



An induced P_3 -packing k -partition number for Benzenoid System

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Abstract

Benzenoid systems are formed by collections of congruent hexagons arranged in the plane such that any two hexagons are either disjoint or share a common edge. These structures are naturally studied through graph-theoretic packing parameters. For a fixed graph H , an H -packing of a graph G is a family of vertex-disjoint subgraphs of G , each isomorphic to H . In this work, we determine the P_3 -packing number and an induced P_3 -packing k -partition number for three standard benzenoid families: the triangular benzenoid system, the rhombic benzenoid system, and the zigzag benzenoid system. For each class, algorithms are provided for computing these parameters, together with justification of their correctness. The results yield exact values for the corresponding packing and partition numbers in these benzenoid structures.

Keywords: P_3 -Packing, Perfect P_3 -packing, Near Perfect P_3 -packing, Induced H -packing k -partition, Triangular Benzenoid System, Rhombic Benzenoid System, and Zigzag Benzenoid System.

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1. Introduction

Let G and H be graphs. An H -packing of a graph G is a family of pairwise vertex-disjoint subgraphs of G , each isomorphic to H [1, 13]. Packing problems generalize matchings and arise in numerous combinatorial and applied settings.

Definition 1.1. A collection $\mathcal{H} = \{H_1, H_2, \dots, H_r\}$ of induced subgraphs of a graph G is said to be *sg-independent* if (i) $V(H_i) \cap V(H_j) = \emptyset$ for all $i \neq j$, and (ii) no edge of G has one endpoint in H_i and the other in H_j , for $i \neq j$. If each H_i is isomorphic to a fixed graph H , then \mathcal{H} is called an *H-independent set*.

Definition 1.2. Let \mathcal{H} be a perfect or almost perfect H -packing of a graph G . A partition $\{\mathcal{H}_1, \dots, \mathcal{H}_k\}$ of \mathcal{H} such that every \mathcal{H}_i is an H -independent set is called an *induced H-packing k-partition*. The minimum such k is the induced H -packing k -partition number of \mathcal{H} , denoted by $\text{ipp}_{\mathcal{H}}(G, H)$.

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The induced H-packing k-partition number of G, written $\text{ipp}(G, H)$, is

$$\text{ipp}(G, H) = \min_{\mathcal{H}} \text{ipp}_{\mathcal{H}}(G, H),$$

where the minimum is taken over all H-packings of G [13].

Packing problems have been studied in several contexts, including scheduling [4], sensor networks [5], wiring-board layout, code optimization [11], and channel assignment in radio communication [17]. When H is a connected graph with at least three vertices, determining the maximum H-packing is NP-complete [28]. Packing in hypercubes [3], induced star packings [14], dense tree packings [27], packings of almost stars [9], and packings in honeycomb and hexagonal structures [22, 20, 1, 6] have been examined extensively. Further studies on packing cycles, dense graph packings, and approximations for maximum P_3 -packing also appear in [2, 15, 16].

Graph partition parameters, including induced matching partitions, have applications in both structural graph theory and interconnection networks [7, 21]. The induced H-packing k-partition problem has been investigated for several classes of graphs and shown to be NP-complete in general [13, 23].

In chemical graph theory, graphs represent molecular structures: vertices correspond to atoms and edges correspond to chemical bonds. These graphs are usually finite, simple, connected, and undirected. For such molecular graphs, packing and partitioning problems reveal structural relations, separation of atomic groups, and independent interaction patterns within the molecule. Induced packings provide disjoint substructures without shared vertices or edges, while partition parameters organize vertex sets into mutually independent subsets, aiding structural characterization and computation.

Benzenoid systems constitute an important class of molecular graphs formed by hexagons arranged on the hexagonal lattice. Their topology influences aromaticity, stability, and electronic behavior. Path-based parameters such as induced P_3 -packings play a role in describing local structural arrangements, resonance patterns, and constraints imposed by the lattice geometry. Studies on induced P_k structures and path-detection algorithms further highlight their relevance in analyzing molecular graphs [12]. Induced P_3 -packing and its associated k-partition parameter have been examined in various network structures, including hypercubes, nanotube lattices, and other chemical graphs [13, 24, 25, 26]. Extending these investigations to benzenoid systems enables a systematic understanding of the distribution of three-vertex paths within these planar molecular structures.

In this work, we study the P_3 -packing number and the induced P_3 -packing k-partition number for three fundamental benzenoid families: triangular, rhombic, and zigzag systems. These parameters reflect the arrangement of independent three-vertex paths within each structure, and their analysis provides insight into the combinatorial organization of the corresponding molecular graphs. Algorithms for determining these values are presented, together with proofs of correctness, thereby establishing exact results for these benzenoid classes.

2. Triangular Benzenoid System

In chemical graph theory and mathematical chemistry, molecular structures are often represented as graphs, where vertices correspond to atoms and edges denote chemical bonds [8]. A triangular benzenoid system exemplifies this representation, as shown in Figure 1. Let T_p represent a triangular benzenoid system, with p indicating the number of hexagons along its base. The total number of hexagons in T_p is calculated as $\frac{1}{2}p(p+1)$ [18]. The number of vertices and edges in T_p are expressed by $|V(T_p)| = P^2 + 4p + 1$ and $|E(T_p)| = \frac{3}{2}p(p+3)$, respectively.

In the following theorem, we determine the induced P_3 -packing k-partition number for the triangular benzenoid system.

Theorem 2.1. [22] *Let G be a graph and H be a subgraph of G. Then the following general inequality holds:*

$$\lambda(G, H) \leq \left\lfloor \frac{|V(G)|}{|V(H)|} \right\rfloor.$$

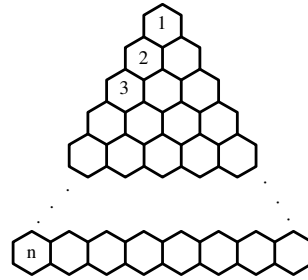


Figure 1: Triangular Benzenoid System

By applying this relation to the triangular benzenoid system, we obtain the following result.

Theorem 2.2. *Let G be a triangular benzenoid system and $H \simeq P_3$. Then induced P_3 packing number satisfies:*

$$\lambda(G, P_3) \leq \left\lfloor \frac{p^2 + 4p + 1}{3} \right\rfloor.$$

Proof. Consider the triangular benzenoid graph T_p which contains $|V(T_p)| = p^2 + 4p + 1$ vertices. Each induced P_3 subgraph involves exactly three distinct vertices, so the maximum number of disjoint P_3 paths cannot exceed one-third of the total vertices in T_p . A triangular benzenoid system is formed by arranging regular hexagons in a triangular pattern where each hexagon shares an edge with one or more neighboring hexagons. This structure can be described in terms of rows: the first row contains a single hexagon, the second row has two, and the i^{th} row contains i hexagons. The two slanting sides of the triangle form the acute edges, while the horizontal base represents the obtuse edge.

Let T_p represent a triangular benzenoid system with p rows of hexagons. For $H \simeq P_3$, we proceed to determine the corresponding H-packing number for this configuration.

Theorem 2.3. *For a triangular benzenoid system T_n with n layers, Algorithm in Triangular Benzenoid System, constructs an induced P_3 -packing of maximum size $\lfloor |V(T_n)|/3 \rfloor$, and produces the corresponding induced P_3 -packing k -partition.*

Procedure: P_3 -Packing Triangular Benzenoid System T_p

Input: The Triangular Benzenoid System T_p and $H \simeq P_3$.

Algorithm:

(i) Label the hexagons of T_p row by row as $R_1, R_2, R_3, \dots, R_n$, where R_i represents the i -th row containing i hexagons. Refer Figure 2.

(ii) Determine the boundary edges of T_p . The two slanted sides form the acute edges, while the horizontal base corresponds to the obtuse edge of the triangle.

(iii) Form the P_3 - packing pattern by selecting appropriate acute and obtuse edges in each row, ensuring that no two chosen edges share a vertex within a hexagon.

(iv) Repeat step (3) across all rows until only one or two vertices remain uncovered in the entire structure.

(v) The packing pattern naturally propagates along the triangular boundaries formed by the acute edges.

If $n \equiv 0 \pmod{3}$, all vertices of T_p are completely covered.

If $n \equiv 1, 2 \pmod{3}$, one or two vertices remain uncovered.

Output: The P_3 -packing number of the triangular benzenoid system T_p satisfies

$$\lambda(T_p, P_3) \leq \left\lfloor \frac{p^2 + 4p + 1}{3} \right\rfloor,$$

where $p = |V(T_p)| = p^2 + 4p + 1$.

Proof of correctness: The proposed algorithm guarantees that all vertices of the hexagons are covered when $n \equiv 0 \pmod{3}$, while only one or two vertices remain uncovered. Hence, the resulting configuration

satisfies the vertex-disjoint condition necessary for a valid P_3 -packing.

In each step of Algorithm in Triangular Benzenoid System, three consecutive vertices along a boundary row or diagonal direction are selected to form an induced P_3 . Since the algorithm marks all used vertices, no vertex is reused, ensuring that the selected P_3 paths are pairwise disjoint. The triangular structure guarantees that these triples induce no additional edges between different P_3 components. The algorithm processes every available row in a layer-by-layer manner, exhausting all maximal disjoint triples. Hence, the number of induced P_3 paths equals $\lfloor |V(T_n)|/3 \rfloor$, proving optimality. □

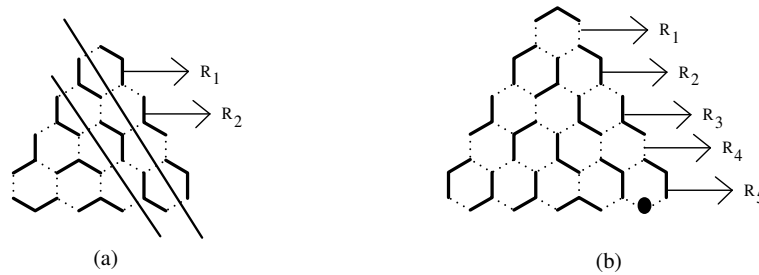


Figure 2: (a) An induced P_3 -packing number for T_4 (b) An induced P_3 -packing number for T_5

Theorem 2.4. *The Induced P_3 -Packing k -Partition number for Triangular Benzenoid System is 3.*

Proof. Let G denote a triangular benzenoid system. To demonstrate that $\text{ipp}(T_P, P_3) = 3$, we describe the following constructive procedure and verify its correctness

Procedure Partition for (T_P, P_3)

Input: The Induced P_3 -packing k -partition number for T_P is 3,

Algorithm:

- (i) Consider T_P and label P_3 -Packing k -Partition number as shown in Figure 3.
- (ii) Label P_3 -packing k -Partition number for region A_1 as $[V_1]$ and $[V_2]$ or $[V_2]$ and $[V_1]$.
- (iii) Label P_3 -packing k -Partition for region A_2 as $[V_3]$ and $[V_2]$ or $[V_1]$ and $[V_3]$.
- (iv) Label region A_3 as $[V_1], [V_2]$ or $[V_2], [V_1]$, or $[V_1], [V_2], [V_3]$ or $[V_2], [V_3], [V_1]$ or $[V_3], [V_1], [V_2]$ etc... according to the labeling of A_2 .
- (v) Continue the same labeling process for A_4, A_5, \dots, A_n until it is possible to obtain 3-partition in G .

Output:

There exists an induced P_3 -packing 3-partition for T_P .

Proof of Correctness: The labeling process described in steps (ii)(v) ensures that the vertices of T_P can be partitioned into three disjoint subsets, each corresponding to an induced P_3 -packing.

Hence $\text{ipp}(T_P) = 3$. □

3. Rhombic Benzenoid System

Consider a benzenoid system in which the hexagons are arranged to form a rhombic shape R_n , consisting of n rows with n hexagons in each row, as shown in Figure 4. The system has $2n(n + 2)$ vertices and $3n^2 + 4n - 1$ edges [19]. The notation R_n is used to denote the rhombic benzenoid system, where n represents the number of rows. The first row represents the top vertex of the rhombus - containing a single hexagon at the apex. Each subsequent row adds one hexagon until the middle row, which forms the widest part of the rhombus. After reaching the middle, each successive lower row symmetrically loses one hexagon on either side. The last row, corresponding to the bottom vertex, again consists of a single hexagon, mirroring the first row.

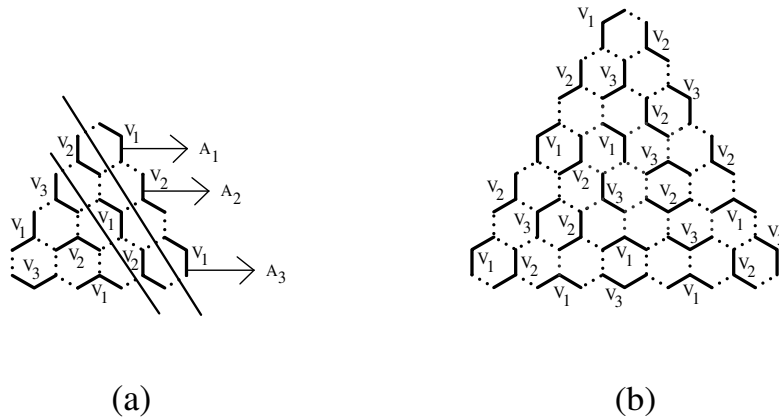


Figure 3: (a) An induced P_3 -packing 3-partition number for T_4 (b) An induced P_3 -packing 3-partition number for T_7

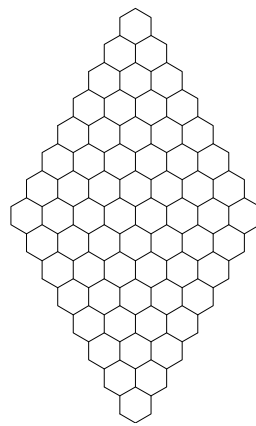


Figure 4: Rhombic Benzenoid System

Thus, the structure begins and ends with one hexagon, preserving symmetry, a closed rhombic boundary, and overall compactness. Hence, R_n forms a diamond-shaped arrangement that starts and ends with a single hexagon.

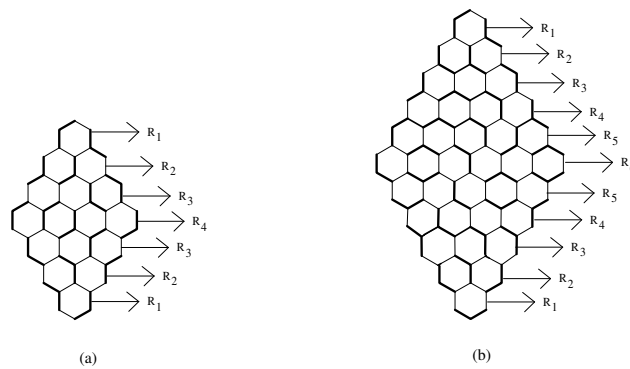


Figure 5: (a) An induced P_3 -packing number for R_4 (b) An induced P_3 -packing number for R_6

Theorem 3.1. Let G be a rhombic benzenoid of size n . Then,

$$\lambda(G, P_3) \leq \left\lfloor \frac{|2n(n+2)|}{3} \right\rfloor.$$

Proof. Let R_n denote a rhombic benzenoid system formed by a parallelogram of hexagons with n rows and let $H \simeq P_3$. We describe a procedure to construct a maximal P_3 -packing of R_n .

Theorem 3.2. For a rhombic benzenoid system R_n , Algorithm produces an induced P_3 -packing of maximum size $\lfloor |V(R_n)|/3 \rfloor$, and yields the corresponding induced P_3 -packing k -partition.

Procedure: P_3 -Packing Rhombic Benzenoid System R_n

Input: Rhombic Benzenoid System R_n and $H \simeq P_3$.

Algorithm:

- (i) Label the hexagon of R_n in row-wise as $R_1, R_2, R_3, R_4, \dots, R_n$ where R_i denotes the i^{th} row of the system as shown in figure 5.
- (ii) Construct an induced P_3 - packing within each row, ensuring that no two selected edges share a common vertex.
- (iv) Any leftover vertices in a row can be paired with vertices in the subsequent row to maintain vertex-disjointness and improve coverage.
- (v) Repeat steps ii and iii for all rows until either all vertices are covered (perfect packing) or one or two vertices remain uncovered.

Output:

The induced P_3 - packing of R_n satisfies

$$\lambda(G, P_3) \leq \left\lfloor \frac{|2n(n+2)|}{3} \right\rfloor.$$

Proof of Correctness: algorithm ensures that all vertices of the hexagons are included when $n \equiv 0 \pmod{3}$. If $n \equiv 1, 2 \pmod{3}$, one or two vertices may remain uncovered. Therefore, the procedure produces a valid induced P_3 - packing satisfying the vertex-disjoint condition.

Every triple selected by Algorithm corresponds to three consecutive vertices along a diagonal or horizontal chain in R_n , forming an induced P_3 . Because the algorithm records all used vertices, no two selected triples share vertices. The rhombic structure ensures that triples chosen on one diagonal do not introduce edges to triples on other diagonals. The algorithm systematically traverses all valid diagonals, selecting all possible vertex-disjoint P_3 components. Therefore, the constructed packing achieves the upper bound $\lfloor |V(R_n)|/3 \rfloor$. □

Theorem 3.3. The Induced P_3 -Packing k -Partition number for Rhombic Benzenoid System is 3.

Proof. Let G be a Rhombic Benzenoid System R_n . We now present a procedure along with a proof of correctness to show that $\text{ipp}(R_p, P_3) = 3$.

Procedure Partition for (R_n, P_3)

Input: Rhombic Benzenoid System R_n and $H \simeq P_3$.

Algorithm:

- (i) Consider R_n and label P_3 -Packing k -Partition number as shown in Figure 6.
- (ii) Label the P_3 -Packing k -Partition number for region R_1 as $[V_1]$ and $[V_2]$ or $[V_2]$ and $[V_1]$.
- (iii) Label P_3 -Packing k -Partition number for R_2 as $[V_3]$ and $[V_2]$ or $[V_1]$ and $[V_3]$.
- (iv) Label R_3 is labeled as $[V_1], [V_2]$ or $[V_2], [V_1]$, or $[V_1], [V_2], [V_3]$ or $[V_2], [V_3], [V_1]$ or $[V_3], [V_1], [V_2]$ etc ... depending on the labeling of R_2 .
- (v) Continue the same procedure for R_4, R_5, \dots, R_n until a 3-partition is obtained for the entire system G .

Output:

There exists an induced P_3 -packing 3-partition for R_n .

Proof of Correctness: The labeling process from steps (ii) to (v) guarantees that the vertices of R_n can be partitioned into three disjoint subsets corresponding to an induced P_3 -packing. Hence $\text{ipp}(R_n) = 3$. □

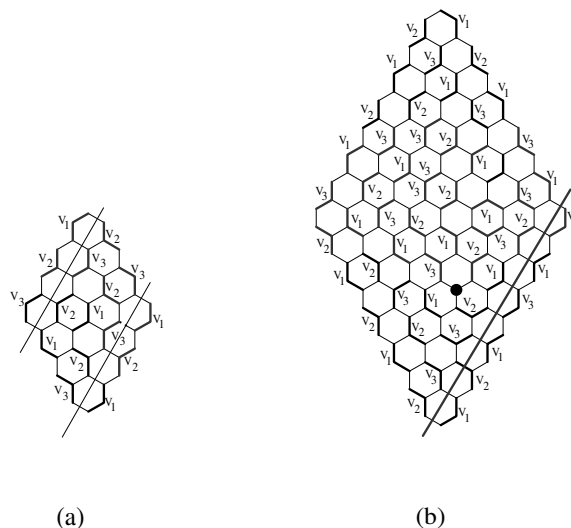


Figure 6: (a) An induced P_3 -packing 3-partition number for R_4 (b) An induced P_3 -packing 3-partition number for R_7

4. Zigzag Benzenoid System

In this subsection, we describe the structural characteristics of the zigzag benzenoid system Z_p and determine its corresponding induced P_3 -packing k -partition number. The zigzag benzenoid system Z_p illustrated in Figure 7, consists of a sequence of hexagons arranged in a zigzag manner. It contains p rows, where each row includes two adjacent hexagons connected along their sides. The total number of vertices in Z_p is $8p + 2$, and the number of edges is $10p + 1$ [19].

In this section, we examine the existence of perfect and near-perfect P_3 -packings and establish the corresponding induced P_3 -packing k -partition number for the zigzag benzenoid chain. These results provide insights into the structural regularity and connectivity patterns of this molecular configuration.

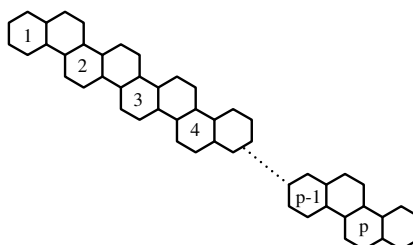


Figure 7: Zigzag Benzenoid System

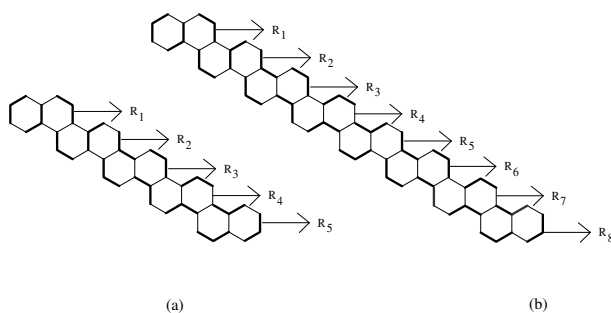


Figure 8: (a) An induced P_3 -packing number for Z_5 (b) An induced P_3 -packing number for Z_8

Theorem 4.1. Let G be a Zigzag Benzenoid System Z_p . Then,

$$\lambda(G, P_3) \leq \left\lfloor \frac{8p+2}{3} \right\rfloor.$$

Proof. A Zigzag Benzenoid System of order p , is a connected hexagonal chain composed of p hexagons joined edge-to-edge, where the outer boundary alternates in a zigzag fashion.

Theorem 4.2. For a zigzag benzenoid system Z_p , Algorithm constructs a maximum induced P_3 -packing of size $\lfloor |V(Z_k)|/3 \rfloor$, together with the induced P_3 -packing k -partition.

Procedure: P_3 -Packing Zigzag Benzenoid System Z_p

Input: A Zigzag Benzenoid System Z_p and $H \simeq P_3$.

Algorithm:

- (i) Label the topmost row as R_1 and the succeeding rows as R_2, R_3, \dots, R_n as in figure 8.
- (ii) In R_1 , select three consecutive outer boundary vertices from each hexagon to form an induced path P_3 .
- (iii) For R_2 , repeat the same packing pattern as in R_1 , ensuring that the selected vertices do not overlap with those in the previous row.
- (iv) Continue the same process for all rows R_3, R_4, \dots, R_n until the structure is completely covered.

Output: There exists a perfect or almost perfect H -packing of Z_p satisfying $\lambda(G, P_3) \leq \left\lfloor \frac{8p+2}{3} \right\rfloor$.

Proof of Correctness: In the Zigzag Benzenoid System, adjacent hexagons share exactly one common edge. Each selected P_3 subgraph consists of three consecutive boundary vertices belonging to a single hexagon, and it does not intersect with the vertices of neighboring hexagons.

By alternating the packing sequence between successive rows, the constructed subgraphs remain vertex-disjoint and collectively cover all vertices, except possibly one or two when $n \equiv 1, 2 \pmod{3}$.

Hence the result $\lambda(G, P_3) \leq \left\lfloor \frac{8p+2}{3} \right\rfloor$ is verified.

Algorithm selects triples of consecutive vertices along each zigzag chain, guaranteeing that each chosen triple forms an induced P_3 . Since vertices are marked as soon as they are used, no two triples overlap. The zigzag structure ensures that adjacent chains do not create edges between distinct triples, preserving the induced property. As the algorithm exhaustively processes each chain, it extracts all possible disjoint triples. Consequently, the packing is maximal and has size $\lfloor |V(Z_p)|/3 \rfloor$, establishing its correctness. \square

Theorem 4.3. The Induced P_3 -Packing k -Partition number for Zigzag Benzenoid system is 3.

Proof. Let G be a Zigzag Benzenoid system Z_p . Let p represent the number of rows in the graph, where each row contains two adjacent hexagons. In the first row, there are two hexagons with a total of twelve edges, among which one edge is shared; hence, the effective count is eleven distinct edges. When the first and second rows are combined, we obtain twenty-four total edges, with three shared edges, resulting in twenty-one unique edges. Continuing this pattern, the general structure of the Zigzag Benzenoid System contains $10p + 1$ edges and $8p + 2$ vertices. Each vertex in the system is of degree either two or three.

We now present a systematic procedure to demonstrate that $\text{ipp}(Z_p, P_3) = 3$.

Procedure: Partition for (Z_p, P_3)

Input: Zigzag Benzenoid system Z_p and $H \simeq P_3$.

Algorithm:

- (i) Consider Z_p and mark the P_3 -Packing k -Partition number as illustrated in Figure 9.
- (ii) Label P_3 -Packing k -Partition number for region R_1 as $[V_1]$ and $[V_2]$ or $[V_2]$ and $[V_1]$.
- (iii) Label P_3 -Packing k -Partition number of R_2 as $[V_3]$ and $[V_2]$ or $[V_1]$ and $[V_3]$.
- (iv) Label R_3 as $[V_1], [V_2]$, or $[V_2], [V_1]$ or $[V_1], [V_2], [V_3]$ or $[V_2], [V_3], [V_1]$ or $[V_3], [V_1], [V_2]$ etc... depending on the labeling pattern of R_2 .

(v) Continue the same labeling approach for R_4, R_5, \dots, R_n until a valid 3-partition of the graph is obtained.

Output:

There exists an induced P_3 -packing 3-partition for Z_p .

Proof of Correctness: The labeling process of (ii)-(v) guarantees that the vertices of Z_p can be divided into three mutually disjoint subsets, each corresponding to an induced P_3 -packing. Therefore, it follows that $\text{ipp}(Z_p) = 3$.

□

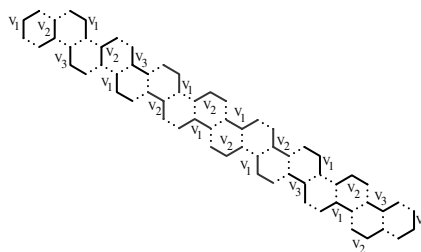


Figure 9: An induced P_3 -packing 3-partition number for Zigzag Benzenoid System

5. Conclusion

In this paper, we have determined the packing number and the induced H -packing k -partition number for three distinct benzenoid systems - Triangular, Rhombic, and Zigzag where $H \simeq P_3$. The results demonstrate that each of these molecular graph structures admits a well-defined induced P_3 -packing partition, revealing underlying regularities in their vertex and edge configurations.

The study highlights how the structural pattern and connectivity of the benzenoid systems influence their induced packing properties. These findings can provide a mathematical basis for understanding molecular stability and connectivity patterns in chemical graph theory. Future investigations may extend this approach to other benzenoid systems or to higher-order path packings P_k , thereby deepening the combinatorial understanding of molecular graph structures.

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