

On metric dimension of circumcoronene series of benzenoid networks

Faryal Chaudhry [#]

Department of Mathematics and Statistics

The University of Lahore

Lahore 54000

Pakistan

Azhar Ali Abbas [§]

Department of Information Technology

College of Computer Science and Information Technology

University of Kerbala

Karbala 56001

Iraq

Mohammed Abdul Jaleel Maktoof [‡]

Department of Computer Technologies Engineering

Al-Turath University

Al Mansour

Baghdad 10013

Iraq

Umar Farooq [†]

Department of Mathematics and Statistics

The University of Lahore

Lahore 54000

Pakistan

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[#] ORCID-ID: 0000-0002-1997-1515

[§] ORCID-ID: 0000-0003-4078-8536

[‡] ORCID-ID: 0000-0002-6591-2903

[†] ORCID-ID: 0000-0002-7301-7853

[#] E-mail: faryal.chaudhry@math.uol.edu.pk

[‡] E-mail: mohammed.jaleel@uoturath.edu.iq

[†] E-mail: 70126471@student.uol.edu.pk

Mohammad Reza Farahani [@]

Mehdi Alaeiyan ^{*}

Department of Mathematics and Computer Science

Iran University of Science and Technology (IUST)

Narmak

Tehran 16844

Iran

Murat Cancan [§]

Department of Mathematics

Faculty of Education

Yuzuncu Yil University

Van

Turkey

Abstract

In molecular topology and chemistry, resolving sets and metric bases are essential concepts. They have numerous applications in computer science, artificial intelligence, chemistry, pharmacy, traffic networking, mathematical modeling, and programming. A division S of the vertex set χ of a linked graph G is said to resolve G if each point of G can be represented from its neighborhood in S . A metric dimension of a graph is the number of the smallest resolving set, also known as the metric basis of the graph. In the current research we will determine the metric dimension and metric basis of the circumcoronene series CS of benzenoid H_k for $k \geq 1$. We prove that a set with three vertices is required to resolve this graph, and therefore, its metric dimension is 3.

Subject Classification: 05C12, 05C76, 05C90, 68R10.

Keywords: Resolving set, Metric basis, Metric dimension, Circumcoronene series, Benzenoid.

1. Introduction

Metric graph theory is a powerful tool for analyzing distance-based systems in the real world. Its implementation in computer sciences, artificial intelligence, industrial chemistry, molecular topology and networking are widely used to facilitate various applications and advancements in these fields [1-2]. It has interesting problems starting from structure and symmetries due to which

[@] ORCID-ID: 0000-0003-2969-4280

^{*} ORCID-ID: 0000-0003-2185-5967

[§] ORCID-ID: 0000-0002-8606-2274

[@] E-mail: mohammad_farahani@mathdep.iust.ac.ir;
mrifarhani88@gmail.com

^{*} E-mail: alaeiyan@iust.ac.ir (Corresponding Author)

[§] E-mail: mcancan@yyu.edu.tr

researchers attracted from different fields and even from mathematics also. The concept of assigning unique identities to nodes, based on a special set, known as a metric basis, and determining the minimum number of elements in that set, called the metric dimension, is consistently advantageous [3-4]. These ideas have been effectively applied in drug patterns to accurately identify specific atoms.

The application of resolving set and metric dimension can be seen in robotic networking, artificial intelligence, engineering, robot manufacturing and navigation, gaming, and traffic signal working, where a lot of observers in a system or robotic network may be there by measuring the distance or length from the position of a selection of SONAR stations (Sound, navigation and ranging), which is given an identical position in networking. The discovery of a robot's precise location is achieved through the application of resolving vectors, a widely recognized approach known as "robot navigation." This problem has received significant attention and has been extensively discussed in the field. The primary objective is to determine a set of resolving vectors that enables accurate localization of the robot within a given space. By identifying the minimum number of essential elements in this set, known as the metric dimension and fault tolerant metric dimension, the process becomes more efficient, reducing both the cost and time required for successful robot navigation [4].

In combinatorial chemistry, a fundamental challenge is to show mathematically a huge set of atoms, molecules, and bounding between atoms of compounds in an identical manner within complex structures.

This is accomplished by assigning labels to the points and edges of a graph, where the points represent the types of atoms and the edges shows the types of bonds either it is single or double bond. Consequently, the goal is to develop distinct mathematical representations for the graph vertices, ensuring that different vertices have different interpretations within the structure. The distance $d(u_1, u_2)$ between the vertices u_1 and u_2 of a graph is equal to the number of edges between u_1 and u_2 in the shortest path. For an ordered set of vertices $S = \{\omega_1, \omega_2, \omega_3, \dots, \omega_n\}$, then-vectors $r\left(\frac{u}{S}\right) = \{d(u, \omega_1), d(u, \omega_2), \dots, d(u, \omega_n)\}$ is the vector representation $r\left(\frac{u}{S}\right)$ of u with respect to S . The set S is called the resolving set of graphs G , if every vector has identical representation [6].

The concept of dimension inspired the idea of making its generalized form for metric dimension was introduced by "Blumenthal" in 1953. Due to the continuous nature, of standard Euclidean space, its application was limited so no work was done in this way until Haray and Melter developed this concept for a distance graph in 1976 [3]. Today we can find a huge literature that shows working on the dimensions of metric space, comparatively, there is no data present in typical metric space. A revolving set with the lowest cardinal number

is known as the bases and the number of elements is known as the dimension of which is represented as $dim(G)$.

We have presented data about the metric dimension concept in different areas of sciences see Figure 1. From Scopus database (<https://www.scopus.com/>) it can be seen most of papers are published in mathematics (42.5%), computers science (25.3%), Engineering (8.4%), Physics (6.4%), Decision sciences (3.1%), and material Science (2.3%).

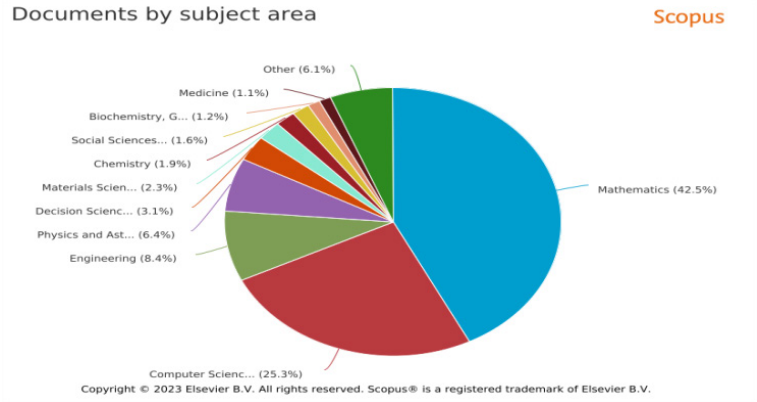


Figure 1

The bibliometric analysis of metric dimension concept in different areas of science

Also we used the scopus data based (<https://www.scopus.com/>) to plot this graph (see Figure 2), which shows that metric dimension concept is interlinked in different countries.

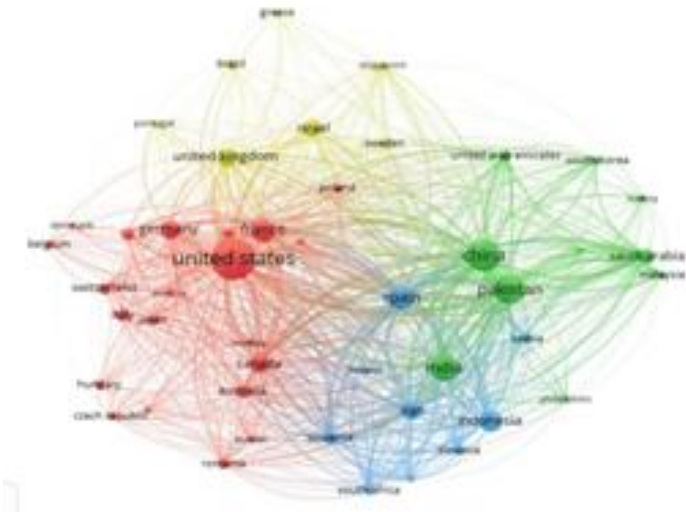


Figure 2

The bibliometric analysis of metric dimension concept in different countries.

The concepts of metric dimension and resolving sets for graphs were initially introduced by Slater. Subsequently, Melter and Harary independently developed these ideas. Further exploring and advancing this idea of resolving set was applied in networking and Games. A graph is stated to exhibit a perpetual metric dimension if the consequence of its dimension does not transformation through the variation of variables. In case of path graph (P_n) the metric dimension remains the same. If graph is complete (K_n) its metric dimension is $n-1$ for all $n>1$, [7-10] and the dimension of cyclic C_n is 2 for $n>1$. In general the metric dimension of Peterson graph(P_n) is calculated, in [18-34] few new consequences about constant metric dimension have been calculated.

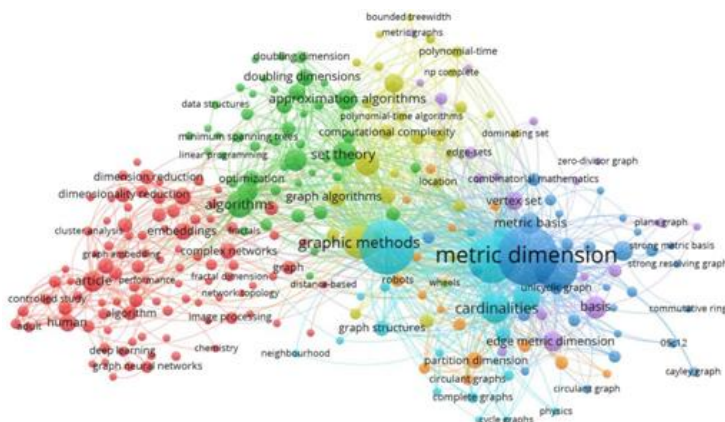


Figure 3
The bibliometric analysis of metric dimension keyword in different networks

A unique and identical dilemma in ‘chemistry in combination’ is to show the group of accurately compounds and molecules in a different way to a structure. Thus, atoms and bonds between the atoms are represented in vertices and edges. These vertices and edges are given specific name according to desired requirement and need. So different atoms are given the position according to their bond connectivity and represented as vertices and bonds are represented by edges [11-17].

These edges and vertices are given different names according to their functions in the network and to interpret the properties of that substance. Benzenoids are a category of organic molecules that are explored in the field of organic chemistry, and they contain at minimum one benzene ring [7]. The resonance within the benzene ring leads to higher levels of stability for these

The resolving set for 2nd cycle is $S = \{\chi_{2,1}, \chi_{2,2}, \chi_{2,5}\}$ for $\rho = 2n$ where $n = 2$ the distance vectors lying on second cycle are

$$\begin{aligned} r(\chi_{2,1}/S) &= (\rho - 4, \rho - 2, \rho), r(\chi_{2,2}/S) = (\rho - 3, \rho - 3, \rho - 1) \\ r(\chi_{2,3}/S) &= (\rho - 2, \rho - 4, \rho - 2), r(\chi_{2,4}/S) = (\rho - 1, \rho - 3, \rho - 3) \\ r(\chi_{2,5}/S) &= (\rho, \rho - 2, \rho - 4), r(\chi_{2,6}/S) = (\rho + 1, \rho - 1, \rho - 3) \\ r(\chi_{2,7}/S) &= (\rho + 2, \rho, \rho - 2), r(\chi_{2,8}/S) = (\rho - 3, \rho + 1, \rho - 1) \\ r(\chi_{2,9}/S) &= (\rho + 4, \rho + 2, \rho), r(\chi_{2,10}/S) = (\rho + 5, \rho + 3, \rho + 1) \\ r(\chi_{2,11}/S) &= (\rho + 4, \rho + 4, \rho + 2), r(\chi_{2,12}/S) = (\rho + 3, \rho + 5, \rho + 3) \\ r(\chi_{2,13}/S) &= (\rho + 2, \rho + 4, \rho + 4), r(\chi_{2,14}/S) = (\rho + 1, \rho + 3, \rho + 5) \\ r(\chi_{2,15}/S) &= (\rho, \rho + 2, \rho + 4), r(\chi_{2,16}/S) = (\rho - 1, \rho + 1, \rho + 3) \\ r(\chi_{2,17}/S) &= (\rho - 2, \rho, \rho + 2), r(\chi_{2,18}/S) = (\rho - 3, \rho - 1, \rho + 1) \end{aligned}$$

The resolving set for 3rd cycle is $S = \{\chi_{3,1}, \chi_{3,2}, \chi_{3,7}\}$ for $\rho = 2n$ where $n = 3$.

The distance vectors lying on 3rd cycle are

$$\begin{aligned} r(\chi_{3,1}/S) &= (\rho - 6, \rho - 4, \rho - 6), r(\chi_{3,2}/S) = (\rho - 5, \rho - 5, \rho - 1) \\ r(\chi_{3,3}/S) &= (\rho - 4, \rho - 6, \rho - 2), r(\chi_{3,4}/S) = (\rho - 3, \rho - 5, \rho - 3) \\ r(\chi_{3,5}/S) &= (\rho - 2, \rho - 4, \rho - 4), r(\chi_{3,6}/S) = (\rho - 1, \rho - 3, \rho - 5) \\ r(\chi_{3,7}/S) &= (\rho, \rho - 2, \rho - 6), r(\chi_{3,8}/S) = (\rho + 1, \rho - 1, \rho - 5) \\ r(\chi_{3,9}/S) &= (\rho + 2, \rho, \rho - 4), r(\chi_{3,10}/S) = (\rho + 3, \rho + 1, \rho - 3) \\ r(\chi_{3,11}/S) &= (\rho + 4, \rho + 2, \rho - 2), r(\chi_{3,12}/S) = (\rho + 5, \rho + 3, \rho - 1) \\ r(\chi_{3,13}/S) &= (\rho + 6, \rho + 4, \rho), r(\chi_{3,14}/S) = (\rho + 7, \rho + 5, \rho + 1) \\ r(\chi_{3,15}/S) &= (\rho + 8, \rho + 6, \rho + 2), r(\chi_{3,16}/S) = (\rho + 9, \rho + 7, \rho + 3) \\ r(\chi_{3,17}/S) &= (\rho + 8, \rho + 8, \rho + 4), r(\chi_{3,18}/S) = (\rho + 7, \rho + 9, \rho + 5) \\ r(\chi_{3,19}/S) &= (\rho + 6, \rho + 8, \rho + 6), r(\chi_{3,20}/S) = (\rho + 5, \rho + 7, \rho + 7) \\ r(\chi_{3,21}/S) &= (\rho + 4, \rho + 6, \rho + 8), r(\chi_{3,22}/S) = (\rho + 4, \rho + 5, \rho + 9) \\ r(\chi_{3,23}/S) &= (\rho + 2, \rho + 4, \rho + 8), r(\chi_{3,24}/S) = (\rho + 1, \rho + 3, \rho + 7) \\ r(\chi_{3,25}/S) &= (\rho, \rho + 2, \rho + 6), r(\chi_{3,26}/S) = (\rho - 1, \rho + 1, \rho + 5) \end{aligned}$$

$$r(\chi_{3,27}/S) = (\rho - 2, \rho, \rho + 4), r(\chi_{3,28}/S) = (\rho - 3, \rho - 1, \rho + 3)$$

$$r(\chi_{3,29}/S) = (\rho - 4, \rho - 2, \rho + 2), r(\chi_{3,30}/S) = (\rho - 5, \rho - 3, \rho + 1)$$

The resolving set for 4th cycle is $S = \{\chi_{4,1}, \chi_{4,2}, \chi_{4,42}\}$ for $\rho = 2n$ where $n=4$. The distance vectors lying on 4th cycle are

$$r(\chi_{4,1}/S) = (\rho - 8, \rho - 6, \rho), r(\chi_{4,2}/S) = (\rho - 7, \rho - 7, \rho - 1)$$

$$r(\chi_{4,3}/S) = (\rho - 6, \rho - 8, \rho - 2), r(\chi_{4,4}/S) = (\rho - 5, \rho - 7, \rho - 3)$$

$$r(\chi_{4,5}/S) = (\rho - 4, \rho - 6, \rho - 4), r(\chi_{4,6}/S) = (\rho - 3, \rho - 5, \rho - 5)$$

$$r(\chi_{4,7}/S) = (\rho - 2, \rho - 4, \rho - 6), r(\chi_{4,8}/S) = (\rho - 1, \rho - 3, \rho - 7)$$

$$r(\chi_{4,9}/S) = (\rho, \rho - 2, \rho - 8), r(\chi_{4,10}/S) = (\rho + 1, \rho - 1, \rho - 7)$$

$$r(\chi_{4,11}/S) = (\rho + 2, \rho, \rho - 6), r(\chi_{4,12}/S) = (\rho + 3, \rho + 1, \rho - 5)$$

$$r(\chi_{4,13}/S) = (\rho + 4, \rho + 2, \rho - 4), r(\chi_{4,14}/S) = (\rho + 5, \rho + 3, \rho - 3),$$

$$r(\chi_{4,15}/S) = (\rho + 6, \rho + 4, \rho - 2), r(\chi_{4,16}/S) = (\rho + 7, \rho + 5, \rho - 1)$$

$$r(\chi_{4,17}/S) = (\rho + 8, \rho + 6, \rho), r(\chi_{4,18}/S) = (\rho + 9, \rho + 7, \rho + 1)$$

$$r(\chi_{4,19}/S) = (\rho + 10, \rho + 8, \rho + 2), r(\chi_{4,20}/S) = (\rho + 11, \rho + 9, \rho + 3)$$

$$r(\chi_{4,21}/S) = (\rho + 12, \rho + 10, \rho + 4), r(\chi_{4,22}/S) = (\rho + 13, \rho + 11, \rho + 5)$$

$$r(\chi_{4,23}/S) = (\rho + 12, \rho + 12, \rho + 6), r(\chi_{4,24}/S) = (\rho + 11, \rho + 13, \rho + 7)$$

$$r(\chi_{4,25}/S) = (\rho + 10, \rho + 12, \rho + 8), r(\chi_{4,26}/S) = (\rho + 9, \rho + 11, \rho + 9)$$

$$r(\chi_{4,27}/S) = (\rho + 8, \rho + 10, \rho + 10), r(\chi_{4,28}/S) = (\rho + 7, \rho + 9, \rho + 11)$$

$$r(\chi_{4,29}/S) = (\rho + 6, \rho + 8, \rho + 12), r(\chi_{4,30}/S) = (\rho + 5, \rho + 7, \rho + 13)$$

$$r(\chi_{4,31}/S) = (\rho + 4, \rho + 6, \rho + 12), r(\chi_{4,32}/S) = (\rho + 3, \rho + 5, \rho + 11)$$

$$r(\chi_{4,33}/S) = (\rho + 2, \rho + 4, \rho + 10), r(\chi_{4,34}/S) = (\rho + 1, \rho + 3, \rho + 9)$$

$$r(\chi_{4,35}/S) = (\rho, \rho + 2, \rho + 8), r(\chi_{4,36}/S) = (\rho - 1, \rho + 1, \rho + 7)$$

$$r(\chi_{4,37}/S) = (\rho - 2, \rho, \rho + 6), r(\chi_{4,38}/S) = (\rho - 3, \rho - 1, \rho + 5)$$

$$r(\chi_{4,39}/S) = (\rho - 4, \rho - 2, \rho + 4), r(\chi_{4,40}/S) = (\rho - 5, \rho - 3, \rho + 3)$$

$$r(\chi_{4,41}/S) = (\rho - 6, \rho - 4, \rho + 2), r(\chi_{4,42}/S) = (\rho - 7, \rho - 5, \rho + 1)$$

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The distance vectors lying on i th cycle is

$$\begin{aligned} r\left(\chi_{i,1}/S\right) &= (\rho - 2i, \rho - 2i + 2, \rho) \quad r\left(\chi_{i,2}/S\right) \\ &= (1 + \rho - 2i, 1 - 2i + \rho, -1 + \rho) \\ r\left(\chi_{i,3}/S\right) &= (\rho - 2i + 2, \rho - 2i, \rho - 2) \quad r\left(\chi_{i,4}/S\right) \\ &= (\rho - 2i + 3, \rho - 2i - 1, \rho - 3) \\ r\left(\chi_{i,5}/S\right) &= (\rho - 2i + 4, \rho - 2i - 2, \rho - 4) \quad r\left(\chi_{i,6}/S\right) \\ &= (\rho - 2i + 5, \rho - 2i - 3, \rho - 5) \\ r\left(\chi_{i,7}/S\right) &= (\rho - 2i + 6, \rho - 2i - 4, \rho - 6), \end{aligned}$$

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Representation of vectors for n th cycle, we have $r\left(\chi_{i,n}/S\right) = (\rho - 2i + n - 1, \dots, \rho - n + 1)$ Now, by putting $\rho = 2n$, we further generalized it, as

$$\begin{aligned} r\left(\chi_{i,n}/S\right) &= (3n - 2i - 1, \rho - 2j + 2) \text{ for } n = 1, n + 1 \\ r\left(\chi_{i,n}/S\right) &= (3n - 2i - 1, \rho - 2j + 1) \text{ for } n = 2, n + 1 \\ r\left(\chi_{i,n}/S\right) &= (3n - 2i - 1, \rho - 2j + n - 3) \text{ for } n \geq 3, n + 1 \end{aligned}$$

The set S will be considered a resolving set for the CS of benzenoid.

Theorem 1: Let H_k be the molecule of CS of benzenoid H_k for $k \geq 1$ networks, we have $\dim(H_k) \geq 3$.

Proof: To show that no set of nodes of cardinality two or fewer may be converted into a resolving set for the CS of benzenoid H_k for $k \geq 1$ thus the idea of producing a set containing just one element is not considered because there is no path to take. We will try to find out the set of two elements that resolves the graph is $\varpi = \{\chi_{\rho,i}, \chi_{\xi,j}\}$. Let us see the following possible options.

First Possibility is, If selected vertices are from the same cycle in ϖ , then

1. In case of $\rho = \xi = 1$ and both vertices are present on the same cycle, we have $r(\chi_{2,2} | \varpi) = r(\chi_{2,25} | \varpi)$, which is a contradiction.
2. In case of $\rho = \xi = 2$ and both selected vertices of ϖ are on 2nd cycle we have $r(\chi_{4,33} | \varpi) = r(\chi_{4,35} | \varpi)$, again this leads to a contradiction.
3. In case of $\rho = \xi = 3$ and selected vertices of ϖ are from 3rd cycle then we have $r(\chi_{6,51} | \varpi) = r(\chi_{6,53} | \varpi)$, leads to a contradiction.
4. In case of $\rho = \xi = 4$ and selected vertices of ϖ are from 4th cycle then we have $r(\chi_{8,71} | \varpi) = r(\chi_{8,73} | \varpi)$, a contradiction.
5. In case of $\rho = \xi = 5$ and selected vertices of ϖ are from 5th cycle then we have $r(\chi_{10,89} | \varpi) = r(\chi_{10,91} | \varpi)$, a contradiction.

6. In case of $\rho = \xi = r$ and selected vertices of ϖ are from r th cycle then we will get $r(\chi_{2r, 19r-6} \mid \varpi) = r(\chi_{2r, 19r-4} \mid \varpi)$, leads to a discrepancy.
7. If designated vertices are from $(r + 1)^{\text{th}}$ succession and r is odd so therefore $\rho = \xi = r + 1$ and we have $r(\chi_{2r+2, 19r+14} \mid \varpi) = r(\chi_{2r, 19r+16} \mid \varpi)$, this shows a contradiction.
8. In circumstances of the designated vertices are on n^{th} cycle then $\rho = \xi = n$ and we prepare $r(\chi_{n-k, 10(n-k)-5} \mid \varpi) = r(\chi_{n-k-1, 2} \mid \varpi)$, for $k=0, 1, \dots, n-2$.

Possibility 2: If selected vertices in ϖ , are from the adjacent or neighboring cycles

1. In case of selected vertices of ϖ are from 1^{st} and 2^{nd} cycles, suppose the 1^{st} one is $\chi_{1,1}$ and 2^{nd} is $\chi_{2,j}$; $1 \leq j \leq 18$ from second cycle Then $\chi_{3,2} = \chi_{3,25}$ or $\chi_{3,2} = \chi_{4,35}$, shows a contradiction.
2. Similarly, if selected vertices of ϖ are from 2^{nd} and 3^{rd} cycles suppose on 2^{nd} cycle selected one is $\chi_{2,1}$ also the vertex on third cycle is $\chi_{3,j}$; $1 \leq j \leq 30$. Then $\chi_{4,2} = \chi_{4,35}$ or $\chi_{4,2} = \chi_{5,45}$ leads to a contradiction.
3. Similarly, if selected vertices of ϖ are from 3^{rd} and 4^{th} cycles we assume, that the vertex from 3^{rd} cycle is $\chi_{3,1}$ and on 4^{th} cycle is $\chi_{4,j}$; $1 \leq j \leq 42$. Then $\chi_{5,2} = \chi_{5,45}$ or $\chi_{5,2} = \chi_{6,55}$, leads to a discrepancy.
4. If 1^{st} vertex of ϖ lies on i^{th} cycle and the 2^{nd} vertex in ϖ is selected from $(i + 1)^{\text{th}}$ cycle where i is odd. Defeat of generality assumedly, the vertex on C_i is $\chi_{i,1}$ and the vertex on C_{i+1} is $\chi_{i+1,j}$; $1 \leq j \leq 12i-6$. Then $\chi_{i+2,2} = \chi_{i+2, I+15}$ or $\chi_{i+2,2} = \chi_{i+3, I+25}$, a discrepancy.
5. Let 1^{st} vertex of ϖ be on $n - 1$ cycle and the second one is from cycle n . Let the vertex from n cycle is $\chi_{n,1}$ and the vertex on $n - 1$ is $\chi_{n-1,j}$; $1 \leq j \leq 12n - 6$. Then $\chi_{n,2} = \chi_{n, 10n-5}$ or $\chi_{n-1,2} = \chi_{n, 10n-5}$, leads to a discrepancy.

Possibility 3: If the nodes are from ϖ , are from unlike cycles which are not neighboring.

1. If selected vertex is from 1^{st} and i^{th} cycle where $3 \leq i \leq n-2$. Devoid of exhausting generalization. Let the vertex from 1^{st} cycle is $\chi_{1,1}$ and the i^{th} cycle is $\chi_{i,j}$ where $1 \leq j \leq 12i - 6$. Then $\chi_{i+1,2} = \chi_{i+1, 12i-6}$ or $\chi_{i+2,2} = \chi_{i+1,3}$ shows a discrepancy.
2. If 1^{st} vertices in ϖ lie on i^{th} cycle and another vertex lies on k^{th} cycle where $1 < i < k < n$. let the vertex on i^{th} cycle is $\chi_{i,1}$ the vertex on k^{th} cycle is $\chi_{k,j}$ where $1 \leq j \leq 10k - 5$. Then $\chi_{i-1,1} = \chi_{i,10i-5}$ or $\chi_{i-1,1} = \chi_{i,2}$ leads to a discrepancy.

We derive from above conversation that a set or any set which has cardinality 2 cannot resolve the CS of benzenoid H_k for $k \geq 1$ so its Dimension is always greater than two.

And we eventually obtain the $\dim(H_K) = 3$.

Conclusions

Resolving sets for a certain robot(chain of networks) or graph contain central data required for the distinctive identity of each module current in the network. We prove that the CS of benzenoid H_k for $k \geq l$ invariable metric dimension three and it is independent from K . People working in the field of nano engineering, nano devices, and micro devised constructed from nano scale materials can benefit from the results established in this article the CS of benzenoid H_k for $k \geq l$. In nano-biotechnology and pharmacy, in pharmacological designs where various nodes have varying degrees of significance, these findings may also be useful.

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