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Fault-Tolerant Metric Dimension in Carbon Networks

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Abstract: In this paper, we study the fault-tolerant metric dimension in graph theory, an important measure against failures in unique vertex identification. The metric dimension of a graph is the smallest number of vertices required to uniquely identify every other vertex based on their distances from these chosen vertices. Building on existing work, we explore fault tolerance by considering the minimal number of vertices needed to ensure that all other vertices remain uniquely identifiable even if a specified number of these vertices fails. We compute the fault-tolerant metric dimension of various chemical graphs, namely fullerenes, benzene, and polyphenyl graphs.

Keywords: fullerene; polyphenol; metric dimension; fault-tolerant metric dimension

1. Introduction

Slater firstly introduced the concept of a resolving set in 1975 ([1]). Subsequently, Harary and Melter [2] proposed a similar notion, terming it a "metric dimension". Chartrand et al. [3] further expanded on this by introducing the concept of metric basis, with the cardinality termed as the metric dimension (MD). Over the recent decade, researchers have widely explored the MD and its associated parameters due to their significant relevance in identifying nodes within graphs and networks. The MD determines the smallest set of vertices required to uniquely identify all other vertices through their distances. With its roots deeply embedded in the study of graph-based networks, the MD has gathered significant attention due to its applications in various fields ranging from computer science to social network analysis [4], transportation systems [5], and molecular biology [6,7]. The MD uses the shortest path distances from a set of landmarks, which are useful in network discovery, verification, and optimization [8]. In social networks, the MD helps in identifying influential nodes and tracking the spread of information or diseases [9]. The MD is also used in navigation systems to simplify complex transportation networks, improving route planning and traffic flow [5]. Chartrand et al. explored some applications of resolving sets in chemistry [3]. The MD of bicyclic graphs was computed by Asad et al. [10]. Furthermore, the applications of the MD span various scientific domains, including robot navigation in autonomous systems [11], geographical route determination, and telecommunications [12].

Recent developments in this context paved the way for a new related concept known as the fault-tolerant metric dimension (FTMD). The concept of fault tolerance in the definition of a resolving set was introduced by Hernando et al. [13]. Calculating the FTMD involves finding the smallest set of nodes such that the remaining network can maintain this identifying property even under specific fault conditions. The issue of vertex failure, which can occur due to errors like experimental inaccuracies and computational limitations or attacks, poses a significant challenge. However, practical applications in physics,

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chemistry, and material science require that these systems remain robust even when certain data points or measurements fail [14]. The study of the FTMD has emerged as a critical domain within network theory, addressing the resilience of networks when faced with node or link failures. This concept extends the traditional notion of the MD by accounting for the network's ability to maintain its navigational integrity even in the presence of faults. The FTMD of a graph is a special and significant parameter that is a generalization of the MD of a graph. The chosen vertex set for the FTMD could be different for different graphs. However, its construction method is uniquely optimal following the definition of the FTMD and can provide alternate optimal solutions. The optimality of a vertex set depends upon the structure of a graph. Different chemical graphs exhibit unique connectivity patterns, affecting the selection of the most representative vertex set. Research on the FTMD focuses on developing algorithms and strategies to find these resilient subsets efficiently, ensuring that networks can function optimally even in the presence of faults or failures. The FTMD finds application in various real-world scenarios, including interconnection and communication networks [15] and wireless system networks [16]. The FTMD of networks with circulant properties, for example, has been investigated in [17–19].

Use of MD and FTMD in Mathematical Chemistry

One area of graph theory that has its own specialization and mathematics is chemical graph theory. It examines different chemical structures through graphical representations. In a chemical graph, vertices represent atoms and edges represent bonds. When chemical structures are vast and complex, the utility of direct analysis may be limited. The chemical graph theory makes this easier by providing valuable insights into the structure and properties of molecules. Fullerenes, benzene, and polyphenyls each play unique roles in carbon networks. Benzene serves as a fundamental aromatic building block, polyphenyls help create intricate and stable carbon-based structures, and fullerenes provide unique molecular forms and the capacity to enclose other substances. Benzene's stable aromatic structure makes it an essential component in polymer production. By adding electron-donating or withdrawing groups, like halogens or hydroxyls, its reactivity can be adjusted to create polymers that are either stronger or more flexible [4]. Modified benzene derivatives also offer better solubility and heat resistance, making them valuable for advanced plastics and protective coatings [3]. Polyphenylene materials are highly resistant to heat and oxidation, making them essential for high-performance polymers. Their mechanical strength and conductivity can be enhanced by cross-linking or incorporating nanomaterials like carbon nanotubes and graphene [4]. Increasing their crystallinity further boosts wear resistance, making them ideal for aerospace and structural applications [10]. Fullerene is the third allotrope of carbon after graphite and diamond. Any molecule composed solely of carbon atoms that can be tube-shaped, hollow spherical, or ellipsoid is called a fullerene. Fullerenes are incredibly stable, both thermally and chemically, which makes them perfect for use in electronics. Scientists have found that adding certain metals to them can boost their electrical conductivity, making them even better for things like superconductors and solar cells [4]. They are also highly resistant to oxidation, which is why they work well in fuel cells and lubricants (see [20]). Fullerenes are composed of a hexagonal and pentagonal cage-like structure, so they are very durable and useful in nanotechnology and protective coatings. Since the fullerene molecule was discovered by Kroto et al. in 1985, fullerene has garnered significant interest across various scientific domains (see [20]). Fullerenes have therapeutic uses in dentistry, drug transport, antioxidant action, and antiviral activity. The six-carbon ring benzene, which has alternating double bonds, is a well-known example of a structure that is explored in graph theory and chemistry. Graph theory and its allied subjects frequently employ the graph representation of benzenes in their numerous

applications. Many well-known drugs that treat pain, cold and flu symptoms, and aid in weight loss contain benzene C_6H_6. A variety of colours, detergents, and medicinal medications are made with benzene. Furthermore, in material science, crystal structures and molecular lattices are studied using the FTMD. This idea aids in the classification and comparison of network architectures in the GeSbTe superlattice, for instance, which is utilized in phase-change memory materials [21]. The MD of dual polar graphs was discussed by Bailey et al. [22]. The FTMD also enhances the reliability of QSAR models, especially in high-dimensional datasets [23]. Umer et al. studied the MD of line graphs of bakelite and subdivided bakelite networks [24]. The FTMD of boron nano-lattices is discussed by Zafar and Mubeen [25]. The FTMD of a two-fold heptagonal-nonagonal circular ladder is revealed by Sharma and Bhat [26]. Lin et al. studied the ultra-efficient heat transport across "2.5D" all-carbon sp^2/sp^3 [27] and hierarchical AlN/erythritol composite phase-change materials with ultra-efficient polarity enhanced heat conduction [28]. The computational complexity of all parameters within the resolvability family is connected to the hardness of non-deterministic polynomial time [3,11,29]. As such, this manuscript delves into the FTMD for five chemical graphs.

2. Preliminaries

Consider a graph $\mho$ of order ζ with the vertex and edge sets as $V(\mho)$ and $E(\mho)$. The distance between two vertices $\gamma, \wp \in V(\mho)$, denoted by $d(\gamma, \wp)$, is the least number of edges in the $\gamma - \wp$ path. For a vertex $\wp \in V(\mho)$, $N(\wp)$ and $N[\wp]$ denote the open neighbourhood and closed neighbourhood of $\wp$ in $\mho$, where $N(\wp) = \{b \in V(\mho) : b \text{ is adjacent to } \wp\}$ and $N[\wp] = N(\wp) \cup \{\wp\}$ (see [30]). Assume that $\Im \subseteq V(\mho)$, where $\Im = \{\Im_1, \Im_2, \ldots, \Im_f\}$. The representation $r(\wp|\Im)$ of a vertex $\wp$ with respect to $\Im$ comprises the f-ordered distances $(d(\wp, \Im_1), d(\wp, \Im_2), \ldots, d(\wp, \Im_f))$. We determine that $\Im$ is the resolving set of $\mho$ if every element of the vertex set has a distinct representation with $\Im$. The MD of $\mho$, represented as $\beta(\mho)$, equals the cardinality of $\Im$ if it is the smallest resolving set of $\mho$. A resolving set $\Im$ for a graph $\mho$ is fault-tolerant if $\Im \setminus \wp$ is also resolving for each $\wp \in \Im$. The fault-tolerant metric dimension of $\mho$, denoted by $\beta^{'}(\mho)$, is the minimum number of members in a fault-tolerant resolving set $\Im$.

The following proposition relates the MD to the FTMD, which will be helpful in our proofs.

Proposition 1 ([31]). *For a connected graph* $\mho$, $\beta^{'}(\mho) \geq \beta(\mho) + 1$.

The remaining sections of this paper are structured as follows: Section 3 explains the methodology, algorithmic approach, and scope of this study. Section 4 focuses on computing the exact values of the FTMD for fullerene graphs. The FTMDs for benzene, ortho, and meta polyphenyl graphs are explored in Section 5. Applications of the FTMD are provided in Section 6. In Section 7, we provide conclusions and outline future research directions.

3. Methodology

The following algorithmic steps can be followed to construct a fault-tolerant resolving set of a given cardinality. Suppose we have a connected graph with n vertices and that we want to check if its fault-tolerant metric dimension is k. We proceed as follows:

Output: A fault-tolerant resolving set $\Im$.

1. Initialization:
   - Start with adjacency matrix $A = [a_{ij}]$ (with $a_{ij} = 1$ if vertices are adjacent; otherwise, $a_{ij} = 0$).

- Compute the distance matrix $D = [d_{ij}]$ (with d_{ij} being the distance between vertices v_i and v_j.

2. Building the fault-tolerant resolving set of a given cardinality k:
   - For $i = 1$ to m (where $m = \binom{n}{k}$).
   - Compute $\Im = \{\Im_1, \Im_2, \ldots, \Im_m\}$ (where each $\Im_i$ contains k number of vertices).
3. Check fault tolerance:
   - For each $\Im_i$, compute the distance vector representations $r(v|\Im_i)$ for all the vertices.
   - If the representations ensure fault tolerance, then STOP $\Im_i$ is the required set.
   - Otherwise, choose the next $\Im_i$ until the list is completely exhausted.
   - If all the $\Im_i$ fail, then start the procedure with $k + 1$.
4. Output:
   - Return the set $\Im_i$ as the fault-tolerant resolving set.

Scope and Limitations

The above algorithmic steps can be implemented in any programming language like MATLAB or Python to compute the fault-tolerant resolving set for a connected graph. However, due to the NP-hardness of the problem, we can effectively use it for smaller graphs. On the other hand, these steps can help to explore bigger families of graphs if there is symmetry and regularity in the graphs. We can use pattern recognition and graph-theoretic properties to compute the resolving sets and distance representations of the vertices. This would enable us to explore the larger and complex graphs. This literature review also indicates that the MD and FTMD have significant uses in the fields of networks, chemistry, optimization, material science, and robotics.

4. Fault-Tolerant Metric Dimension of Fullerene Graph

We calculate the FTMD of fullerene graph classes in this section. The faces of a $(k, 6)$-fullerene graph are k and 6 in size. There is only a $(k, 6)$-fullerene graph for $k = 3$, 4, and 5. There are cycles of orders four and six in a $(4, 6)$-fullerene graph.

4.1. FTMD of Fullerene Graph $G_1[\zeta]$

A $(4, 6)$-fullerene graph denoted by $G_1[\zeta]$ has order 8ζ. The $G_1[\zeta]$ has vertex set $V(G_1[\zeta]) = \{x_1, x_2, \ldots, x_{4\zeta}\} \cup \{y_1, y_2, \ldots, y_{4\zeta}\}$. The edge set of $E(G_1[n]) = X \cup X_1 \cup Y \cup Y_1 \cup X_2$, where $X = \{x_\tau x_{\tau+1} : 1 \leq \tau \leq 4\zeta - 1\}$, $X_1 = \{x_{2\tau-1}x_{4\zeta-\tau+1} : 1 \leq \tau \leq 2\zeta - 1\}$, $Y = \{y_\tau y_{\tau+1} : 1 \leq \tau \leq 4\zeta - 1\}$, $Y_1 = \{y_{2\tau-1}y_{4\zeta-\tau+1} : 1 \leq \tau \leq 2\zeta - 1\}$ and $X_2 = \{x_\tau y_\tau : 1 \leq \tau \leq 4\zeta\}$. The graph of $G_1[4]$ is shown in Figure 1.

The MD of fullerene graph $G_1[n]$ is computed in [32].

Lemma 1 ([32]). *The MD of fullerene graph $G_1[\zeta]$ is 3 for $\zeta \geq 2$.*

We compute $\beta'(G_1[\zeta])$ in the subsequent theorem.

Theorem 1. *For a fullerene graph denoted as $G_1[\zeta]$ with $\zeta \geq 2$, the FTMD is 4.*

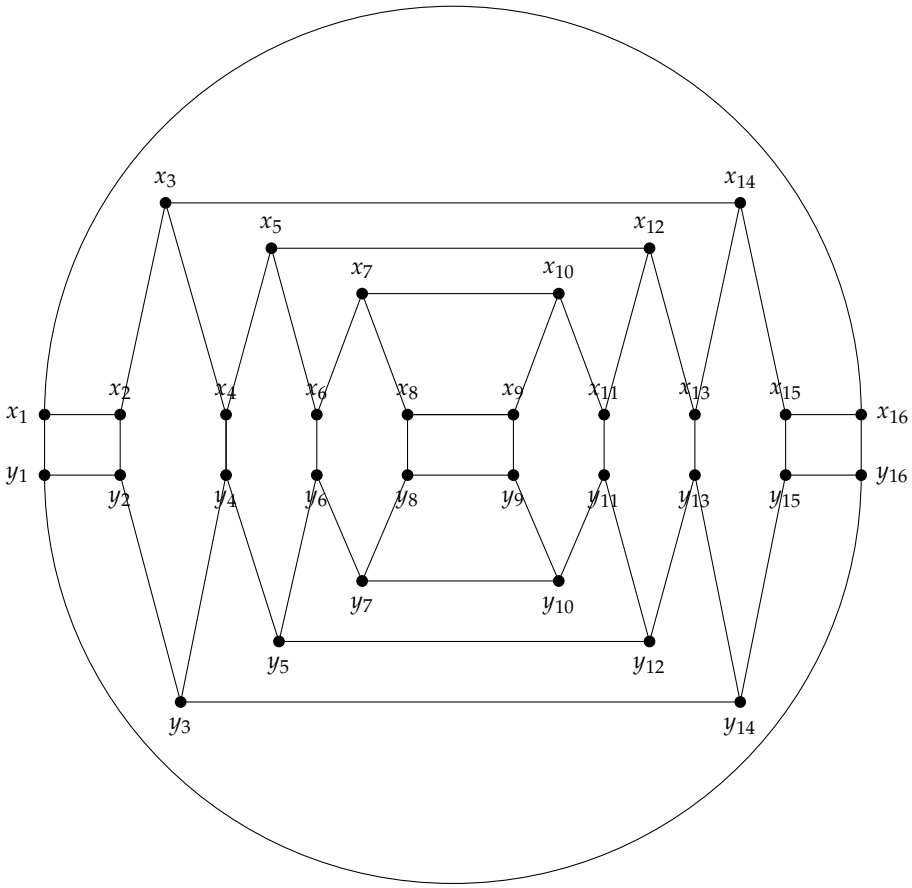


Figure 1. Fullerene graph $G_1[4]$.

Proof. To demonstrate that $\beta^{'}(G_1[\zeta]) = 4$, we begin by showing that $\beta^{'}(G_1[\zeta]) \leq 4$. Consider $\Omega = \{x_1, x_{2\zeta-1}, x_{2\zeta+2}, x_{4\zeta}\}$ to be a resolving set of $V(G_1[\zeta])$. The $r(x|\Omega)$ values are provided as follows:

$$r(x_\varrho|\Omega) = \begin{cases} (0, 2\zeta-2, 2\zeta-1, 1) & \text{for } \varrho = 1; \\ (\varrho-1, 2\zeta-\varrho-1, 2\zeta-\varrho, \varrho) & \text{for } 2 \leq \varrho \leq 2\zeta-2; \\ (2\zeta-2, 0, 1, 2\zeta-1) & \text{for } \varrho = 2\zeta-1; \\ (2\zeta-1, 1, 2, 2\zeta) & \text{for } \varrho = 2\zeta; \\ (2\zeta, 2, 1, 2\zeta-1) & \text{for } \varrho = 2\zeta+1; \\ (2\zeta-1, 1, 0, 2\zeta-2) & \text{for } \varrho = 2\zeta+2; \\ (4\zeta-\varrho+1, \varrho-2\zeta-1, \varrho-2\zeta-2, 4\zeta-\varrho) & \text{for } 2\zeta+3 \leq \varrho \leq 4\zeta-1; \\ (1, 2\zeta-1, 2\zeta-2, 0) & \text{for } \varrho = 4\zeta. \end{cases}$$

The $r(y|\Omega)$ values are provided as follows:

$$r(y_\varrho|\Omega) = \begin{cases} (\varrho, 2\zeta-\varrho, 2\zeta-\varrho+1, \varrho+1) & \text{for } 1 \leq \varrho \leq 2\zeta-2; \\ (2\zeta-1, 3, 4, 2\zeta) & \text{for } \varrho = 2\zeta-1; \\ (2\zeta, 2, 3, 2\zeta+1) & \text{for } \varrho = 2\zeta; \\ (2\zeta+1, 3, 2, 2\zeta) & \text{for } \varrho = 2\zeta+1; \\ (2\zeta, 4, 3, 2\zeta-1) & \text{for } \varrho = 2\zeta+2; \\ (4\zeta-\varrho+2, \varrho-2\zeta, \varrho-2\zeta-1, 4\zeta-\varrho+1) & \text{for } 2\zeta+3 \leq \varrho \leq 4\zeta. \end{cases}$$

The unique representations above confirm that Ω is a fault-tolerant resolving set of $G_1[\zeta]$. Therefore, $\beta^{'}(G_1[\zeta]) \leq 4$. Also, by Lemma 1, $\beta(G_1[\zeta]) = 3$. Thus, by Proposition 1, $\beta^{'}(G_1[\zeta]) \geq 4$. Therefore, we conclude by establishing a connection between the two inequalities. Hence, $\beta^{'}(G_1[\zeta]) = 4$. □

4.2. FTMD of Fullerene Graph $G_2[\zeta]$

A $(4,6)$-fullerene graph denoted by $G_2[\zeta]$ has order $8\zeta+4$. The $G_2[\zeta]$ has vertex set $V(G_1[\zeta]) = \{x_1, x_2, \ldots, x_{4\zeta+2}\} \cup \{y_1, y_2, \ldots, y_{4\zeta+2}\}$. The edge set of $E(G_2[n]) = X \cup X_1 \cup Y \cup Y_1 \cup X_2$, where $X = \{x_\tau x_{\tau+1} : 1 \leq \tau \leq 4\zeta+1\}$, $X_1 = \{x_{2\tau-1}x_{4\zeta-\tau+3} : 1 \leq \tau \leq 2\zeta-1\}$, $Y = \{y_\tau y_{\tau+1} : 1 \leq \tau \leq 4\zeta+1\}$, $Y_1 = \{y_{2\tau-1}y_{4\zeta-\tau+3} : 1 \leq \tau \leq 2\zeta-1\}$ and $X_2 = \{x_\tau y_\tau : 1 \leq \tau \leq 4\zeta+2\}$. The graph of $G_2[4]$ is shown in Figure 2.

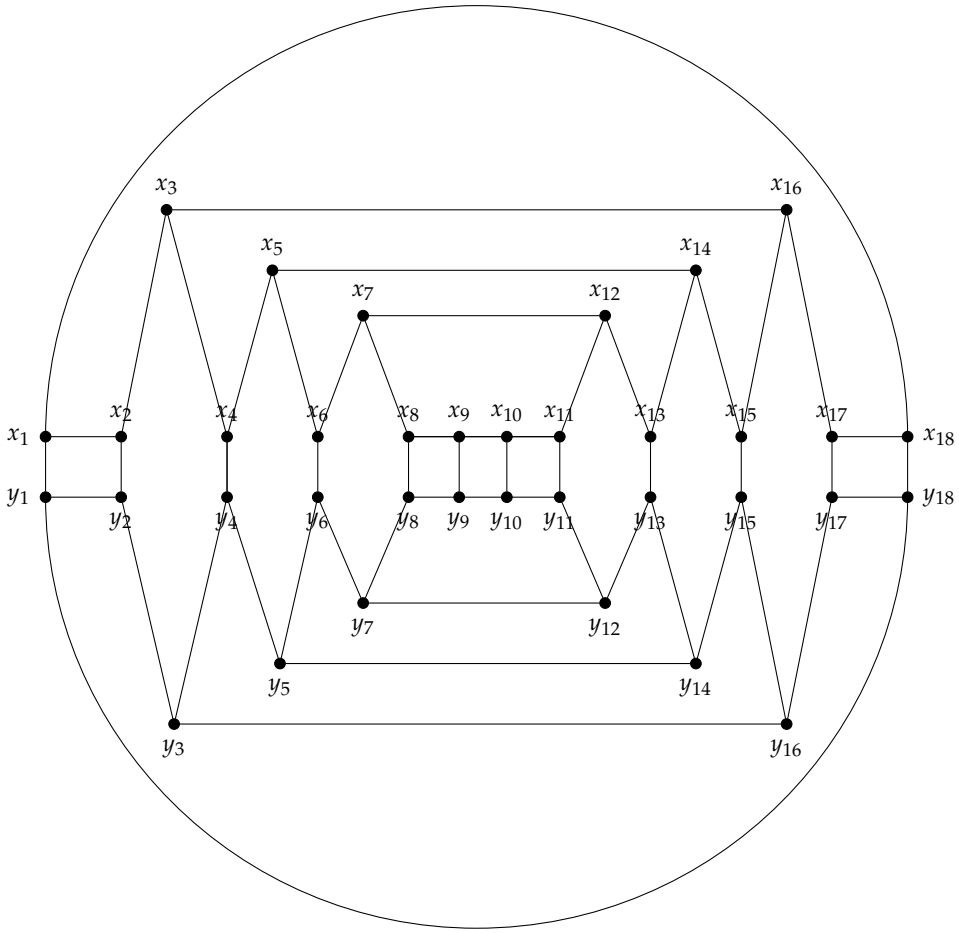


Figure 2. Fullerene graph $G_2[4]$.

The MD of fullerene graph $G_2[n]$ is computed in [32].

Lemma 2 ([32]). *The MD of fullerene graph $G_2[\zeta]$ is 3 for $\zeta \geq 2$.*

Theorem 2. *For a fullerene graph denoted as $G_2[\zeta]$ with $\zeta \geq 2$, the FTMD is 4.*

Proof. To demonstrate that $\beta'(G_2[\zeta]) = 4$, we begin by showing that $\beta'(G_2[\zeta]) \leq 4$. Consider $\Omega = \{x_1, x_{2\zeta}, x_{2\zeta+2}, y_{2\zeta}\}$ to be a resolving set of $V(G_2[\zeta])$, where $\zeta \geq 2$.

$$r(x_\varrho|\Omega) = \begin{cases} (0, 2\zeta-1, 2\zeta+1, 2\zeta) & \text{for } \varrho = 1; \\ (\varrho-1, 2\zeta-\varrho, 2\zeta-\varrho+2, 2\zeta-\varrho+1) & \text{for } 2 \leq \varrho \leq 2\zeta-1; \\ (2\zeta-1, 0, 2, 1) & \text{for } \varrho = 2\zeta; \\ (2\zeta, 1, 1, 2) & \text{for } \varrho = 2\zeta+1; \\ (2\zeta+1, 2, 0, 3) & \text{for } \varrho = 2\zeta+2; \\ (2\zeta, 3, 1, 4) & \text{for } \varrho = 2\zeta+3; \\ (4\zeta-\varrho+3, \varrho-2\zeta-2, \varrho-2\zeta-2, \varrho-2\zeta-1) & \text{for } 2\zeta+4 \leq \varrho \leq 4\zeta+2; \end{cases}$$

The $r(y|\Omega)$ values are provided as follows:

$$r(y_\varrho|\Omega) = \begin{cases} (\varrho, 2\zeta-\varrho+1, 2\zeta-\varrho, 2\zeta-1) & \text{for } 1 \leq \varrho \leq 2\zeta-1; \\ (2\zeta, 1, 3, 0) & \text{for } \varrho = 2\zeta; \\ (2\zeta+1, 2, 2, 1) & \text{for } \varrho = 2\zeta+1; \\ (2\zeta+2, 3, 1, 2) & \text{for } \varrho = 2\zeta+2; \\ (2\zeta+1, 4, 2, 3) & \text{for } \varrho = 2\zeta+3; \\ (2\zeta, 3, 3, 2) & \text{for } \varrho = 2\zeta+4; \\ (4\zeta-\varrho+4, \varrho-2\zeta-1, \varrho-2\zeta-1, \varrho-2\zeta-2) & \text{for } 2\zeta+5 \leq \varrho \leq 4\zeta+2; \end{cases}$$

The above unique representations verify that Ω is a fault-tolerant resolving set of $G_2[\zeta]$. Therefore, $\beta^{'}(G_2[\zeta]) \leq 4$. Also, by Lemma 2, $\beta(G_2[\zeta]) = 3$. Thus, by Proposition 1, $\beta^{'}(G_2[\zeta]) \geq 4$. Therefore, we conclude by establishing a connection between the two inequalities. Therefore, $\beta^{'}(G_2[\zeta]) = 4$. □

5. Fault-Tolerant Metric Dimension of Benzene-Based Graphs

This section contains the FTMD of ζ-linear benzene, ortho-polyphenyl chain, and meta-polyphenyl chain.

5.1. FTMD of ζ-Linear Benzene

Now, we calculate the FTMD of the graph corresponding to ζ times concatenated benzene molecule C_6H_6. This graph is denoted by B_ζ. It has $4\zeta+2$ vertices: $2\zeta+4$ are of degree 2, and $2\zeta-2$ are of degree 3. The B_ζ has a vertex set $V(B_\zeta) = \{x_1, x_2, \ldots, x_{2\zeta+1}\} \cup \{y_1, y_2, \ldots, y_{2\zeta+1}\}$ and an edge set $E(B_\zeta) = X \cup Y \cup Z$, where $X = \{x_\tau x_{\tau+1} : 1 \leq \tau \leq 2\zeta\}$, $Y = \{y_\tau y_{\tau+1} : 1 \leq \tau \leq 2\zeta\}$ and $Z = \{x_\tau y_\tau : 1 \leq \tau \leq 2\zeta+1\}$. The graph of B_5 is shown in Figure 3.

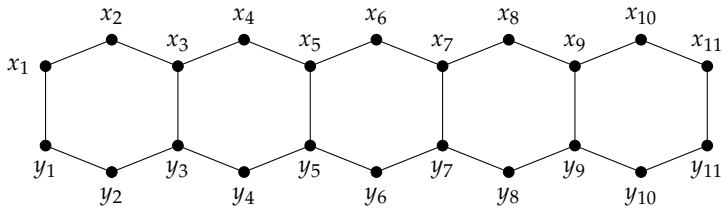


Figure 3. Five-linear benzene B_5.

We compute the $\beta^{'}(B_\zeta)$ in the subsequent theorem.

Theorem 3. *For a benzene graph denoted as B_ζ, the fault-tolerant metric dimension is* 4.

Proof. To demonstrate that $\beta^{'}(B_\zeta) = 4$, we begin by showing that $\beta^{'}(B_\zeta) \leq 4$. Assume $\Omega = \{x_1, y_1, y_2, y_{2\zeta}\}$ to be a resolving set of $V(B_\zeta)$. The $r(x|\Omega)$ values are provided as follows:

$$r(x_\varrho|\Omega) = \begin{cases} (0, 1, 2, 2\zeta) & \text{for } \varrho = 1; \\ (1, 2, 3, 2\zeta-1) & \text{for } \varrho = 2; \\ (\varrho-1, \varrho, \varrho-1, 2\zeta-\varrho+1) & \text{for } 3 \leq \varrho \leq 2\zeta-1; \\ (\varrho, \varrho+1, \varrho, 3) & \text{for } \varrho = 2\zeta; \\ (\varrho, \varrho+1, \varrho, 2) & \text{for } \varrho = 2\zeta+1; \end{cases}$$

The $r(y|\Omega)$ values are provided as follows:

$$r(y_\varrho|\Omega) = \begin{cases} (1,0,1,2\zeta-1) & \text{for } \varrho = 1; \\ (2,1,0,2\zeta-2) & \text{for } \varrho = 2; \\ (\varrho,\varrho-1,\varrho-2,2\zeta-\varrho) & \text{for } 3 \leq \varrho \leq 2\zeta-1; \\ (2\zeta,2\zeta-1,2\zeta-2,0) & \text{for } \varrho = 2\zeta; \\ (2\zeta+1,2\zeta,2\zeta-1,1) & \text{for } \varrho = 2\zeta+1. \end{cases}$$

The above unique representations verify that Ω is a fault-tolerant resolving set of B_ζ. Therefore, $\beta^{'}(B_\zeta) \leq 4$.

Now, to corroborate that $\beta^{'}(B_\zeta) \geq 4$, we obtain $\beta^{'}(B_\zeta) \neq 3$ by a contradiction. Among $V(B_\zeta)$, x_{2w+1} and y_{2w+1}, $1 \leq w \leq \zeta-1$ are vertices of degree 3, and the remaining vertices are of degree 2. We discuss the ensuing cases in support of the contradiction.

Case 1: Here, Ω contains at least one vertex of degree 3. Consider that x_{2w+1} is a vertex of degree 3 with neighbours $x_{2w}, x_{2w+2}, y_{2w+1}$, where $1 \leq w \leq \zeta-1$.

Case 1(a) If x_{2w+1} and two of its neighbours are in Ω. For simplicity, consider $\Omega = (x_{2w+1}, x_{2w}, x_{2w+2})$. Representations of the neighbouring vertices of x_{2w+1} are $r(x_{2w}|\Omega) = (1,0,1)$, $r(x_{2w+2}|\Omega) = (1,2,0)$, and $r(y_{2w+1}|\Omega) = (1,2,2)$. As vertices x_{2w+2} and y_{2w+1} have two identical positions, this contradicts the results.

Case 1(b) If x_{2w+1} and one of its neighbour is in Ω. For simplicity, consider $\Omega = (x_{2w+1}, x_{2w}, \delta)$, where $\delta = V(B_\zeta) \setminus x_{2w+2}, y_{2w+1}$. Representations of the neighbouring vertices of x_{2w+1} are $r(x_{2w}|\Omega) = (0,1,p)$, $r(x_{2w+2}|\Omega) = (2,1,q)$, and $r(y_{2w+1}|\Omega) = (2,1,r)$. As vertices x_{2w+2} and y_{2w+1} have two identical positions, this contradicts the results.

Case 1(c) If x_{2w+1} is in Ω but none of its neighbour is in Ω. For simplicity, consider $\Omega = (x_{2w+1}, \alpha, \delta)$, where $\alpha, \delta = V(B_\zeta) \setminus x_{2w}, x_{2w+2}, y_{2w+1}$. Therefore, representations of its neighbouring vertices are $r(x_{2w}|\Omega) = (1,p,q)$, $r(x_{2w+2}|\Omega) = (1,p_1,q_1)$, and $r(y_{2w+1}|\Omega) = (1,p_2,q_2)$. Two of the vertices from x_{2w}, x_{2w+2} and b_{2w+1} will have two identical positions. Considering Figure 3, $\Omega = (x_1, x_3, y_{11})$, $r(x_2|\Omega) = (1,1,10)$, $r(x_4|\Omega) = (3,1,8)$, and $r(y_3|\Omega) = (3,1,8)$. As vertices x_4 and y_3 have two identical positions, this contradicts the results.

Case 2: In this scenario, Ω does not contain any vertex of degree 3. Thus, the representation of y_{2w+1} will be the same at two positions with the representation of one of x_{2w} and x_{2w+2}. Considering Figure 3, $\Omega = (x_1, x_2, y_{11})$, $r(x_2|\Omega) = (1,0,10)$, $r(x_4|\Omega) = (3,2,8)$, and $r(y_3|\Omega) = (3,2,8)$. As vertices x_4 and y_3 have two identical positions, this contradicts the results.

Case 3: In this scenario, Ω contains all the three neighbours x_{2w}, x_{2w+2} and y_{2w+1} of x_{2w+1}, where $1 \leq w \leq \zeta-1$. Representations of two of three neighbours x_{2a}, x_{2a+2} and y_{2a+1} of x_{2a+1}, where $1 \leq a \leq \zeta-1$ and $w \neq a$, will be the same at the two positions. Considering Figure 3, $\Omega = (x_2, x_4, y_3)$. Considering a vertex x_7 of degree 3 with neighbours x_6, x_8 and y_7, $r(x_6|\Omega) = (4,2,4)$, $r(x_8|\Omega) = (6,4,4)$, and $r(y_7|\Omega) = (6,4,4)$. As vertices x_8 and y_7 have two identical positions, this contradicts the results.

In each of the aforementioned cases, it is evident that $\beta^{'}(B_\zeta)$ is greater than or equal to 4. Therefore, we conclude by establishing a connection between the two inequalities. Thus, $\beta^{'}(B_\zeta) = 4$. □

5.2. FTMD of Ortho-Polyphenyl Chain

The ortho-polyphenyl chain is denoted by O_ζ. The order of O_ζ is 6ζ. The vertex set of this polyphneyl chain is $V(O_\zeta) = \{x_1, x_2, \ldots, x_{2\zeta}\} \cup \{y_1, y_2, \ldots, y_{2\zeta}\} \cup \{z_1, z_2, \ldots, z_{2\zeta}\}$. The edge set of O_ζ is $E(O_\zeta) = X \cup Y \cup Z \cup X_1$, where $X = \{x_\tau x_{\tau+1}\}$, where $\tau = 1, 3, 5, \ldots, 2\zeta - 1$, $Y = \{z_\tau z_{\tau+1} : 1 \leq \tau \leq 2\zeta - 1\}$, $Z = \{x_\tau y_\tau : 1 \leq \tau \leq 2\zeta\}$ and $X_1 = \{y_\tau z_\tau : 1 \leq \tau \leq 2\zeta\}$. The graph of ortho-polyphenyl chain O_4 is shown in Figure 4.

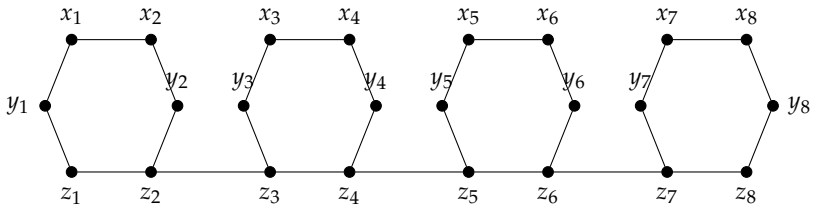


Figure 4. Ortho-polyphenyl chain O_4.

We compute $\beta'(O_\zeta)$ in the subsequent theorem.

Theorem 4. *For a ortho-polyphenyl chain denoted as O_ζ, the fault-tolerant metric dimension is* 4.

Proof. To establish that $\beta'(O_\zeta) = 4$, we start by showing that $\beta'(O_\zeta) \leq 4$. Assume $\Omega = \{y_1, z_1, y_{2\zeta-1}, x_{2\zeta-1}\}$ to be a resolving set of $V(O_\zeta)$. The $r(x|\Omega)$ values are provided as follows:

$$r(x_\varrho|\Omega) = \begin{cases} (\varrho, \varrho+1, 2\zeta-\varrho+2, 2\zeta-\varrho+3) & \text{for } 1 \leq \varrho \leq 2; \\ (\varrho+2, \varrho+1, 2\zeta-\varrho+2, 2\zeta-\varrho+3) & \text{for } 3 \leq \varrho \leq 2\zeta-2; \\ (2\zeta+1, 2\zeta, 1, 0) & \text{for } \varrho = 2\zeta-1; \\ (2\zeta+2, 2\zeta+1, 2, 1) & \text{for } \varrho = 2\zeta. \end{cases}$$

The $r(y|\Omega)$ values are provided as follows:

$$r(y_\varrho|\Omega) = \begin{cases} (0, 1, 2\zeta, 2\zeta+1) & \text{for } \varrho = 1; \\ (\varrho+1, \varrho, 2\zeta-\varrho+1, 2\zeta-\varrho+2) & \text{for } 2 \leq \varrho \leq 2\zeta-2; \\ (2\zeta, 2\zeta-1, 0, 1) & \text{for } \varrho = 2\zeta-1; \\ (2\zeta+1, 2\zeta, 3, 2) & \text{for } \varrho = 2\zeta. \end{cases}$$

The $r(z|\Omega)$ values are provided as follows:

$$r(z_\varrho|\Omega) = \begin{cases} (1, 0, 2\zeta-1, 2\zeta) & \text{for } \varrho = 1; \\ (\varrho, \varrho-1, 2\zeta-\varrho, 2\zeta-\varrho+1) & \text{for } 2 \leq \varrho \leq 2\zeta-1; \\ (2\zeta, 2\zeta-1, 2, 3) & \text{for } \varrho = 2\zeta. \end{cases}$$

The above unique representations verify that Ω is a fault-tolerant resolving set of O_ζ. Thus, $\beta'(O_\zeta) \leq 4$.

Now, to corroborate that $\beta'(O_\zeta) \geq 4$, we obtain $\beta'(O_\zeta) \neq 3$ by a contradiction. Among $V(O_\zeta)$, z_w vertices (where $2 \leq w \leq 2\zeta - 1$) are vertices of degree 3, and the remaining vertices are of degree 2. We discuss the ensuing cases in support of the contradiction.

Case 1: Here, Ω contains at least one vertex of degree 3. Consider z_w to be a vertex of degree 3 with neighbours z_{w-1}, z_{w+1}, y_w, where $2 \leq w \leq 2\zeta - 1$.

Case 1(a) If z_w and two of its neighbours are in Ω. For simplicity, consider $\Omega = (z_w, z_{w-1}, z_{w+1})$. Representations of the neighbouring vertices of z_w are $r(z_{w-1}|\Omega) = (1, 0, 2)$, $r(z_{w+1}|\Omega) = (1, 2, 0)$, and $r(y_w|\Omega) = (1, 2, 2)$.

As vertices z_{w+1} and y_w have two identical positions, this contradicts the results.

Case 1(b) **If z_w and one of its neighbour is in Ω.** For simplicity, consider $\Omega = (z_w, z_{w-1}, \delta)$, where $\delta = V(O_\zeta) \setminus z_{w+1}, y_w$. Representations of the neighbouring vertices of z_w are $r(z_{w-1}|\Omega) = (1, 0, p)$, $r(z_{w+1}|\Omega) = (1, 2, q)$, and $r(y_w|\Omega) = (1, 2, r)$. As vertices z_{w+1} and y_w have two identical positions, this contradicts the results.

Case 1(c) **If z_w is in Ω but none of its neighbour is in Ω.** For simplicity, consider $\Omega = (z_w, \alpha, \delta)$, where $\alpha, \delta = V(O_\zeta) \setminus z_{w-1}, z_{w+1}, y_w$. Therefore, representations of its neighbouring vertices are $r(z_{w-1}|\Omega) = (1, p, q)$, $r(z_{w+1}|\Omega) = (1, p_1, q_1)$, and $r(y_w|\Omega) = (1, p_2, q_2)$. Two of the vertices from z_{w-1}, z_{w+1} and y_w will have two identical positions. Considering Figure 4, $\Omega = (z_2, x_3, y_6)$, $r(z_1|\Omega) = (1, 4, 6)$, $r(z_3|\Omega) = (1, 2, 4)$, and $r(y_2|\Omega) = (1, 5, 6)$. As vertices z_1 and y_2 have two identical positions, this contradicts the results.

Case 2: In this scenario, Ω does not contain any vertex of degree 3. Thus, the representation of y_w will be the same at two positions with the representation of one of z_{w-1} and z_{w+1}. Considering Figure 4, $\Omega = (x_1, x_2, y_8)$, $r(z_1|\Omega) = (2, 3, 8)$, $r(z_3|\Omega) = (4, 3, 6)$, and $r(y_2|\Omega) = (2, 1, 8)$. As vertices z_1 and y_2 have two identical positions, this contradicts the results.

Case 3: In this scenario, Ω contains all the three neighbours z_{w-1}, z_{w+1} and y_w of x_w, where $2 \leq w \leq 2\zeta - 1$. Representations of two of three neighbours z_a, z_{a+1} and y_a of z_a, where $2 \leq a \leq 2\zeta - 1$ and $w \neq a$, will be the same at two positions. Considering Figure 4, $\Omega = (z_1, z_3, y_2)$. Considering a vertex z_7 of degree 3 with neighbours z_6, z_8 and y_7, $r(z_6|\Omega) = (5, 3, 5)$, $r(z_8|\Omega) = (7, 5, 7)$, and $r(y_7|\Omega) = (7, 5, 7)$. As vertices z_8 and y_7 have two identical positions, this contradicts the results.

In each of the aforementioned cases, it is evident that $\beta'(O_\zeta)$ is greater than or equal to 4. Therefore, we conclude by establishing a connection between the two inequalities. Thus, $\beta'(O_\zeta) = 4$. □

5.3. FTMD of Meta-Polyphenyl Chain

The meta-polyphenyl chain is denoted by M_ζ. The order of M_ζ is 6ζ. This polyphneyl chain has a vertex set $V(M_\zeta) = \{x_1, x_2, \ldots, x_{3\zeta}\} \cup \{y_1, y_2, \ldots, y_{3\zeta}\}$. The edge set of M_ζ is $E(M_\zeta) = X \cup Y \cup Z$ where $X = \{x_\tau x_{\tau+1} : i \leq \tau \leq i+1\}$, where $i = 1, 4, 7 \ldots, 3\zeta - 2$, $Y = \{y_\tau y_{\tau+1} : 1 \leq \tau \leq 3\zeta - 1\}$ and $Z = \{x_\tau y_\tau : 1 \leq \tau \leq \zeta\}$. The graph of meta-polyphenyl M_4 is shown in Figure 5.

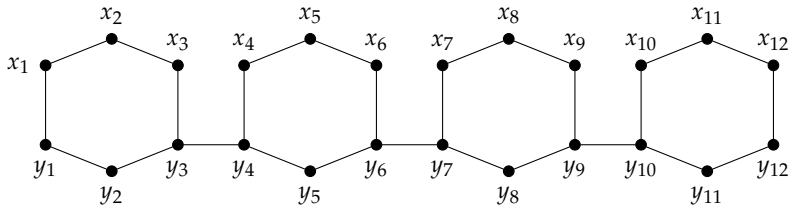


Figure 5. Meta-polyphenyl chain M_4.

We compute $\beta'(M_\zeta)$ in the subsequent theorem.

Theorem 5. *For a meta-polyphenyl chain denoted as M_ζ, the fault-tolerant metric dimension is* 4.

Proof. To establish that $\beta^{'}(M_\zeta) = 4$, we begin by showing that $\beta^{'}(M_\zeta) \leq 4$. Assume $\Omega = \{y_1, y_2, x_{3\zeta-2}, x_{3\zeta-1}\}$ to be a resolving set of $V(M_\zeta)$. The $r(x|\Omega)$ values are provided as follows:

$$r(x_\varrho|\Omega) = \begin{cases} (1,2,3\zeta-1,3\zeta) & \text{for } \varrho = 1; \\ (2,3,3\zeta-2,3\zeta-1) & \text{for } \varrho = 2; \\ (3,2,3\zeta-3,3\zeta-2) & \text{for } \varrho = 3; \\ (\varrho,\varrho-1,3\zeta-\varrho,3\zeta-\varrho+1) & \text{for } 4 \leq \varrho \leq 3\zeta-3; \\ (3\zeta-2,3\zeta-3,0,1) & \text{for } \varrho = 3\zeta-2; \\ (3\zeta,3\zeta-1,2,1) & \text{for } \varrho = 3\zeta-1; \\ (3\zeta-1,3\zeta-2,1,0) & \text{for } \varrho = 3\zeta. \end{cases}$$

The $r(y|\Omega)$ values are provided as follows: $V(M_\zeta)$. The $r(x|\Omega)$ values are provided as follows:

$$r(y_\varrho|\Omega) = \begin{cases} (0,1,3\zeta-2,3\zeta-1) & \text{for } \varrho = 1; \\ (1,0,3\zeta-3,3\zeta-2) & \text{for } \varrho = 2; \\ (\varrho-1,\varrho-2,3\zeta-\varrho-1,3\zeta-\varrho) & \text{for } 3 \leq \varrho \leq 3\zeta-2; \\ (3\zeta-2,3\zeta-3,2,3) & \text{for } \varrho = 3\zeta-1; \\ (3\zeta-1,3\zeta-2,3,2) & \text{for } \varrho = 3\zeta. \end{cases}$$

The unique representations above confirm that Ω is a fault-tolerant resolving set of M_ζ. Thus, $\beta^{'}(M_\zeta) \leq 4$.

Now, to corroborate that $\beta^{'}(M_\zeta) \geq 4$, we obtain $\beta^{'}(M_\zeta) \neq 3$ by a contradiction. Among $V(M_\zeta)$, y_{3w}, y_{3w+1} vertices (where $1 \leq w \leq \zeta-1$) are vertices of degree 3, and the remaining vertices are of degree 2. We discuss the ensuing cases in support of the contradiction.

Case 1: Here, Ω contains at least one vertex of degree 3. Consider y_{3w} to be a vertex of degree 3 with neighbours $x_{3w}, y_{3w-1}, y_{3w+1}$, where $1 \leq w \leq \zeta-1$.

Case 1(a) If y_{3w} and two of its neighbours are in Ω. For simplicity, consider $\Omega = (y_{3w}, x_{3w}, y_{3w-1})$. Representations of the neighbouring vertices of y_{3w} are $r(x_{3w}|\Omega) = (1,0,2)$, $r(y_{3w-1}|\Omega) = (1,2,2)$, and $r(y_{3w+1}|\Omega) = (1,2,2)$. As vertices x_{3w} and y_{2w-1} have two identical positions, this contradicts the results.

Case 1(b) If y_{3w} and one of its neighbour is in Ω. For simplicity, consider $\Omega = (y_{3w}, x_{3w}, \delta)$, where $\delta = V(M_\zeta) \setminus y_{3w-1}, y_{3w+1}$. Representations of the neighbouring vertices of y_{3w} are $r(x_{3w}|\Omega) = (1,0,p)$, $r(y_{3w-1}|\Omega) = (1,2,q)$, and $r(y_{3w+1}|\Omega) = (1,2,r)$. As vertices y_{3w-1} and y_{3w+1} have two identical positions, this contradicts the results.

Case 1(c) If y_{3w} is in Ω but none of its neighbours are in Ω. For simplicity, consider $\Omega = (y_{3w}, \alpha, \delta)$, where $\alpha, \delta = V(M_\zeta) \setminus x_{3w}, y_{3w-1}, y_{3w+1}$. Thus, representations of its neighbouring vertices are $r(x_{3w}|\Omega) = (1,p,q)$, $r(y_{3w-1}|\Omega) = (1,p_1,q_1)$, and $r(y_{3w+1}|\Omega) = (1,p_2,q_2)$. Two of the vertices from x_{3w}, y_{3w-1} and y_{3w+1} will have two identical positions. Considering Figure 5, $\Omega = (x_1, x_5, y_{11})$, $r(x_3|\Omega) = (2,4,9)$, $r(y_2|\Omega) = (2,4,9)$, and $r(y_4|\Omega) = (4,2,7)$. As vertices x_3 and y_2 have two identical positions, this contradicts the results.

Case 2: In this scenario, Ω does not contain any vertex of degree 3. Thus, the representation of y_{3w-1} will be the same at two positions with the representation of one of x_{3w} and y_{3w-1}. Considering Figure 5, $\Omega = (x_1, x_2, y_{12})$, $r(x_3|\Omega) = (2,1,10)$,

$r(y_2|\Omega) = (2,3,10)$, and $r(y_4|\Omega) = (4,3,8)$. As vertices x_3 and y_2 have two identical positions, this contradicts the results.

Case 3: In this scenario, Ω contains all the three neighbours x_{3w}, y_{3w-1} and y_{3w+1} of y_{3w}, where $1 \leq w \leq \zeta - 1$. Representations of two of three neighbours x_{3a}, y_{3a-1} and y_{3a+1} of y_{3a}, where $1 \leq a \leq \zeta - 1$ and $w \neq a$, will be same at the two positions. Considering Figure 5, $\Omega = (x_6, y_5, y_7)$. Considering a vertex y_7 of degree 3 with neighbours y_6, y_8 and x_7, $r(y_6|\Omega) = (1,1,1)$, $r(y_8|\Omega) = (3,3,1)$, and $r(x_7|\Omega) = (3,3,1)$. As vertices y_8 and x_7 have two identical positions, this contradicts the results.

In each of the aforementioned cases, it is evident that $\beta'(M_\zeta)$ is greater than or equal to 4. Therefore, we conclude by establishing a connection between the two inequalities. Thus, $\beta'(M_\zeta) = 4$. □

6. Application

In drug discovery, maintaining the stability of molecular interactions and therapeutic efficacy is crucial, especially when disruptions occur in drug–target binding or metabolic pathways. The target's goal is to find out the minimum number of optimized drug molecules (or structural modifications) needed to guarantee that each target site retains a distinct and reliable interaction profile and whether, even if some binding sites fail, the remaining ones will still allow the drug to function effectively.

Consider that a molecular interaction network is arranged in the form of an ortho-polyphenyl chain, as shown in Figure 4, where drug molecules are at vertices y_1, z_1, y_7 and x_7. Note that those are vertices of a resolving set given in Theorem 4. The representations of the vertices are provided as follows: $r(x_1|\Omega) = (1,2,9,10)$, $r(x_2|\Omega) = (2,3,8,9)$, $r(x_3|\Omega) = (5,4,7,8)$, $r(x_4|\Omega) = (6,5,6,7)$, $r(x_5|\Omega) = (7,6,5,6)$, $r(x_6|\Omega) = (9,7,4,5)$, $r(x_7|\Omega) = (9,8,1,0)$, $r(x_8|\Omega) = (10,9,2,1)$. $r(y_1|\Omega) = (0,1,8,9)$, $r(y_2|\Omega) = (3,2,7,8)$, $r(y_3|\Omega) = (4,3,6,7)$, $r(y_4|\Omega) = (5,4,5,6)$, $r(y_5|\Omega) = (6,5,4,5)$, $r(y_6|\Omega) = (7,6,3,4)$, $r(y_7|\Omega) = (8,7,0,1)$, $r(y_8|\Omega) = (9,8,3,2)$. $r(z_1|\Omega) = (1,0,7,8)$, $r(z_2|\Omega) = (2,1,6,7)$, $r(z_3|\Omega) = (3,2,5,6)$, $r(z_4|\Omega) = (4,3,4,5)$, $r(z_5|\Omega) = (5,4,3,4)$, $r(z_6|\Omega) = (6,5,2,3)$, $r(z_7|\Omega) = (7,6,1,2)$, $r(z_8|\Omega) = (8,7,2,3)$. The above distinct representations elaborate that each target site retains a distinct and reliable interaction profile and that, even if some binding sites fail, the remaining ones still allow the drug to function effectively.

7. Conclusions

The objective of this study was to calculate the FTMD of chemical graphs. Our findings indicate that the FTMD of the families discussed is 4 and that our methodology can be used to explore the graphs that have symmetry and regularity. The concept of fault tolerance can enhance other chemical graph exploration methodologies, like molecular graph theory, automated graph-based exploration, and modelling chemical reactions, in several significant ways. Fault tolerance enhances chemical graph exploration by ensuring analysis remains valid despite vertex failures or inaccuracies. It aids in detecting molecular stability and key atoms or bonds that influence reactivity. Integrating fault tolerance boosts reliability, resilience to errors, and scalability in the analysis of complex chemical networks. The para-polyphenyl graph is recognized for its complex structural properties, which pose considerable computational challenges when attempting to model its FTMD accurately. The following open problem might be interesting to tackle using our approach.

Open Problem 1. *To explore the FTMD of a para-polyphenyl graph.*

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