selected edges are on a middle cube, which is neither the outermost cube nor the central cube.

Assume that the central cube C_m contains two arbitrarily selected edges, as illustrated in Figure 8. Let the eight vertices of C_m be denoted by $c, a_1, a_2, \dots, a_7$, and its edges by e_i for $i \in \{1, 2, \dots, 12\}$.

As established in case VI, each vertex is incident to three edges of C_m . Consequently, following a similar argument as discussed in Case VI, it follows that the pair is strongly resolved by at least one vertex from S_E .

Case VIII: When the pair of arbitrarily selected edges consists of one edge situated on a cube and the other acting as a bridge edge connecting adjacent cubes.

In this case, two subcases arises:

Subcase I: If the distance between the central most cube and the above selected bridge edge is smaller than the distance between the central most cube and the above selected edge on the cube. In this subcase the vertices from the set S_E that lies on the outermost cube, which is at the shortest distance from the

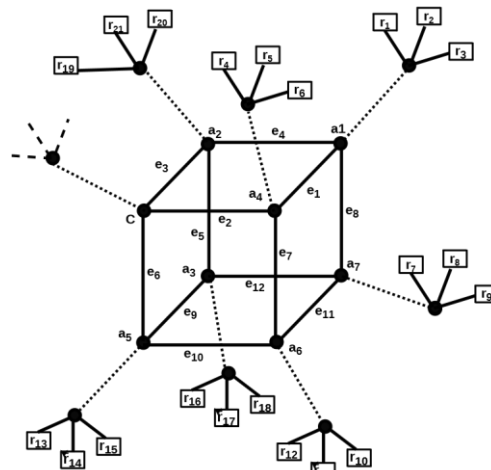


Figure 8: Central cube C_m

selected edge on the cube, will strongly resolve that pair of edge.

Subcase II: If the distance between the central most cube and the above selected bridge edge is greater than the distance between the central most cube and the above selected edge on the cube. In

this subcase the vertices from the set S_E that lies on the outermost cube, which is at the shortest distance from the selected bridge edge, will strongly resolve that pair of edge.

From all of the above cases, it follows that $\text{sedim}(\Gamma(n)) \leq 7^{n-2} \times 24$.

Also from theorem 1, it follows that $sedim(\Gamma(n)) \geq 7^{n-2} \times 24$ and thus $sedim(\Gamma(n)) = 7^{n-2} \times 24$, $n \geq 2$.

4 Conclusion

In this paper, we investigated the graph-theoretic properties of certain carbon-based crystal structures, focusing on the determination of their strong edge metric dimension. By analyzing the structural characteristics and distance-based representations of the network, we successfully established exact formulas (and/or sharp bounds) for the strong edge metric generators across various structural layers. Our findings reveal that the strong edge metric dimension provides a robust, uniquely identifying framework for distinguishing chemical bonds (edges) in complex carbon architectures. A natural direction for future research includes extending these resolvability parameters to other higher-dimensional carbon networks, evaluating fault-tolerant strong edge metric dimensions, and exploring their practical applications in QSAR/QSPR modeling within computational chemistry.

5 Declarations

Competing Interests

The authors declare no conflict of interest regarding the publication of this manuscript.

Ethical Approval Not applicable.

Authors' Contributions

All authors' contributed equally in this work

Data Availability

No datasets or software were generated, utilized, or analyzed to support the conclusions of this study.

References

- 1 Trinajstić N *Chemical Graph Theory* CRC Press (1983)
- 2 Slater P J 1975 Leaves of trees *Congr. Numer.* **14** 549-559
- 3 Chartrand G, Eroh L, Johnson M A and Oellermann O R 2000 Resolvability in graphs and the metric dimension of a graph *Discrete Appl. Math.* **105** 99-113
- 4 Melter R A and Tomescu I 1984 Metric bases in digital geometry *Comput. Gr. Image Process* **25** 113-21
- 5 Sebő A and Tannier E 2004 On metric generators of graphs *Math. Oper. Res.* **29**(2) 383-93
- 6 Khuller S, Raghavachari B and Rosenfeld A 1996 Landmarks in graphs, *Disc. Appl. Math.* **70** 217-29
- 7 Peterin, I., & Yero, I. G. (2020). Edge Metric Dimension of Some Graph Operations: I. Peterin, IG Yero. Bulletin of the Malaysian Mathematical Sciences Society, 43(3), 2465-2477.
- 8 Okamoto F, Crosse L, Phinezy B, and Zhang P 2010 The local metric dimension of a graph *Math. Bohem.* 135 239-55
- 9 Kelenc A, Kuziak D, Taranenko A and Yero I G 2017 Mixed metric dimension of graphs *Appl. Math. Comput.* **314** 420-38
- 10 Kelenc A, Tratnik N and Yero I G 2018 Uniquely identifying the edges of a graph: the edge metric dimension *Discret. Appl. Math.* **251** 204-20
- 11 Hernando M C, Mora M, Slater P J and Wood D R 2008 Fault-tolerant metric dimension of graphs *Convexity Discrete Struct.* **5** 81-5
- 12 Liu X, Ahsan M, Zahid Z and Ren S 2021 Fault-tolerant edge metric dimension of certain families of graphs *AIMS Math.* **6** 1140-52
- 13 Chartrand G and Zhang P 2006 The theory and applications of resolvability in graphs: A survey. In: Proceedings of the 34th Southeastern International Conference on Combinatorics, Graph Theory and Computing *Congr. Numer.* **160** 47-68
- 14 Raza H, Hayat S and Pan X F 2019 On the fault-tolerant metric dimension of certain interconnection networks *J. Appl. Math. Comput.* **60** 517-35
- 15 Somasundari M and Raj F S 2019 Fault-tolerant resolvability of oxide interconnections *Int. J. Innov. Tech. Explor. Eng.* **8** 1-15
- 16 Krishnan S and Rajan B 2016 Fault-tolerant resolvability of certain crystal structures *Appl. Math.* **7** 599-604

- 17 Sharma S and Bhat V K 2022 Fault-tolerant metric dimension of zero-divisor graphs of commutative rings *AKCE Int. J. Graphs Comb.* **19** 24-30
- 18 Sharma S K and Bhat V K 2022 Fault-tolerant metric dimension of two-fold heptagonal-nonagonal circular ladder, *Discrete Math. Algorithms Appl.* 2150132 <https://doi.org/10.1142/S1793830921501329>.
- 19 Song, Z., Fang, Z., & Fang, C. (2017). (d-2)-dimensional edge states of rotation symmetry protected topological states. *Physical review letters*, 119(24), 246402.
- 20 Knor, Martin, Snježana Majstorović, Aoden Teo Masa Toshi, Riste Škrekovski, and Ismael G. Yero. "Graphs with the edge metric dimension smaller than the metric dimension." *Applied Mathematics and Computation* 401 (2021): 126076.
- 21 Raza H, Hayat S and Pan X F 2018 On the fault-tolerant metric dimension of convex polytopes *Appl. Math. Comput.* **339** 172–85
- 22 Liu J B, Munir M, Ali I, Hussain Z and Ahmed A Fault tolerant metric dimension of wheel related graphs, *Hal Archives* Hal-1857316v2 <https://hal.archives-ouvertes.fr/hal01857316v2/document>
- 23 Mojgan A, Strong Edge Metric Dimension
- 24 Raza H, Hayat S, Imran M and Pan X F 2019 Fault-tolerant resolvability and extremal structures of graphs *Mathematics* **7** 78–97
- 25 Azhar K, Zafar S, Kashif A, Aljaedi A and Albalawi U 2022 The Application of Fault-Tolerant Partition Resolvability in Cycle-Related Graphs *Appl. Sci.* **12(19)** 9558 <https://doi.org/10.3390/app12199558>
- 26 Gao W, Siddiqui M K, Naeem M and Rehman N A 2017 Topological characterization of carbon graphite and crystal cubic carbon structures *Molecules* **22** 1496 <https://doi.org/10.3390/molecules22091496>
- 27 Baig A Q, Imran M, Khalid W and Naeem M 2017 Molecular description of carbon graphite and crystal cubic carbon structures *Can. J. Chem.* **95** 674-86
- 28 Imran M, Naeem M, Baig A Q, Siddiqui M K, Zahid M A and Gao W 2019 Modified eccentric descriptors of crystal cubic carbon *J. Discret. Math. Sci. Cryptogr.* **22(7)** 1215-28
- 29 Yang H, Naeem M, Baig A Q, Shaker V and Siddiqui S K, Vertex Szeged index of crystal cubic carbon structure *J. Discret. Math. Sci. Cryptogr.* **22** 1177-87
- 30 Zhang X and Naeem M 2021 Metric dimension of crystal cubic carbon structure *J. Math.* 3438611 <https://doi.org/10.1155/2021/3438611>
- 31 Sattar A and Javaid M 2022 Topological characterizations of crystal cubic carbon structures *Can. J. Chem.* **100** 828-39
- 32 Yang H, Siddiqui M K, Naeem M and Rehman N A 2020 Molecular properties of carbon crystal cubic structures, *Open Chem.*, **18** 339-46
- 33 Zahid M A, Naeem M, Baig A Q and Gao W 2018 General fifth M-Zagreb indices and fifth M-Zagreb polynomials of crystal cubic carbon *Util. Math.* **109**. <https://utilitasmathematica.com/index.php/Index/article/view/1284>
- 34 Yang H, Siddiqui M K, Arshad M and Naeem M 2018 Degree-distance based topological indices of crystal cubic carbon <https://doi.org/10.3390/atoms6040062>
- [35] Sharma S, Bhat V K and Lal S 2023 Multiplicative Topological Indices of the Crystal Cubic Carbon Structure *Cryst. Res. Technol.* **58** 2200222 <https://doi.org/10.1002/crat.202200222>
- [36] Sharma S, Bhat V K and Lal S 2023 Edge resolvability of crystal cubic carbon structure *Theor. Chem. Acc.* **142** 24 <https://doi.org/10.1007/s00214-023-02964-3>