L(2,1) - Labeling of Chemical Graphs

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ABSTRACT

An $L(2,1)$-labeling of a graph $G(V,E)$ is a function $f: V(G) \to \{0,1,2,\dots\}$ is a set of non- negative integers such that $|f(x) - f(y)| \geq 2$ if $d(x,y) = 1$ and $|f(x) - f(y)| \geq 1$ if $d(x,y) = 2$, where $d(x,y)$ is the distance between the vertices x and y in the graph G. $L(2,1)$-labeling number, represented as $\lambda_{2,1}$ is the smallest number k such that the $L(2,1)$-labeling exists with a maximum label k. In this manuscript, we have determined the bounds for $L(2,1)$-labeling number of Melem structure and Cyclen-Pyrene Dendrimers.

Keywords:$L(2,1)$-labeling, chemical graphs, Melem structure, Cyclen-Pyrene Dendrimers.

1 Introduction

The channel assignment problem is to assign a channel (non-negative integer) to each radio transmitter so that interfering transmitters are assigned channels whose separation is not in a set of disallowed separations.The Frequency Assignment Problem (FAP) is at the core of optimizing wireless networks, where the goal is to allocate specific frequencies to transmitters. In this context, each transmitter is assigned a dedicated frequency channel for broadcasting. One of the primary challenges arises when adjacent transmitters operate on frequencies that are closely positioned, potentially leading to interference. This problem has far-reaching implications in real-world applications, spanning telecommunications, satellite communication, and mobile networks.Initially presented by Hale in 1912, the problem was formulated as a graph coloring issue, introducing the concept of T-coloring. L(2,1)-labeling, an alternative approach, was introduced by Griggs et al[1] in 1992. They observed that, for any graph G with a maximum degree Δ, employing a greedy algorithm results in $\lambda_{(2,1)}(G) \leq 1 + 2\Delta + \Delta^2$. Furthermore, when $\Delta \geq 2$, a conjecture was proposed positing that $\lambda_{(2,1)}(G) \leq \Delta^2$, and it was demonstrated that $\lambda_{(2,1)}(G) \leq 2\Delta + \Delta^2$. Chang et al[2]. improved these bounds to $\Delta^2 + \Delta$ presenting a polynomial-time algorithm for trees and a linear-time algorithm for cographs. Kral et al.[3] further refined the bound to $\Delta^2 + \Delta - 1$. In 2008, Goncalves [4] enhanced the bound by further reducing it to $\Delta^2 + \Delta - 2$. It is important to note that, for general graphs, solving the $L(2,1)$-labeling problem is NP-hard.

In 1991, Roberts proposed a modified version of the frequency assignment problem, emphasizing the need for closely located transmitters to use distinct channels. Additionally, very close transmitters were required to have channels at least two units apart. Typically, transmitters are represented as vertices in a graph, with adjacency indicating closeness, and a distance of two signifying being 'close.' The parameter $\lambda_{(2,1)}$ denotes the bounds, systematically calculated for specific graphs such as hypercubes[6], tree dendrimers, circular arc graphs[7,8], block graphs[9], generalized Petersen graphs[10], permutation graphs[11], silicate and oxide networks[12], and chordal graphs[13].In this paper we have investigated the bounds for L(2,1)-labeling number of Melem structure and Cyclen-Pyrene Dendrimers.

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2 Melem's Structure and Significance

Melem, a trimer derived from melamine, boasts exceptional photo-catalytic and photo responsive properties, presenting a realm of possibilities for diverse applications. With attributes including high stability, low cell toxicity, and remarkable efficiency, Melem emerges as a cutting-edge, metal-free, and environmentally friendly blue-emitting material. Defined by the molecular formula $C_6N_7(NH_2)_3$, its unit cell intricately weaves together three hexagons in a triangular arrangement known as a heptazine [14, 15,16]. The diagrams vividly showcase the melem chain and ring structures, constructed by assembling unit cells into linear and circular forms. The dynamic melem chain, denoted as MC[s], and the corresponding melem ring, denoted as MR[s], symbolize not only structural elegance but also hold promise for innovative applications in materials science. See Figure 1 and 2.

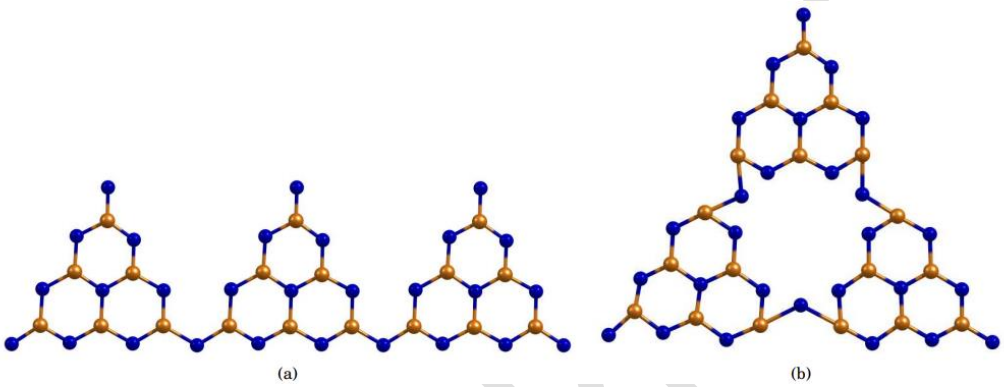

Figure 1:*Melem structure with three units (a) Chain form (b) Ring form.*

2.1 Historical Background and Significance of Melem in Material Science

Melem, recognized as one of the earliest synthetic organic materials, possesses a rich historical background spanning nearly two centuries. First examined by Liebig in 1834, its molecular structure remained enigmatic for over a century due to its insolubility. The breakthrough came in 1937 when Pauling and Sturdivant postulated its formula. However, it wasn't until 2003 that Schnick and colleagues reported Melem's crystal structure and provided crucial spectroscopic details, solidifying its role as a pivotal intermediate in the thermal condensation of melamine to $g - C_3N_4$ [17]. Beyond its role in materials synthesis, Melem's nucleophilic NH_2-groups enable reactions with electrophiles, resulting in various Melem derivatives with innovative functionalities. This historical perspective highlights the challenges and triumphs in understanding and harnessing the potential of Melem, underscoring its enduring significance in materials science[18]. As researchers continue to explore its reactivity and applications, Melem stands as a testament to the enduring curiosity and ingenuity of scientists throughout history, paving the way for advancements in diverse scientific fields.

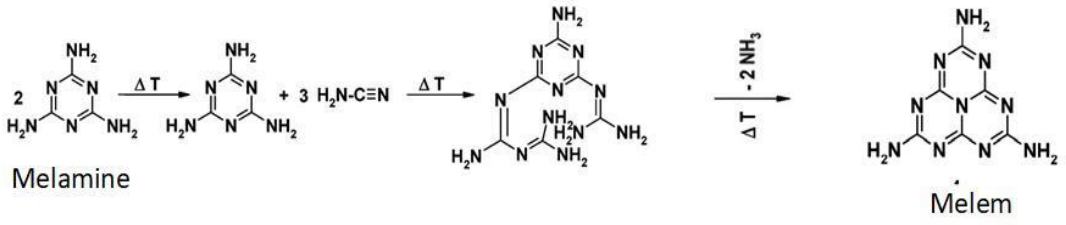

Figure 2:*Possible formation of melem*

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3 Results and Discussion

Theorem 3.1: The L(2,1)-Labelling of Melem structure $C_6N_7(NH_2)_3$(m) is 6.

Proof: Let $G = C_6N_7(NH_2)_3$(m) denote the m copies of melem structure. The function $f: V(G) \rightarrow \{0,1,2,3, \dots\}$ assigns non-negative integer labels to the vertices of the melem structure G.

Claim: Then, the L(2,1) labeling number of vertices of the melem structure satisfies $\lambda_{2,1}(G)$ is 6. Let v_j^{i} denote the vertices, where j represents the levels of the vertices refer figure 2.2 and i denotes the position of the vertex at each level , where $1 \leq i \leq n, 1 \leq j \leq 4$.The $\lambda_{2,1}$ labeling for each levels in the m copies melem structure is given by as follows

Base Case (m = 1): Consider the base case of a single copy, $m = 1$, of the melem structure $C_6N_7(NH_2)_3$. We will analyze the labeling for each level individually:

Level 1: At the first level, there is one vertex, denoted as v_1^1, which is uniquely labeled with 6. This label satisfies the L(2,1) condition as there are no adjacent vertices at this level.

Level 2: For the second level, we have three vertices, denoted as v_2^1, v_2^2, and v_2^3. They are labeled as follows: $v_2^1 = 0$, $v_2^2 = 2$, $v_2^3 = 4$. These labels are distinct and fulfill the L(2,1) condition since they are at least 2 apart from each other.

Level 3: At the third level, we find five vertices, denoted as v_3^1, v_3^2, v_3^3, v_3^4, and v_3^5. They are labeled as follows: $v_3^1 = 1, v_3^2 = 3, v_3^3 = 6, v_3^4 = 1, v_3^5 = 5$. These labels are distinct and fulfill the L(2,1) condition since they are at least 2 apart from each other.

Level 4: At the fourth level, we have seven vertices, denoted as v_4^1, v_4^2, v_4^3, v_4^4, v_4^5, v_4^6, and v_4^7. They are labeled as follows: $v_4^1 = 6$, $v_4^2 = 4$, $v_4^3 = 2$, $v_4^4 = 0$, $v_4^5 = 4$, $v_4^6 = 2$, $v_4^7 = 6$. These labels are distinct and fulfill the L(2,1) condition since they are at least 2 apart from each other.The base case for $m = 1$ satisfies the L(2,1) labeling condition with $\lambda_{2,1} is\ 6$.

Inductive Step: Assume that for $m = k$, the melem structure $C_6N_7(NH_2)_3(k)$ can be labeled with $\lambda 2,1 \leq 6$. We want to show that this holds for $m = k + 1$.

For the $(k+1)$-th Copy: Let's consider the $(k+1)$-th case, where we add another copy of the melem structure to the existing k copies. We will analyze the labeling for each level of the $(k+1)$-th copy:

Level 1: At the new first level, there is one new vertex, labeled as $v_{1_{(k+1)}}^1 = 6$. This label is distinct from the labels in the previous copies and satisfies the L(2,1) condition.

Level 2: For the second level of the $(k+1)$-th copy, there are three new vertices, denoted as $v_{2_{(k+1)}}^1$, $v_{2_{(k+1)}}^2$, and $v_{2_{(k+1)}}^3$. They are labeled as follows: $v_{2_{(k+1)}}^1 = 0$, $v_{2_{(k+1)}}^2 = 2$, $v_{2_{(k+1)}}^3 = 4$. These labels are distinct from the labels in the previous copies and fulfill the L(2,1) condition.

Level 3: At the third level of the $(k+1)$-th copy, there are five new vertices, denoted as $v_{3_{(k+1)}}^1$, $v_{3_{(k+1)}}^2$, $v_{3_{(k+1)}}^3$, $v_{3_{(k+1)}}^4$, and $v_{3_{(k+1)}}^5$. They are labeled as follows: $v_{3_{(k+1)}}^1 = 1$, $v_{3_{(k+1)}}^2 = 3$, $v_{3_{(k+1)}}^3 = 6$, $v_{3_{(k+1)}}^4 = 1$, $v_{3_{(k+1)}}^5 = 5$. These labels are distinct from the labels in the previous copies and fulfill the L(2,1) condition.

Level 4: At the fourth level of the $(k+1)$-th copy, there are seven new vertices, denoted as $v^1_{4_{(k+1)}}$, $v^2_{4_{(k+1)}}$, $v^3_{4_{(k+1)}}$, $v^4_{4_{(k+1)}}$, $v^5_{4_{(k+1)}}$, $v^6_{4_{(k+1)}}$, and $v^7_{4_{(k+1)}}$. They are labeled as follows: $v^1_{4_{(k+1)}} = 6, v^2_{4_{(k+1)}} = 4, v^3_{4_{(k+1)}} = 2,\ v^4_{4_{(k+1)}} = 0,\ v^5_{4_{(k+1)}} = 4,\ v^6_{4_{(k+1)}} = 2,\ v^7_{4_{(k+1)}} = 6$. These labels are distinct from the labels in the previous copies and fulfill the L(2,1) condition.Thus, for the $(k+1)^{th}$ copy, all levels maintain distinct labels and satisfy the L(2,1) condition with $\lambda_{2,1} = 6$.By induction, we have shown that for any m copies of the melem structure $C_6N_7(NH_2)_3$, the L(2,1) labeling condition is satisfied with $\lambda_{2,1}$ is 6. Hence, the aforementioned labeling criteria are applicable to multiple instances of the melem ring structure, meeting the conditions specified for L(2,1) labeling. This observation is valid for m repetitions of the melem ring structure, where the labeling conditions outlined are consistently satisfied.It is shown that the melem structure G satisfy the L(2,1)-Labeling conditions with $\lambda_{2,1}$ is 6. See Figure 3 and 4.

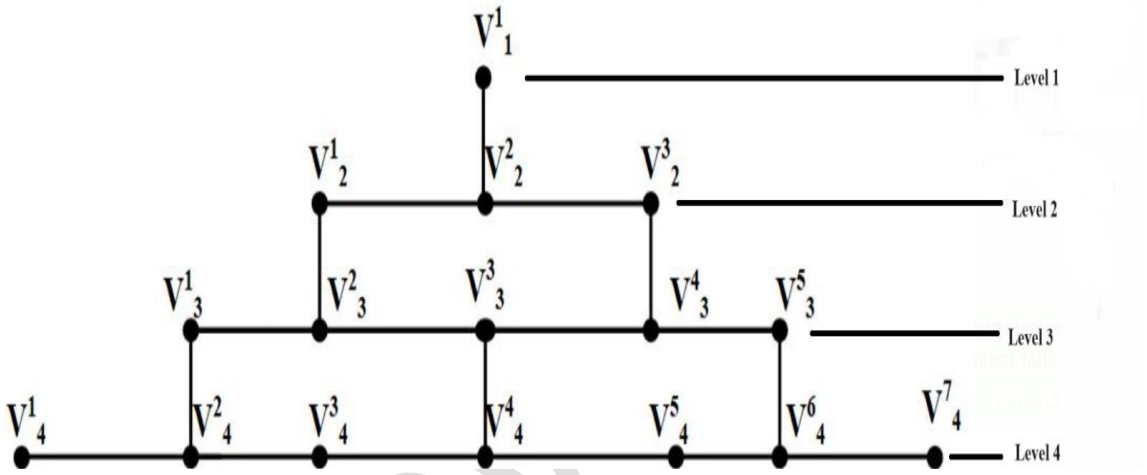

Figure 3:*Labeling pattern of melem structure*

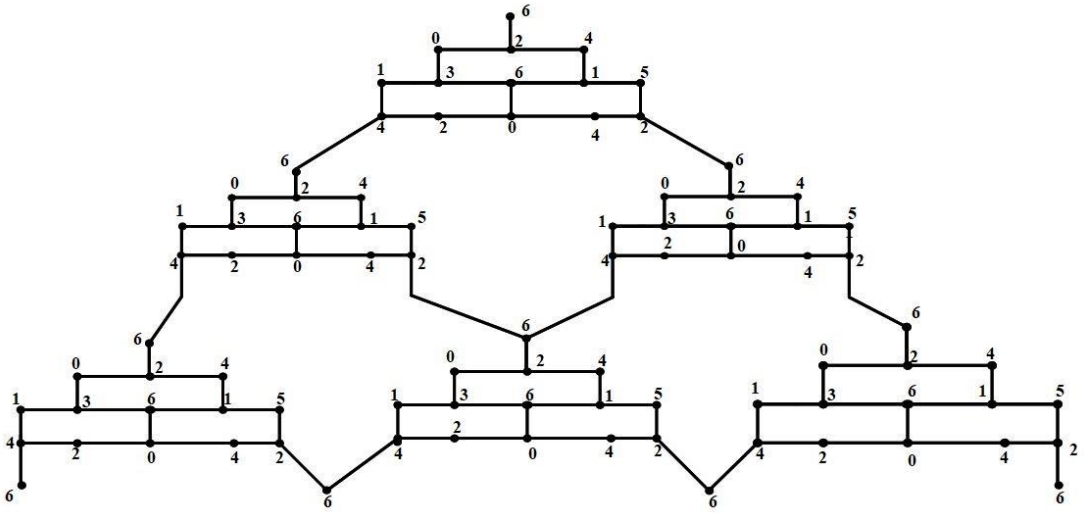

Figure 4:*L(2,1) Labeling of melem structure*

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4 Cyclen-Pyrene Dendrimers

Cyclen, a macrocycle identified as (1, 4, 7, 10-tetraazacyclododecane), has attracted considerable attention in current research. Its derivatives play a crucial role due to their strong coordination with a diverse range of metal ions. The adaptability of cyclen is underscored by its role as a central element in photoactive dendrimers, maintaining a subtle presence in absorption and emission spectra. Its ability to interact with dendrons or intricate metal structures allows for the modification of dendrimer photophysical properties.Research on cyclens spans various applications, including therapeutic interventions for human immunodeficiency virus (HIV)[20], the development of luminescent probes[22], the creation of magnetic resonance imaging (MRI) agents[21], utilization in positron emission tomography (PET) imaging, and applications in photoactive hydrogels[23] and bio-sensing. The strategic control of molecular design facilitates the targeted use of cyclen in applications[24], enhancing characteristics such as stability, solubility, and biocompatibility[25]. Pyrene emerges as a focal point in scientific investigation, celebrated for its remarkable photochemical attributes. Widely employed across diverse scientific domains, pyrene is integrated into various chemical structures, serving both as core and surface groups in dendrimers to confer specific functionalities.

5 A Study of Frechet-Type Cyclen-Cored Dendrimers with Varied Pyrene Units

Dendrimers with tailored surface functionalities play a pivotal role in diverse applications. We synthesized and studied three generations of Frechet-type dendrimers with cyclen as the core and varying numbers of pyrene units in the periphery: CyPy4, CyPy8, and CyPy16. These generations represent dendrimers with four, eight, and sixteen pyrene units, respectively. This systematic variation allows for a controlled exploration of structure-property relationships.

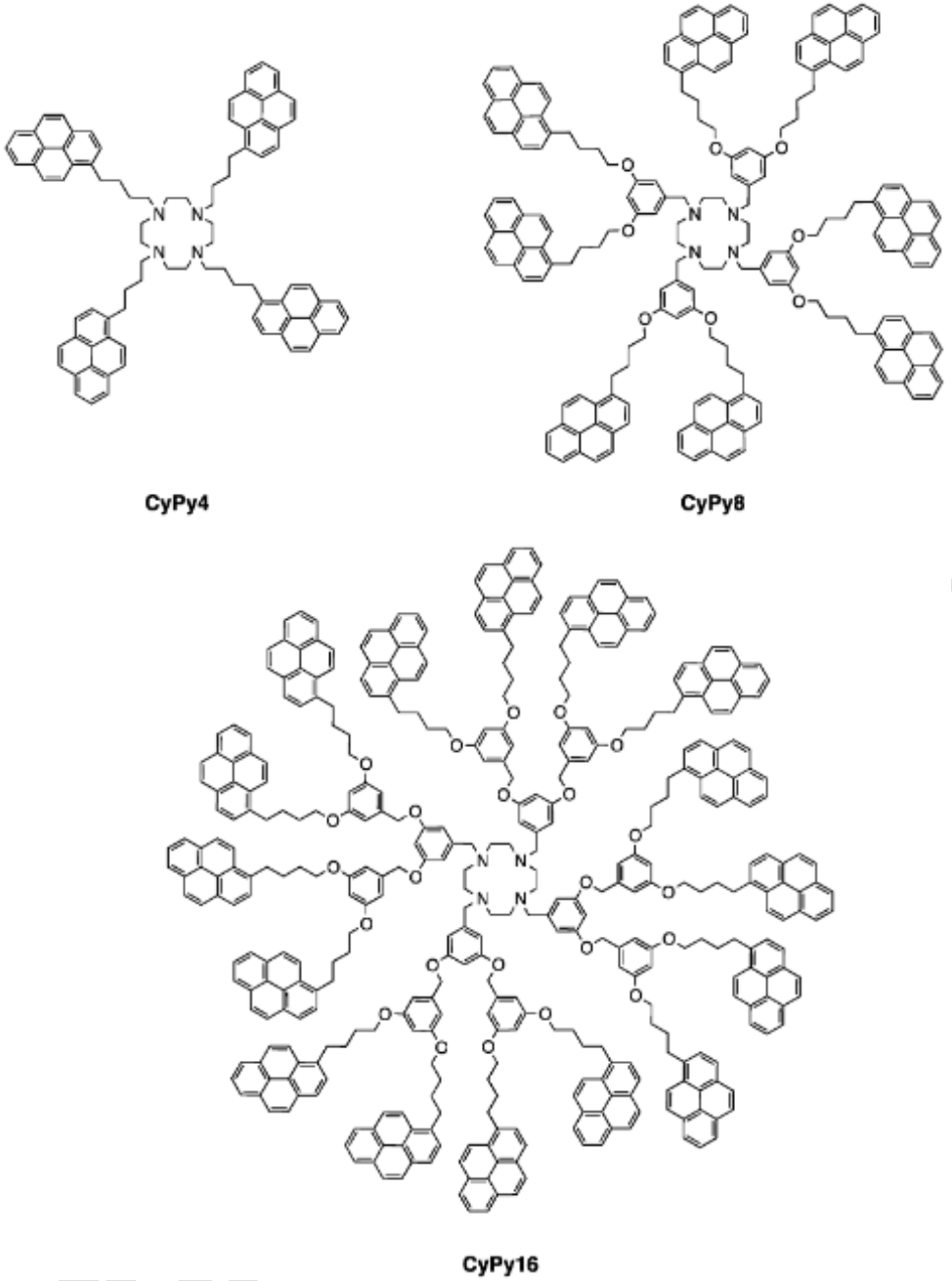

Figure 5:*Frechet type cyclen–pyrene dendrimer CyPy*2^n

The resulting dendrimers hold promise for versatile applications, offering a platform for the development of functional materials in various fields.The zeroth generation of the Frechet-type cyclen-pyrene dendrimer is denoted as CyPy2^2, represented by CyPy4 [5, 26,]. Subsequent generations include the first generation CyPy2^3, the second generation CyPy2^4, and so forth.The Frechet-type cyclen-pyrene dendrimer of zero generation is denoted as CyPy2^2, with CyPy4 as its precursor. See Figure 5. Subsequent generations are labeled as follows: firstgeneration (CyPy2^3), second generation (CyPy2^4), and so on. The graph CyPy2^n possesses $29 \times 2^n - 24$ vertices and $34 \times 2^n - 28$ edges [19].

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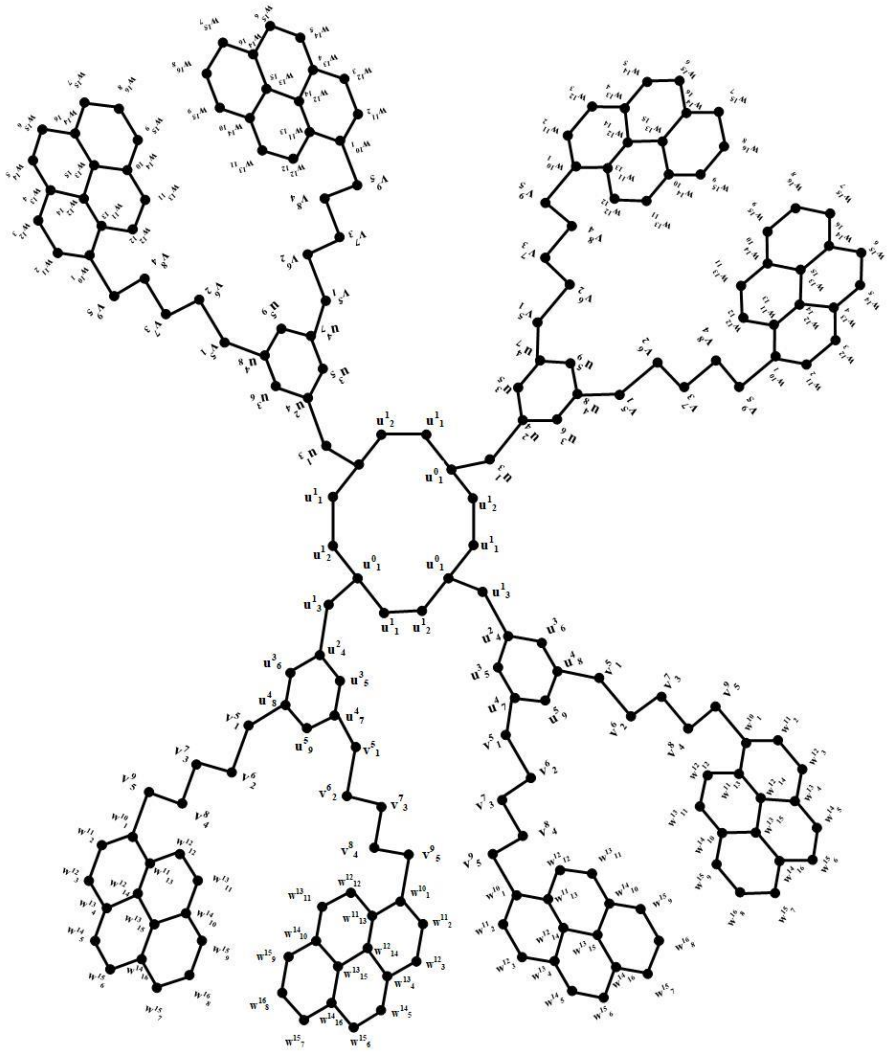

Figure 6:*Labeling pattern of cyclen-pyrene CyPy8*

Theorem 5.1:The L(2,1)-labeling of CyPy2^n for $n > 3$ is 6.

Proof: The cyclen Pyrene dendrimer graph denoted by CyPy2^n.First, we name the vertices in the first generation which are adjacent to the center vertex u_1^0 as u_1^1, u_2^1, u_3^1. Next, we name the vertices in the second generation as u_4^2 in the same order as did previously. Similarly, we name the vertices of 3^{rd}, 4^{th}, ..., n-1 th generations as v_j^{i}, w_j^{i}.Foru_j^{i},where j denote the vertex number and i denote the generation of the vertex from the central vertex.

Claim: For any number of copies n of the Cyclen-Pyrene dendrimer graph, denoted by CyPy2^n, the graph satisfies the L(2,1)-labeling condition.

Base Case (n = 1): The base case of a single copy of the Cyclen-Pyrene dendrimer graph. In this graph, the vertices in the first generation surrounding the central vertex u_1^0 are labeled as u_1^1, u_2^1, u_3^1, and so forth. The labels are assigned as follows: The central vertex u_1^0 is labeled as 0. The first generation vertices u_1^1, u_2^1, u_3^1 are labeled as 4, 2, and 3 respectively. The second generation vertex u_4^2 is labeled as 6. The third generation vertices u_5^3 and u_6^3 are labeled 1 and 2 respectively. The fourth generation vertices u_7^4 and u_8^4

are labeled 3 and 4 respectively. The fifth generation vertex u_9^5 is labeled 6. Continuing this pattern for u_j^{i} up to the n-th generation, all labels are at least 2 apart, satisfying the L(2,1) condition.

Labeling of v_j^{i}: Starting from the fifth generation, the labeling proceeds as follows: The 5^{th} generation vertex v_1^5 is labeled 0. The 6^{th} generation vertex v_2^6 is labeled 5. The 7^{th} generation vertex v_3^7 is labeled 3. The 8^{th} generation vertex v_4^8 is labeled 0. The 9^{th} generation vertex v_5^9 is labeled 5. All labels maintain a separation of at least 2, satisfying the L(2,1) condition.

Labeling of w_j^{i}: Starting from the tenth generation, the labeling proceeds as follows: The 10^{th} generation vertex w_1^{10} is labeled 3. The 11^{th} generation vertex w_2^{11} is labeled 6. The 12^{th} generation vertices are labeled as: w_{12}^{12} is labeled $6w_3^{12}$ is labeled $2w_{14}^{12}$ is labeled 4. The 13^{th} generation vertices are labeled as: w_4^{13} is labeled $0w_{11}^{13}$ is labeled $3w_{15}^{13}$ is labeled 2. The 14^{th} generation vertices are labeled as: w_5^{14} is labeled $3w_{10}^{14}$ is labeled $0w_{16}^{14}$ is labeled 6. The 15^{th} generation vertices are labeled as: w_6^{15} is labeled $1w_7^{15}$ is labeled $3w_9^{15}$ is labeled 4. The 16^{th} generation vertex w_8^{16} is labeled 1. All labels maintain a separation of at least 2, satisfying the L(2,1) condition.

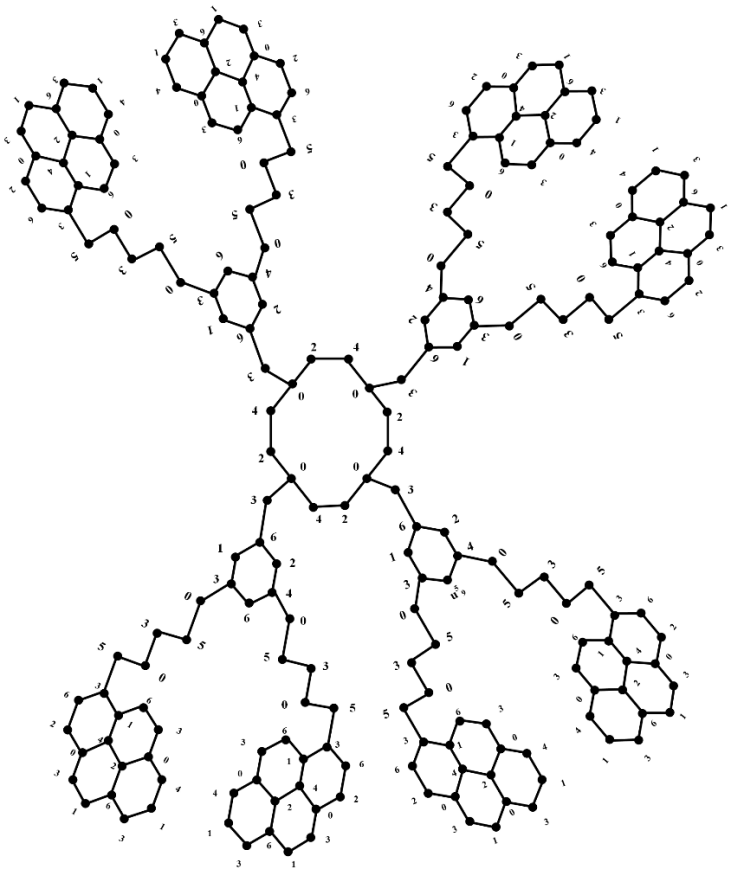

Figure 7: *L(2,1)-Labeling of cyclen-pyrene CyPy8*

Inductive Step: Having established this for the n-th copy, we proceed with the inductive step.Assume the L(2,1) labeling condition holds for $n = k$, we aim to prove it for $n = k + 1$. Extending the labeling schemeas described for the $(k + 1)$-th copy, we ensure that adjacent vertices have labels at least 2 apart, thus maintaining the L(2,1) condition. Thus, by induction, we have shown that for any number of copies n

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of the Cyclen-Pyrene dendrimer graph, CyPy2^n, the graph satisfies the L(2,1) labeling condition with $\lambda_{2,1}$ is 6.See Figure 6 and 7.

6 Potential Limitations

The study on L(2,1)-labeling of Melem and Cyclen-Pyrene dendrimers has a few drawbacks. It uses idealistic graph structures that may not entirely replicate real-world molecule arrangements, limiting the conclusions' generalizability. Labeling big or complicated graphs is computationally costly, which may limit the investigation to smaller structures, and the distance-based labeling approach may not adequately capture chemical interactions. Furthermore, the employment of various techniques may produce varied results, and theoretical bounds may not be compatible with practical chemical systems. The study also ignores unique network features, potential labeling process optimizations, and experimental validation, all of which may have an impact on the application of its conclusions. Finally, the two-dimensional graph model used does not account for the three-dimensional nature of dendrimer molecules, which may lead to differences with real-world structures.

7 Conclusion

This investigation examines in the upper bounds of L(2,1) labeling in chemical structures, with a concentrate on Melem and Cyclen-Pyrene Dendrimers. The findings are relevant to Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) research, which aid in chemical hazard estimation, drug discovery, and molecular design. The paper also covers channel assignment issues such as radio number and geometric radio labeling, stressing their importance in understanding molecular structures and practical applications.

8 Declarations

8.1 Competing Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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