Pendant Graphs: Unveiling Regularity, Irregularity, and Support Vertices

Suji Elizabeth Mathew, Sunny Joseph Kalayathankal, Baiju Thankachan*, Bibin Mathew

***Abstract*—This paper investigates Pendant Graphs, which are graphs that contain pendant vertices. It introduces a new perspective on the regularity and irregularity of pendant graphs, and discusses their relationship with Highly Irregular Graphs. Additionally, this work introduces a novel graph based on the concept derived from (m, k) Regular Graphs. The (m, k) regular graphs are closely related to Pendant Graph. The paper also delves into the nature and characteristics of pendant vertices. By exploring the characteristics of pendant vertices and defining the Cyclic Dendrimer Graph, the paper significantly contributes to both Graph Theory and Chemical Graph Theory.**

***Index Terms*—Chemical Graph Theory, Pendant Graph, Pendant vertices, $(1, k)$ Regular Graph, Cyclic Dendrimer Graph.**

I. Introduction

Chemical Graph Theory is a branch of Mathematical Chemistry [19] that helps chemists to find out the Quantitative Structure-Property Relationship (QSPR) or Quantitative Structure-Activity Relationship (QSAR) of compounds through its mathematical modeling. The mathematical modeling of compounds/ molecules is practicable with the help of Graph Theory. The structure of the compound/ molecule can be converted to graph, with atoms as vertices and bonds between atoms as edges. The mathematical modeling of these compounds into graphs is generally known as Chemical Graphs, in which only hydrogen suppressed graphs are considered.

Majority of the Chemical Graphs are graphs with pendant vertices. The presence of the pendant vertices in the Chemical Graph of the underlying compound acknowledges the existence of functional groups attached to the compounds. For example, consider the anti cancer drugs Pomalidomide, Thioguanine, Mercaptopurine, Streptozocin, Anastrozole and their corresponding Chemical Graphs in Figure 3 to Figure 8.

The functional groups Amino group and Carbonyl group in Pomalidomide are represented by pendant vertices in the corresponding chemical graph. The pendant vertices corresponding to the chemical graph of Thioguanine represents

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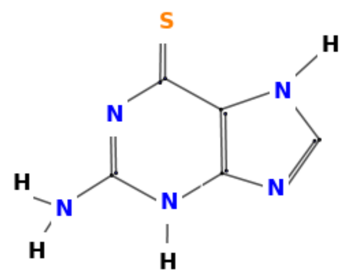

Fig. 1. Thioguanine

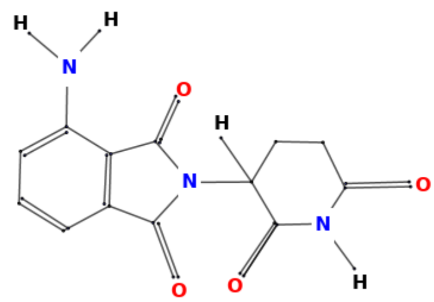

Fig. 2. Pomalidomide

Amino group and Thiocarbonyl group. Similarly, the functional group Cyano group and Propyl group, Alcoholic group and Carbonyl Amino group of Anastrozole and Streptozocin are represented by pendant vertices in their corresponding chemical graphs. In all these cases, pendant vertices represents functional groups of the underlying compound.

Suji et al. [14] defined graphs with pendant vertices as P Graphs. Based on the support vertex degrees of pendant vertices, P Graphs can be mainly classified into Pendant Regular Graph and Pendant Irregular Graph. This paper gives a new perspective to the concept on regularity and irregularity of graphs containing pendant vertices in relation to their support vertices. Currently, the investigation of graph irregularity is an active area of research. Utilizing metrics such as degree distance [16], path of length k [18], neighborhood degree [3], etc., researchers have identified several classes of irregular graphs. By defining irregularity indices, different physico - chemical properties of compound/molecule can be predicted. The Wiener Index [7], as well as the first and second Zagreb Indices [5], and the Albertson Index [2] stand as pioneering irregularity measures/indices. Some of the applications irregularity indices are discussed in [8], [20]–[24].

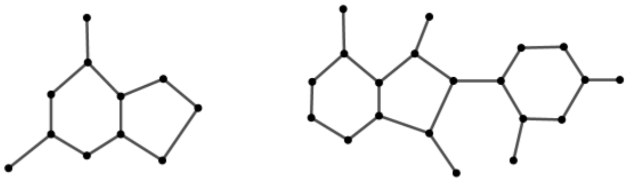

Fig. 3. Chemical Graphs of Thioguanine and Pomalidomide.

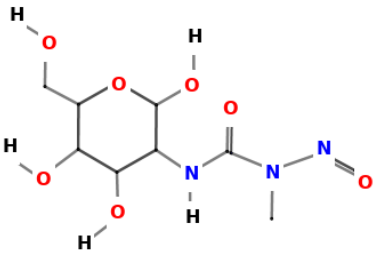

Fig. 4. Streptozocin

II. Preliminaries and Basic Definitions

For a graph G, denote $V(G)$ and $E(G)$ as vertex and edge set respectively. Denote degree of a vertex u as $d(u)$ and the neighbourhood of a vertex u as $N(u)$. $d_d(u)$ denotes number of vertices at a distance d from u. Hence $d_1(u) = d(u)$

Definition 1: [14] Support Vertex is the vertex adjacent to a pendant vertex. Let U denote set of support vertices and $|U|$ denote its cardinality.

Definition 2: [12] A graph G is (d, k) - Regular , if $d_d(v) = k$ for all vertices v in G. $(1, k)$ - Regular Graph represents the k - regular graph.

Definition 3: [14] A graph with single pendant vertex is called a Trivial Pendant Graph. K_2 and m - Pangraph are examples of Trivial Pendant Graph.
Figure 8 is an example of Chemical Graph of compound which comes under the category of Trivial Pendant Graph.

Definition 4: [14] A Pendant graph is Pendant Regular, if all the support vertices should have same degree. Pendant Regular Graph be abbreviated as PR Graph.

Note 1: Path Graph $P_n, n \geq 3$, Star Graph $K_{1,n}, n \geq 2$, Pineapple graph, m-ary tree, Banana graph, n - Sunlet graph, Webgraphs are some examples of PR Graph. The graph is Pendant k - Regular, if all the degrees of support vertices are k, $k \in N$. Figure 9 is an example of Pendant 2-Regular Graph.

Figure 3 is an example of Chemical Graphs of compounds which comes under the category of PR Graph.

Definition 5: [14] A pendant graph is Pendant Irregular, if at least two support vertices have different degree. PIR graphs refer to Pendant Irregular Graphs.
Pendant Irregular graphs can be classified into two as follows;

Definition 6: A Pendant Graph is m-Partitioned Pendant Irregular, if there exist $m, m \geq 2$, distinct support vertex degrees and at least two pendant vertices should have same support vertex degrees. m - Partitioned pendant irregular graph can be simply represented as m - PPIR Graph or simply PPIR Graph.

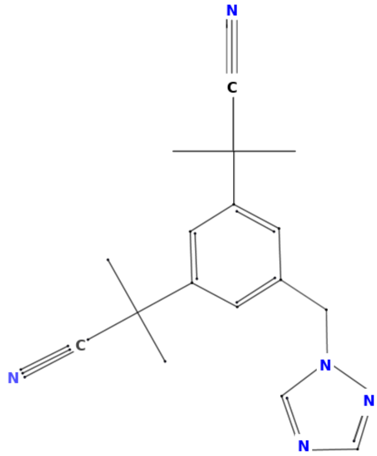

Fig. 5. Anastrozole

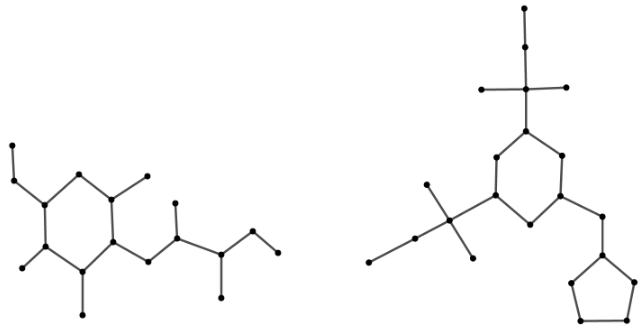

Fig. 6. Chemical Graph of Streptozocin and Anastrozole

Figure 6 is an example of Chemical Graphs of compounds which comes under the category of PPIR Graph.

Definition 7: A Pendant Graph is Completely Pendant Irregular, if there exists at least two support vertices with exactly one pendant edge attached to it and the support vertex degrees are distinct w.r.t each pendant vertices. That is, $d(u_i) \neq d(u_j)$ for any support vertices u_i and u_j and for all i, j. Completely Pendant Irregular Graphs can be abbreviated as CPIR Graph.

Definition 8: [1] The connected graph G is said to be Highly Irregular if for every vertex v, there exist $u, w \in N(v)$, $u \neq w$, implies that $d(u) \neq d(w)$.
i.e., every vertex in G is adjacent only to vertices with distinct degrees.

Proposition 1: [1] For every positive integer $n \neq 3, 5$ or 7, there exists a Highly Irregular Graph of order n.
An example of Highly Irregular Graphs is given in Figure II.

Proposition 2: [1] The size of a Highly Irregular Graph of order n is at most $\dfrac{n(n+2)}{8}$, with equality possible for n even.

Proposition 3: [1] A Highly Irregular Graph having maximum degree d has at least $2d$ vertices.
This paper establishes the relationship between P-Graphs and other classes of pendant graphs, such as $(1, k)$ Regular Graphs and Highly Irregular Graphs.

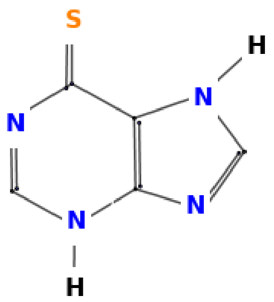

Fig. 7. Mercaptopurine

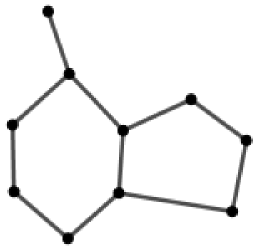

Fig. 8. Chemical graph of Mercaptopurine

III. (1,K) Regular Graphs and Pendant Graphs

As mentioned in the introductory part, P - Graph is Pendant k - Regular if all support vertices have same degree. Based on the concept of (m,k) - Regular Graph, we can redefine Pendant k - Regular graph in terms of (1, k) - Regular Graph. Even though (m, k) - Regular Graph is defined in terms of all vertices of graph, we restrict this concept to support vertices only.

Definition 9: A graph is Pendant Regular, if each support vertices $u_i, i < n$ is $(1, k)$ - Regular. In other words, $d_1(u_i) = k \ \forall i$. That is, number of vertices at a distance 1 from each support vertex is k.

Theorem 4: The smallest order of (1, k) Pendant Regular Graph containing m Star graphs $K_{1,p}$ is $m(p+1)$

Proof: Let $K_{1,p}$ be star graphs of order 1 + p. $p_1, p_2, ...p_p$ are the pendant vertices incidents on a support vertex u_1. Let $K_{1,p}^m$ denote m copies of $K_{1,p}$ with vertex set $V(K_{1,p}^m)$.
$V(K_{1,p}^m)$ = $\{p_1^m, p_2^m, p_3^m ...p_p^m, u_i^m, m \geq 1, i \geq 1\}$
Let G be a graph with vertex set and edge set as follows:

$$V(G) = \bigcup_{m \geq 1} V(K_{1,p}^m) = \{p_i^m, u_j^m, 1 \leq i \leq p, 1 \leq j \leq m\}$$

$$E(G) = \bigcup_{m \geq 1} E(K_{1,p}^m) \bigcup \{u_1u_2, u_2u_3, u_3u_4 ...., u_mu_1\}$$

The resulting graph G contains $K_{1,p}$ as an induced sub graph. These m copies of $K_{1,p}$ makes the least order of G as $m(p+1)$. ■

Corollary 1: The cycle length of smallest graph of (1, k) - Pendant Regular Graph containing m star graph $K_{1,p}$ is m.

Proof: If we take m copies of $K_{1,p}$ from the above

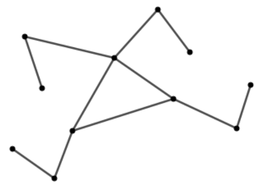

Fig. 9. Example for k - Regular Graphs

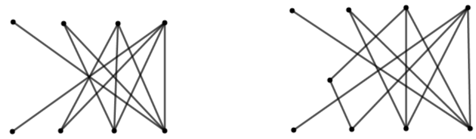

Fig. 10. Highly Irregular Graphs of order 8 and 9

theorem 4, we get

$$V(G) = \bigcup_{m \geq 1} V(K_{1,p}^m) = \{p_i^m, u_j^m, 1 \leq i \leq p, 1 \leq j \leq m\}$$

$$E(G) = \bigcup_{m \geq 1} E(K_{1,p}^m) \bigcup \{u_1u_2, u_2u_3, u_3u_4 ...., u_mu_1\}$$

The edges $u_1u_2, u_2u_3, u_3u_4 ...., u_mu_1$ will generate a cycle whose length is m. ■

Corollary 2: Any $(1, k)$ - Pendant Regular Graph with r support vertices has at least rk vertices.

Proof: By theorem 4, G contains induced sub graph $K_{1,p}$ with $V(G) = \bigcup_{m \geq 1} V(K_{1,p}^m)$. This makes order of G as at least $r(p+1)$. In general, order of any $(1, k)$ - Pendant Regular Graph has at least rk vertices.
Since the graph resembles to dendrimers, we name the above constructed graph as Cyclic Dendrimer Graph. An example of Cyclic Dendrimer Graph is given in Figure 11. ■

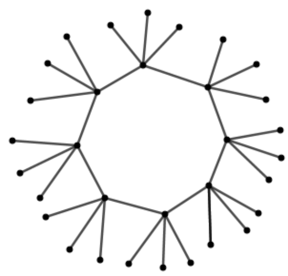

Fig. 11. The Cyclic Dendrimer Graph $K_{1,3}^8$

Proposition 5: The general pattern of adjacency matrix of Cyclic Dendrimer Graph is as follows:

$$\begin{array}{c|cccccccccccccccccccccccccc}
 & u_1 & u_2 & u_3 & u_4 & \dots & u_{m-1} & u_m & p_1^1 & p_2^1 & p_3^1 & p_4^1 & \dots & p_p^1 & p_1^2 & p_2^2 & p_3^2 & p_4^2 & \dots & p_p^2 & \dots & p_1^m & p_2^m & p_3^m & p_4^m & \dots & p_p^m \\
u_1 & 0 & * & 0 & 0 & \dots & 0 & * & * & * & * & * & \dots & * & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
u_2 & * & 0 & * & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & * & * & * & * & \dots & * & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
u_3 & 0 & * & 0 & * & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
u_4 & 0 & 0 & * & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
u_m & * & 0 & 0 & 0 & \dots & * & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & * & * & * & * & \dots & * \\
p_1^1 & * & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
p_2^1 & * & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
p_3^1 & * & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
p_4^1 & * & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
p_p^1 & * & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
p_1^2 & 0 & * & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
p_2^2 & 0 & * & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
p_3^2 & 0 & * & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
p_4^2 & 0 & * & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
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p_p^2 & 0 & * & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
p_1^m & 0 & 0 & 0 & 0 & \dots & 0 & * & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
p_2^m & 0 & 0 & 0 & 0 & \dots & 0 & * & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
p_3^m & 0 & 0 & 0 & 0 & \dots & 0 & * & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
p_4^m & 0 & 0 & 0 & 0 & \dots & 0 & * & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
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. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
p_p^m & 0 & 0 & 0 & 0 & \dots & 0 & * & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0
\end{array},$$

where * denotes the non zero element 1.
The determinant of the matrix of any size can be calculated through the determinant calculator : https://m.matrix.reshish.com/determinant.php

Note 2: The order of a Cyclic Dendrimer Graph is $(m+pm)\times(m+pm)$

Theorem 6: Determinant of Cyclic Dendrimer Graph with $K_{1,p}$, $p \geq 2$ is always zero.

Proof: The result is trivial from the adjacency matrix. In the adjacency matrix of Cyclic Dendrimer Graph, the rows of each $p_1^i, p_2^i ... p_p^i, i \geq 1$ is same. Since two rows are identical, determinant is zero. ∎

Theorem 7: The spectrum of smallest Cyclic Dendrimer Graph is 6.5

Proof: The smallest Cyclic Dendrimer Graph G is constructed with three copies of $K_{1,1}$. The adjacency matrix of such a graph is as follows;

$$A: \begin{array}{c} \\ u_1 \\ u_2 \\ u_3 \\ p_1 \\ p_2 \\ p_3 \end{array} \begin{array}{c} \begin{array}{cccccc} u_1 & u_2 & u_3 & p_1 & p_2 & p_3 \end{array} \\ \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} \end{array}$$

Arrange the rows through the following steps. Swap the first and second rows inversing determinant sign. Eliminate elements in the first column under first element. Eliminate elements in the second column under second element. Eliminate elements in the third column under the third element. Eliminate elements in the first column under fourth element. Swap the fifth and sixth rows inversing determinant. This makes the triangle into an upper triangular matrix with diagonal elements $1, 1, (-2), (\frac{-1}{2}), (-1), (-1)$. Since the spectrum is sum of absolute values of eigenvalues, here it is 6.5. ∎

Theorem 8: The adjacency matrix of Cyclic Dendrimer Graph is non singular iff $p = 1$ for each $K_{1,p}$.

Proof: Consider a Cyclic Dendrimer Graph G with vertex set

$$V(G) = \bigcup_{m \geq 1} V(K_{1,p}^m) = \{p_i^m, u_j^m, 1 \leq i \leq p, 1 \leq j \leq m\}$$

Assume that adjacency matrix of Cyclic Dendrimer Graph is non singular. p_i^1 represents the pendant vertices p_1^1, p_2^1, $p_3^1 ... p_p^1$ which incidents on the support vertex u_1 in $K_{1,p}^1$. p_i^2 represents the pendant vertices $p_1^2, p_2^2, p_3^2 ... p_p^2$ which incidents on the support vertex u_2 in $K_{1,p}^2$ etc. In the adjacency matrix of G, $u_1p_1^1, u_1p_2^1, ...u_1p_p^1$ and $u_2p_1^2, u_2p_2^2, ...u_2p_p^2$ etc is 1. The rows representing pendant vertices contains only a single element. Thus the column representing u_1 contains m identical elements or otherwise the rows representing p_1^1, p_2^1, $p_3^1 ... p_p^1$ are identical so that the adjacency matrix become singular. Since we assumed that graph is non singular, this is not possible.Therefore there should exist only one pendant vertex p_1^1 w.r.t u_1 in $K_{1,p}^1$. Similarly for $K_{1,p}^2$, $K_{1,p}^3$,...$K_{1,p}^m$. Conversely assume that $p = 1$ in each $K_{1,p}^m$. Each of $K_{1,p}$ has exactly a single pendant edge. The support vertices and pendant vertices in $K_{1,p}^m$ makes an adjacency matrix as explained in Theorem 8. The determinant value -1 makes the adjacency matrix as a non singular matrix. ∎

Theorem 9: The chromatic number of Cyclic Dendrimer Graph is $\chi(G)$= $\begin{cases} 2, & m = \text{even},\ m\ \epsilon N \\ 3, & m = \text{odd},\ m\ \epsilon N \end{cases}$

Proof: Since the chromatic number of star graph is 2, assign colour 1 for u_1. Assign colour 2 to p_1^1, p_2^1, $p_3^1 ... p_p^1$ and for u_m and u_2. Assign colour 1 to p_1^2, p_2^2, $p_3^2 ... p_p^2$ and u_3. Assign colour 2 to p_1^3, p_2^3, $p_3^3 ... p_p^3$ and u_4. Continue this process of colouring. As mentioned in corollary 1 of Theorem 4, the cycle length of $K_{1,p}^m$ is m. The chromatic number of a cycle graph is 2, if cycle length is even and 3, if cycle length is odd. Thus the chromatic number of cyclic dendrimer graph exactly depends on the length of the cycle. ∎

Corollary 3: The girth of cyclic dendrimer graph is m.

Theorem 10: The chromatic polynomial of Cyclic Dendrimer Graph is; $P_n(\lambda) = \lambda(\lambda - 1)$

Proof: By theorem 9, the chromatic number of Cyclic Dendrimer Graph is 2,

$$\therefore \quad P_n(\lambda) = \sum_{i=1}^{n} \binom{\lambda}{i} c_i$$

$\because \chi(G) = 2$, $c_1 = 0$ and $i = 2$

$$P_n(\lambda) = 0 + \binom{\lambda}{2} c_2 = \lambda(\lambda - 1)$$

∎

Theorem 11: For a Cyclic Dendrimer Graph, the cardinality of vertex cover is $|M|$ = m

Proof: The construction of Cyclic Dendrimer Graph is from m -copies of $K_{1,p}$. For a star graph, to cover all the p edges, only support vertices are enough. This yields that $|M|$ = 1, for star graphs. Since Cyclic Dendrimer Graph have m copies of $K_{1,p}$, m support vertices will cover the edges of the graph. $\therefore |U|$ = $|M| = m$. ∎

IV. Highly Irregular Graphs and Pendant Graphs

In this section, we discuss how Highly Irregular Graphs are related to pendant vertices. Some properties related to Highly Irregular Graphs are also explored here.

Theorem 12: Every Highly Irregular Graphs are P - Graphs.

Proof: In Highly Irregular Graph, if v is a vertex of maximum degree d in a Highly Irregular Graph G, then v is adjacent to exactly one vertex of degree k for $1 \leq k \leq d$.

$$\sum_i d(v_i) = d + (d-1) + ... + 1$$
$$= \frac{d(d+1)}{2}$$
$$\leq 2d$$

A Highly Irregular Graph G with maximum degree d has at least $2d$ vertices. That is, the graph G should have at least two vertices of same degree. Hence the graph G should contain at least two vertices with degree 1. Therefore G is a graph with pendant vertices and hence G is a P - Graph. ∎

Theorem 13: Every Highly Irregular Graphs are either pendant k - regular or m - partitioned pendant irregular.

Proof: The construction of Highly Irregular Graphs is obtained as in [1]. Two vertices have maximum degree $\frac{n}{2}$ and these vertices are support vertices with a single pendant edge. Since both support vertices have same degree $\frac{n}{2}$, the graph becomes an Pendant $\frac{n}{2}$ -Regular Graph.
There exists trees in which at least degrees of two vertices are repeating which are also Highly Irregular Graphs. Figure IIis an example of Highly Irregular Graph and at the same time the graphs are 2- PPIR Graph and Pendant 2-Regular Graph. ∎

Theorem 14: The Highly Irregular Tree with $o(G)$ minimum is the pendant 1 - regular or simply PR graph.

Proof: K_2 is the Highly Irregular Tree and PR Graph in which $o(G)$ is minimum. The next minimum tree is P_4 in which for every vertex, neighbourhood degrees are different and two support vertices have same degree. Thus P_4 is the highly irregular and also 2 - regular graph. ∎

Theorem 15: The least Highly Irregular Graph which has at least one cycle is the pendant 3 - regular graph.

Proof: If we consider the least cycle C_3 with two pendant edges attached to two vertices, we get a 3 - regular P Graph. But this graph won't be highly irregular. Instead of C_3, if we consider C_4 the graph becomes highly irregular with at least one cycle and at the same time 3 regular Pendant Graph also. ∎

Theorem 16: The chromatic number of Highly Irregular Graph is

$$\chi(G) = \begin{cases} 2, & n = \text{even}, n\ \epsilon N \\ 3, & n = \text{odd},\ n\ \epsilon N \end{cases}$$

Proof: From the construction of Highly Irregular Graph G, it is clear that G is bipartite for $n \geq 3$. For a bipartite graph, $\chi(G) = 2$. Thus for $n = even$, $\chi(G) = 2$. To colour the vertex v_2 on the subdivision of the edge v_2u_{d-1}, one more colour is needed. Thus for $n = odd$, $\chi(G)$ is one more than number of colours required for $n = even$.
$\therefore \chi(G) = 2 + 1 = 3$ ∎

Theorem 17: The chromatic polynomial of Highly Irregular Graph is

$$P_n(\lambda) = \begin{cases} \lambda(\lambda - 1), & n = \text{even}, n\ \epsilon N \\ \lambda(\lambda^2 - 3\lambda + 2), & n = \text{odd},\ n\ \epsilon N \end{cases}$$

Proof: From Theorem 16, $\chi(G) = 2, n = even$. Hence $c_1 = 0$ and $i = 2$
Therefore

$$P_n(\lambda) = \sum_{i=1}^{n} \binom{\lambda}{i} c_i$$
$$= 0 + \binom{\lambda}{2} c_2 = \lambda(\lambda - 1)$$

For n = odd, $c_1 = c_2 = 0$ and $i = 3$
$\therefore$

$$P_n(\lambda) = \sum_{i=1}^{n} \binom{\lambda}{i} c_i = 0 + 0 + \binom{\lambda}{3} c_3$$
$$= \frac{\lambda(\lambda-1)(\lambda-2)}{3!} 3!$$
$$= \lambda(\lambda^2 - 3\lambda + 2)$$

∎

Theorem 18: For $n \geq 8$, every Highly Irregular Graph have

$$\alpha = |M| = \begin{cases} \frac{n}{2}, & n = \text{even},\ n\ \epsilon N \\ \lceil \frac{n}{2} \rceil, & n = \text{odd}, n\ \epsilon N \end{cases}$$

Proof: Since Highly Irregular Graph is bipartite, $\frac{n}{2}$ vertices are needed to cover $\frac{\frac{n}{2}\left(\frac{n}{2}+1\right)}{2}$ edges, for $n = even$. In the case of $n = odd$, one more vertex is needed to cover $\frac{\frac{n}{2}\left(\frac{n}{2}+1\right)}{2} + 1$edges. The vertex v_2 on the subdivision of edge v_2u_{d-1} is sufficient to cover the edges incident on v_2 and u_{d-1}. Thus for $n = odd$, $\frac{n-1}{2} + 1$ vertices or simply $\lceil \frac{n}{2} \rceil$ vertices are needed to cover all edges.
$\therefore$

$$\alpha = |M| = \begin{cases} \frac{n}{2}, & n = \text{even},\ n\ \epsilon N \\ \lceil \frac{n}{2} \rceil, & n = \text{odd}, n\ \epsilon N \end{cases}$$

∎

V. Nature of Pendant Vertices

As mentioned in introductory part, the motivation for the study of Pendant graphs [14] is from the Chemical Graphs of anticancer drugs. Designing new drugs in cancer treatment is inevitable. The majority of the anticancer drug compounds are pendant graphs. Counting the pendant vertices will give somewhat an idea of the number of functional groups attached to a compound. Functional groups are atoms or clusters of atoms within a compound. The naming, behavior and properties of a compound depend on the functional groups present in that compound [9]. Since pendant vertices represent functional groups, counting the pendant vertices is a matter of concern. In organic compounds, various studies of even and odd numbers of carbon atoms are executed [6], [10], [11], [13], [15], [17]. In this section, the nature of pendant vertices is revealed. Before that, the following facts should be remembered: 1. Sum of an even number of degrees is even. 2. The sum of an odd number of degrees is odd. 3. The sum of even number of odd degrees is even.

A. Pendant Vertices in PR Graphs

In PR Graphs, the degree of all support vertices are same. From the first theorem of graph theory,

$$\sum_{v \in V(G)} d(v) = 2e \tag{1}$$

The vertex set V can be partitioned into 3 sets; P, U and

W. Set of pendant vertices as P, support vertices as U and all other vertices as W. Thus $P \cup U \cup W = V$ and $P \cap W = P \cap U = U \cap W = \phi$. Let $p \in P$, $u \in U$ and $w \in W$.
By equation 1,

$$|P| + \sum_{u \in U} d(u) + \sum_{w \in W} d(w) = 2e$$

$$|P| = 2e - \sum_{u \in U} d(u) - \sum_{w \in W} d(w) \qquad (2)$$

Now we shall consider two cases; Pendent graph with vertex sets (i) P and U, (ii) P, U and W

a) Case-i: PR Graphs with P&U From 2, we have,

$$|P| = 2e - \sum_{u \in U} d(u) - \sum_{w \in W} d(w)$$

If $W = \phi$,

$$|P| = 2e - \sum_{u \in U} d(u) \qquad (3)$$

For PR Graphs, all support vertices have same degree. Let k be the number of support vertices.

Then $|P| = 2e - kd(u)$
Subcase-1 : k = even & $d(u)$ = even $\implies |P|$ is even
Subcase-2 : k = even & $d(u)$ = odd $\implies |P|$ is even
Subcase-3 : k = odd & $d(u)$ = odd $\implies |P|$ is even
Subcase-4 : k = odd & $d(u)$ = odd $\implies |P|$ is odd
It can be understood from the following representation;

$$|P| = \begin{matrix} \\ k = even \\ k = odd \end{matrix} \begin{matrix} d(u) = even & d(u) = odd \\ \left(\begin{matrix} even \\ even \end{matrix} \right. & \left. \begin{matrix} even \\ odd \end{matrix} \right) \end{matrix}$$

b) Case ii: PR Graph with P, U and W
We have,

$$|P| = 2e - \sum_{u \in U} d(u) - \sum_{w \in W} d(w)$$

$$= 2e - kd(u) - \sum_{d(w)=even} d(w) - \sum_{d(w)=odd} d(w)$$

Let

$$\sum_{d(w)=even} d(w) = s \qquad and \qquad \sum_{d(w)=odd} d(w) = t$$

$$|P| = 2e - kd(u) - s - t$$

s is always even. The above expression is depending on k, $d(u)$ and number of odd degrees of w.

Subcase 1:- $k = d(u) = t = even \implies |P|\ is\ even$
Subcase 2:- $k = d(u) = even, t = odd \implies |P|\ is\ odd$
Subcase 3:- $k - t = even, d(u) = odd \implies |P|\ is\ even$
Subcase 4:- $k = even, d(u) = t = odd \implies |P|\ is\ odd$
Subcase 5:- $d(u) = t = even, k = odd \implies |P|\ is\ even$
Subcase 6:- $d(u) = even, k = t = odd \implies |P|\ is\ odd$
Subcase 7:- $t = even, d(u) = k = odd, \implies |P|\ is\ odd$
Subcase 8:- $k = d(u) = t = odd \implies |P|\ is\ even$

The subcases can be represented as follows;

$$\begin{matrix} \\ k = d(u) = even \\ k = even,\ \ d(u) = odd \\ k = odd,\ \ d(u) = even \\ k = d(w) = odd \end{matrix} \begin{matrix} t = odd & t = even \\ \left(\begin{matrix} odd \\ odd \\ odd \\ even \end{matrix} \right. & \left. \begin{matrix} even \\ even \\ even \\ odd \end{matrix} \right) \end{matrix}$$

B. Pendant Vertices in CPIR Graphs

From equation 2,

$$|P| = 2e - \sum_{u \in U} d(u) - \sum_{w \in W} d(w)$$

Case i CPIR Graph with vertex set P, U, and $W = \phi$
Therefore,

$$|P| = 2e - \sum_{u \in U} d(u)$$

For CPIR Graph, degree of support vertex will never repeat. They may be even or odd.

$$|P| = \sum_{d(u)=even} d(u) - \sum_{d(u)=odd} d(u) \qquad (4)$$

Let

$$\sum_{d(u)=even} d(u) = s \quad and \quad \sum_{d(u)=odd} d(u) = t$$

s is always even and t is depending on the number of odd degrees.

$$|P| = 2e - s - t$$

Subcase 1 :- $t = odd \implies |P|\ \ is\ \ odd$
Subcase 2 :- $t = even \implies |P|\ \ is\ \ even$
Case ii CPIR Graph with vertex set P, U and W

Using equation 4;

$$|P| = 2e - \sum_{d(u)=even} d(u) - \sum_{d(u)=odd} d(u) - \sum d(w)$$

$\sum d(w)$ may be even or odd.
Let

$$\sum_{d(w)=even} d(w) = x \quad and \quad \sum_{d(w)=odd} d(w) = y$$

$$|P| = 2e - s - t - x - y$$

s and x are always even. Nature of P is depending on the number of odd degrees.
Subcase 1:- $k = odd, \ \ y = even \implies |P|\ \ is\ \ odd$
Subcase 2:- $t = y = odd, \ \ \implies |P|\ \ is\ \ even$
Subcase 3:- $t = y = even \implies |P|\ \ is\ \ even$
Subcase 4:- $t = even, y = odd \implies |P|\ \ is\ \ odd$

The representation of subcases are as follows:

$$|P| = \begin{matrix} \\ t = odd \\ t = even \end{matrix} \begin{matrix} y = even & y = odd \\ \left(\begin{matrix} odd \\ even \end{matrix} \right. & \left. \begin{matrix} even \\ odd \end{matrix} \right) \end{matrix}$$

C. Pendant Vertices in PPIR Graphs

Let ${u_1}^{m_1}, {u_2}^{m_2}, ...{u_k}^{m_k}$ be the support vertices of PPIR Graph. $m_1, m_2...m_k$ be the repeating number of support vertices of $u_1, u_2...u_k$ respectively.
Case i PPIR Graph with vertex set P, U and $W = \phi$
From equation 3,

$$|P| = 2e - \sum_{u \in U} d(u)$$

$$= 2e - m_1 d(u_1) - m_2 d(u_2) ... m_k d(u_k)$$

Add separately the even support vertex degrees and odd support vertex degrees.

$$|P| = 2e - \sum_{d(u_i)=even} d(u_i) - \sum_{d(u_j)=odd} d(u_j), \qquad i \neq j$$

Let

$$\sum_{d(u_i)=even} d(u_i) = s \quad and \quad \sum_{d(u_j)=odd} d(u_j) = t$$

$$|P| = 2e - s - t \tag{5}$$

Since s is even, $|P|$ is depending on t.
Subcase 1:- $t = even \Longrightarrow |P| \ \ is \ \ even$
Subcase 2:- $t = odd \Longrightarrow |P| \ \ is \ \ odd$
Case ii PPIR Graph with vertex sets P, U and W
Using equation 5,

$$|P| = 2e - s - t - \sum_{d(w)=even} d(w) - \sum_{d(w)=odd} d(w)$$

As in the case of CPIR Graph, let

$$\sum_{d(w)=even} d(w) = x \quad and \quad \sum_{d(w)=odd} d(w) = y$$

The subcases are similar as in the case of CPIR Graph.

$$|P| = \begin{array}{c} \\ t = odd \\ t = even \end{array} \begin{array}{cc} y = even & y = odd \\ \left(\begin{array}{c} odd \\ even \end{array} \right. & \left. \begin{array}{c} even \\ odd \end{array} \right) \end{array}$$

The graph theoretical work related to the nature of pendant vertices will help in generating new compounds or drugs with given properties. An algorithm to identify all functional groups in an organic compound is discussed in [4].

VI. Conclusion

This paper explores a new angle on graph regularity and irregularity by focusing on pendant graphs. The relation between pendant graphs with existing graph classes like Highly Irregular Graphs, (m, k) regular graphs is established. By delving into the nature of pendant vertices and introducing the Cyclic Dendrimer Graph, the paper offers valuable contributions to both graph theory and Chemical Graph Theory. Future research directions include exploring further graph-theoretic properties of Cyclic Dendrimer Graphs.

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