

SOME RESULTS ON PENDANT REGULAR GRAPHS

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ABSTRACT. Let $G = (V, E)$ be a simple connected graph with $o(G) = n$ and $s(G) = m$. A graph with pendant vertices is called Pendant Graphs or simply P - Graphs. In this paper we define the regularity of Pendant Graphs w.r.t. the degrees of support vertex of each pendant vertices. Sufficient conditions for pendant graphs are discussed in this paper.

1. INTRODUCTION

Throughout this paper we deal with finite, simple connected graph with pendant vertices. Let $G = (V, E)$ be a graph with pendant vertices $p_1, p_2 \dots p_r$ with support vertices $u_1, u_2 \dots u_k, k \leq r$. For a vertex $v \in V$, $d(v)$ denotes the number of edges incident on it. P and U denotes set of pendant vertices and set of support vertices respectively. A *pendant vertex* is a vertex of degree one. The *support vertex* is the adjacent vertex of pendant vertex. In this paper, we consider PR Graph of Pendant Graph, which is the regular graph in terms of support vertices.

Definition 1.1. A simple, connected graph with pendant vertices is called *Pendant Graphs* or simply *P - Graphs*. We denote a graph with single pendant vertex as *Trivial Pendant Graph*.

The motivation for the study of Pendant Graph is from the observations of chemical graphs. Author analysed 156 anticancer drugs and their corresponding chemical graphs. The observations are as follows;

- a) 95% of them are graphs with atleast one cycle.
- b) They are not regular.
- c) 99% of them are graphs with pendant vertices.

These arises a question; whether pendant vertices have any crucial role in chemical graphs for determining the properties of a molecule/compound?. In the chemical graph of organic compounds, the pendant vertices are either carbon or functional groups. The functional groups have major role in determining the properties of a compound and so the pendant vertices have a role among chemical graphs.

From the literature, it was studied that graphs with pendant vertices are always belongs to several kinds of irregular graphs [1–7]. Since pendant vertices have crucial role in determining the physico chemical nature, we are classifying Pendant graphs into Pendant Regular Graph and Pendant Irregular Graph w.r.t degrees of support vertices.

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Definition 1.2. A Pendant graph is *Pendant Regular*, if all the support vertices should have same degree. Pendant Regular Graph can be shortly represented as PR Graph.

Path Graph, Star Graph, r - Pangraph, 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 , $k \in \mathbb{N}$. We consider Trivial Pendant Graph as Pendant 1- Regular graph or simply PR Graph. K_2 and m - Pangraph are examples of Trivial Pendant Graph. Figure 5.1 is an example of Pendant 3-regular, Pendant 1-regular and Pendant 4-regular graphs respectively.

Definition 1.3. A Pendant Graph is *Pendant Irregular*, if atleast two support vertices should have different degree. Pendant Irregular Graph can be simply represented as PIR Graph.

The aim of this article is the characterization of PR Graphs and introduction of a novel graph and its properties.

2. CHARACTERISATIONS OF PENDANT REGULAR GRAPHS

In this section we present characterisations of pendant regular graphs. Based on the degrees of support vertices, Pendant Regular Graph can be realised through the following propositions;

Proposition 2.1. K_2 is the smallest Pendant k -Regular graph.

Proof

For $o(G) = 1$, G is an isolated vertex with degree zero. If $o(G) = 2$, a single edge is attached to two pendant vertices p_1 and p_2 . If we are considering p_1 , p_2 is the support vertex and vice versa. In that case degree of the support vertex is 1 and K_2 becomes the least pendant 1-regular graph.

Proposition 2.2. For any given n , the bounds for k in a Pendant k - Regular graph which is a tree, is $2 \leq k \leq (n-1)$.

The result is trivial. Pendant Regular graph with minimum support vertex degree 2 is the path graph and maximum support vertex degree $(n-1)$ is a star graph.

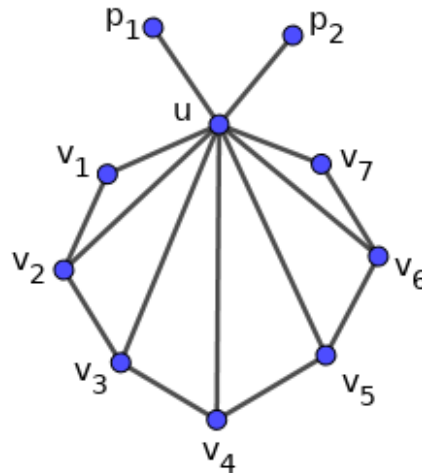
Proposition 2.3. For any given n , we can construct cyclic Pendant Regular Graph with

- (i) max length of cycle as $n-2$
- (ii) max degree of support vertex as $n-1$
- (iii) girth as 3

Proof

(i) By the definition of Pendant Regular Graph, atleast two pendant vertices should have same support vertex degree. Choose the least case of pendant vertices and it is 2. The remaining $(n-2)$ vertices shall form a cycle. If the two pendant vertices are attached to two different support vertices, clearly the degree of support vertices is 3. If two pendant vertices are attached together to a support vertex, the support vertex degree, is 4. In both cases the cycle length is $n-2$.

(ii) For any given n , construct a cycle as mentioned in (i) with two pendant vertices attached to same support vertex of C_{n-2} . Construct edges between the support vertex to non adjacent set of vertices (In geometry, this is exactly the number of diagonals drawn from a vertex of polygon with r sides, which is equal to $(r-3)$). These $(n-2)-3$ edges together with two pendant edges and two adjacent edges of support vertex will contribute $(n-5)+2+2 = n-1$ degree to the support vertex. Since the graph resembles to the insect ladybug, we name it as Ladybug graph or simply LB Graph. An example of LB Graph is given in Figure 2.1 Lady bug graph is the Pendant Regular graph with max degree of support vertex and with maximum cycle

FIGURE 2.1. LB Graph with $o(G) = 10$

length for any given $n, n \geq 5$.

(iii) From the constructions in (ii), edges between support vertex to nonadjacent set of vertices, will form C_3 's. Thus, the girth of ladybug graph is 3.

Proposition 2.4. *For any given n , we can construct Pendant Regular graph with support vertex u such that $3 \leq d(u) \leq n - 1$.*

Proof

A cyclic Pendant Regular graph with maximum degree of support vertex is mentioned in Proposition 2.3. Let p_1, p_2 and u are the pendant and support vertices respectively. Let $\{v_1, v_2, \dots, v_{n-3}\}$ is the remaining set of vertices.

To construct cyclic Pendant Regular graph with $d(u) < n - 1$, we start from the ladybug graph. For the ladybug graph, $d(u) = n - 1$. To construct a Pendant Regular graph with $d(u) = n - 2$, remove an edge from the support vertex to any of the v_i 's and join the edges from v_1 to v_{n-3} .

In the similar manner, for $d(u) = (n - 3), d(u) = (n - 4), \dots, d(u) = 4$, remove edges from support vertex and join the edges $v_1 v_{n-4}, v_1 v_{n-5}, \dots, v_1 v_3$. These construction will generate Pendant Regular graph with required degree of support vertex.

Proposition 2.5. *Pendant Graph with exactly one pair of support vertex and same number of pendant vertices attached to each support vertex is a Pendant k - Regular Graph.*

Proof

Pendant Graph with exactly one pair of support vertex and same number of pendant vertices attached to each support vertex can be constructed as follows; For any given n choose maximum value of k as;

$$k = \begin{cases} \frac{n}{2}, & n = \text{even} \\ \lfloor \frac{n}{2} \rfloor, & n = \text{odd} \end{cases}$$

The construction can be done in two cases.

Case - 1, $n = \text{even}$

Make a Star Graph $K_{1,k-1}$. Attach an edge directly between two support vertices. This will produce our required Pendant k -Regular Graph.

The result is also true in the case of a cyclic P -Graph with $n = \text{even}$. To construct our required cyclic P -Graph, choose the least cycles C_3 or C_4 . Fix any of the two vertices as support vertices u_1 and u_2 . For $n = \text{even}$, choose C_4 . Otherwise, $n - |C_3|$ or $n - 3$ will be odd, and we cannot split the pendant vertices equally to u_1 and u_2 . For $n = \text{even}$, a cycle C_4 with a pair of $\frac{n-4}{2}$ pendant vertices incidents to u_1 and u_2 which will be our required Pendant k -Regular graph. An example is given in Figure 2.2

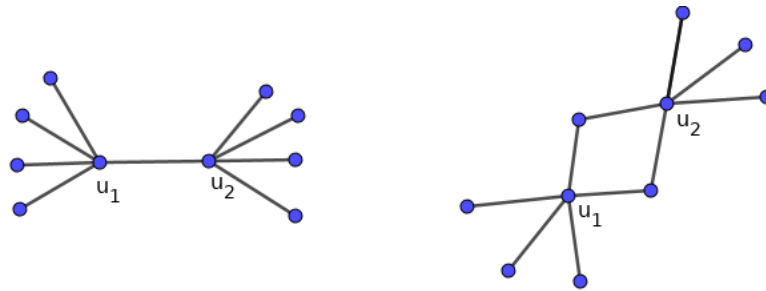


FIGURE 2.2. Example for Pendant 4 - Regular Graph

Case - 2, $n = \text{odd}$

If $n = \text{odd}$, in the similar manner as above, make a pair of Star Graph with $k - 1$ pendant vertices. Let the remaining vertex be x . Attach the edges u_1x and xu_2 . This will be our required Pendant k -Regular Graph, which is a tree. For $n = \text{odd}$, we can construct our required cyclic graph with C_3 . Fix any two vertices of C_3 as support vertices. Split the $n - |C_3|$ or $n - 3$ vertices equally into a pair of $\frac{n-3}{2}$ vertices. Attach each set of vertices as pendant vertices in u_1 and u_2 respectively. This will generate our required Pendant k -Regular Graph, which is cyclic. An example is given in Figure 2.3

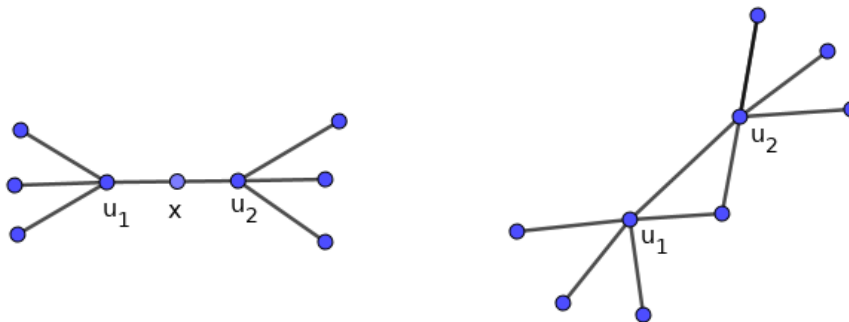


FIGURE 2.3. Example for Pendant 5- Regular Trees

Proposition 2.6. For any given n , Pendant k -Regular tree with exactly one pair of support vertex and same number of pendant vertices attached to each support vertex, $\frac{n}{2} < k < n - 1$ is not possible.

Proof

We prove this by the method of contradiction. Assume that we can construct Pendant $(n - 2)$ -Regular graph. A Star graph is Pendant $(n - 1)$ -Regular graphs. Denote p_1, p_2, \dots, p_{n-1} as pendant vertices and u

as the support vertex. Remove any of the pendant edge with pendant vertex p_1 (say) so that $d(u_1) = n - 2$. The removed pendant edge should be attached to any of the pendant vertices p_2, p_3, \dots, p_n . This will make degree of support vertex of p_1 as 2. From the definition of PR Graphs, two different degrees for support vertices is not possible. This leads to the contradiction. So the bound of k should be less than $\frac{n}{2}$.

Proposition 2.7. Let X, Y be adjacency matrices corresponding to two PR graphs;

- (i) Generally $X \pm Y$ generally need not be Pendant Regular. $X + Y$ is Pendant Regular only if at least one of the label of support vertex degrees of both graphs are same.
- (ii) The product XY will not be PR Graph.

We can explain this idea with the help of three P - Graphs G_1, G_2, G_3 as in Figure 2.4

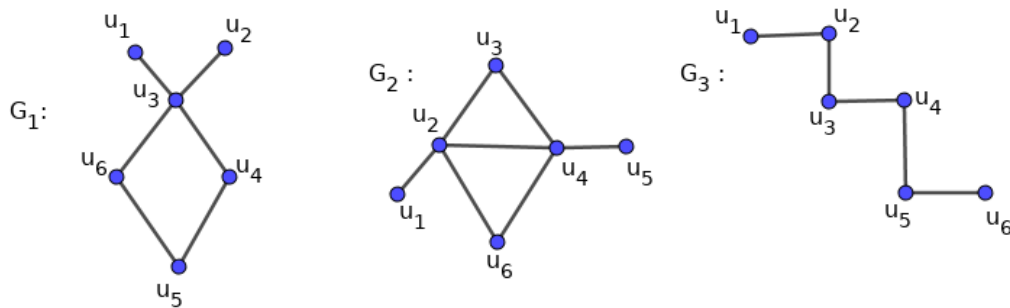


FIGURE 2.4. PR Graphs

Let X and Y be the corresponding adjacency matrices of G_1 and G_2 .

$$X : \begin{matrix} & u_1 & u_2 & u_3 & u_4 & u_5 & u_6 \\ \begin{matrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{matrix} & \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 1 & 0 \end{pmatrix} \end{matrix}$$

$$Y : \begin{matrix} & u_1 & u_2 & u_3 & u_4 & u_5 & u_6 \\ \begin{matrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{matrix} & \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \end{matrix}$$

(i) While adding X and Y , each row will contain more than one element. This is not possible in the adjacency matrix of Pendant Graphs. There is exactly one element in the row containing a pendant vertex.

Consider the case of G_2 and G_3 and let Y and Z be the corresponding adjacency matrices. Here, $Y + Z$ is a PR Graph.

If at least one of the labels of support vertex degrees of both graphs are same, the sum should be a PR Graph.

(ii) While multiplication of X and Y , atleast one of $u_{ii} \neq 0$. This will generate loop in the XY graph. Since our considerations are simple graphs, the product will not satisfy the definition of PR Graph.

3. PROPERTIES OF LADY BUG GRAPH

As we see in the above section, Lady bug graph is the Pendant Regular graph with maximum degree of support vertex and with maximum cycle length for any given $n, n \geq 5$. In this section some of the properties of Lady Bug graph is discussing.

Proposition 3.1. *The girth of LB Graph is 3 and the number of C_3 's are $n - 4$.*

Proof

In the construction of LB Graph, the edges from support vertex to its nonadjacent set of vertices will generate cycles of length 3. From (ii) of proposition 2.3 in section 2, number of edges drawn from support vertex to its nonadjacent set of vertices is $n - 5$. These $n - 5$ edges will partition the cycle of length C_{n-2} into $(n - 4)$ cycles of length 3.

Proposition 3.2. *The chromatic number of LB Graph is $\chi = \begin{cases} 3, n = \text{even} \\ 4, n = \text{odd} \end{cases}$*

Proof

Let p_1, p_2 be the pendant vertices and u_1 be the support vertex. Let u_1 is coloured with 1. u_1 is adjacent to all vertices so that we cannot colour any of the remaining vertices with 1. Let p_1, p_2 can be coloured with another colour 2. Pair the vertices u_2 and u_3 so that u_2 and u_3 are adjacent to u_1 and they are in anticlockwise and clockwise position with u_1 . Again pair the vertices u_4 which are adjacent to u_2 and u_5 , which are adjacent to u_3 as same as above. Continue this process until one or two vertices will remain. u_2 and u_3 can be coloured with 2. u_4 and u_5 can be coloured with a new colour 3. u_6 and u_7 can be coloured with 2 etc. If the number of vertices in the cycle is even, exactly one vertex will remain and it is a pair of support vertex. Since u_1 is colored with 1, the existing pair can be colored with 2 or 3.

If the number of vertices in the cycle is odd, exactly a pair of vertices will remain. One of the vertex can be coloured with 2 or 3. The neighbourhood of uncoloured vertex is already coloured with 1, 2 and 3. So the remaining vertex can be coloured with a different colour, say 4. In total, 4 colours are needed in vertex colouring for $n = \text{odd}$.

Proposition 3.3. *The chromatic polynomial of LB Graph is;*

$$P_n(\lambda) = \begin{cases} \lambda^3 - 3\lambda^2 + 2\lambda, & n = \text{even} \\ \lambda^4 - 7\lambda^3 + 14\lambda^2 - 8\lambda, & n = \text{odd} \end{cases}$$

Proof

From the above proposition, the chromatic number of LB Graph is 3, if $n = \text{even}$. Hence $c_1 = c_2 = 0$ and $i = 3$

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

For $n = \text{odd}$, the chromatic number of LB Graph is 4. Hence $c_1 = c_2 = c_3 = 0$ and $i = 4$

$$\begin{aligned} \therefore P_n(\lambda) &= \sum_{i=1}^n \binom{\lambda}{i} c_i = 0 + 0 + 0 + \binom{\lambda}{4} c_4 \\ &= \frac{\lambda(\lambda-1)(\lambda-2)(\lambda-3)}{4!} 4! \\ &= \lambda^4 - 7\lambda^3 + 14\lambda^2 - 8\lambda \end{aligned}$$

Proposition 3.4. *The general pattern of adjacency matrix of LB graph is as follows;*

$$A : \begin{matrix} & v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & . & . & v_{n-3} & v_{n-2} & v_{n-1} & v_n \\ \begin{matrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \\ v_8 \\ . \\ . \\ . \\ v_{n-2} \\ v_{n-1} \\ v_n \end{matrix} & \left(\begin{array}{cccccccccccccccc} 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & * & 0 & 1 & 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ * & * & 0 & * & * & * & * & * & * & \dots & * & * & * & * \\ 0 & 0 & * & 0 & * & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & * & * & 0 & * & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & * & 0 & * & 0 & * & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & * & 0 & 0 & * & 0 & * & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & * & \dots & 0 & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . & . & . \\ 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & \dots & * & 0 & * & 0 \\ 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & * & 0 & * \\ 0 & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & * & 0 \end{array} \right), \end{matrix}$$

where * denotes the non zero element 1.

Proposition 3.5. *Determinant of LB Graph, $n \geq 5$ is always zero.*

The result is trivial. Since the first two rows of the adjacency matrix are linearly dependent, $\Delta = 0$

Proposition 3.6. *Spectrum of LB Graph is $\xi_{LB}(G) = \begin{cases} n-2, & n = \text{even} \\ n-1, & n = \text{odd} \end{cases}$*

By converting the adjacency matrix of LB Graph into Upper Triangular Matrix, the diagonal elements are $(n-2)$ times 1, for $n = \text{even}$ and $(n-1)$ times 1, for $n = \text{odd}$. Thus the spectrum of LB Graph can be defined easily.

4. COMPLIANCE WITH ETHICAL STANDARDS

This manuscript is original and not published before. There is no conflict of interest associated with this publication. There has been no financial support for this work.

5. ANNEXURE

Some of the examples of PR graphs are given below;

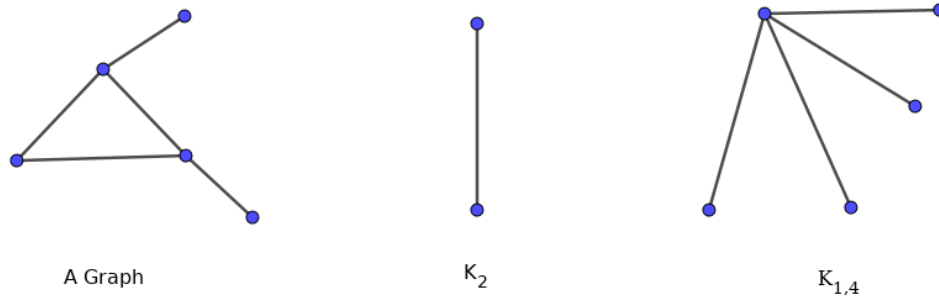
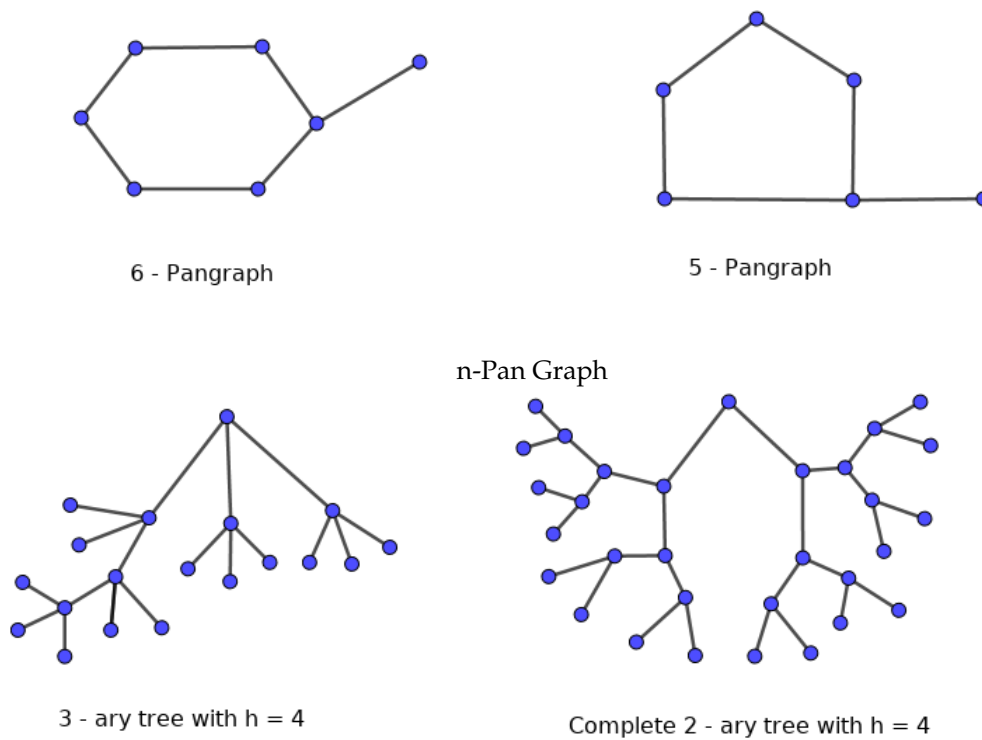
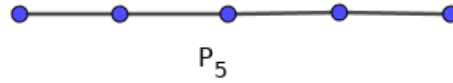
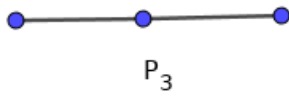


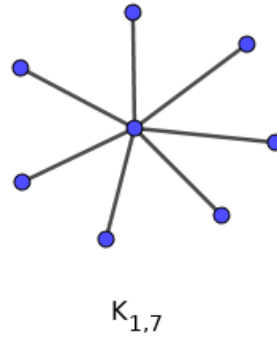
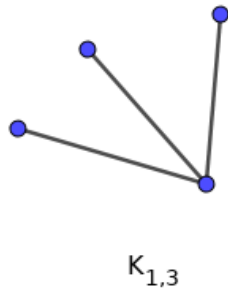
FIGURE 5.1. Example for k - Regular Graphs



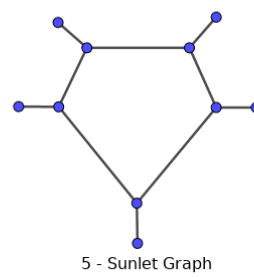
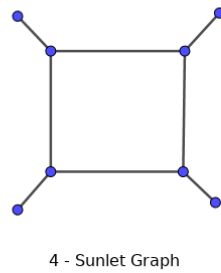
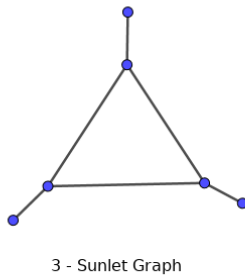
3 - ary and complete 3- ary tree



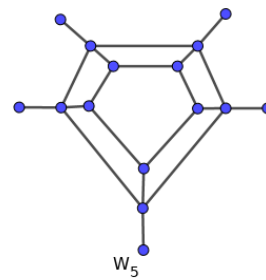
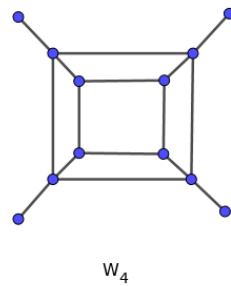
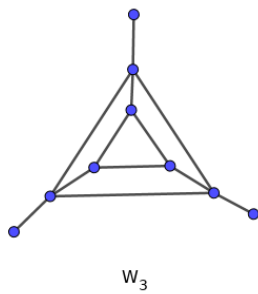
Path Graph



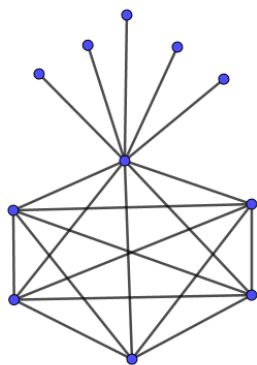
Star Graph



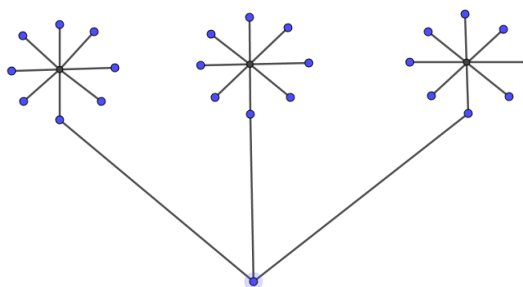
Sunlet Graph



Web Graph

The Pineapple Graph : G_6^5

Pineapple Graph

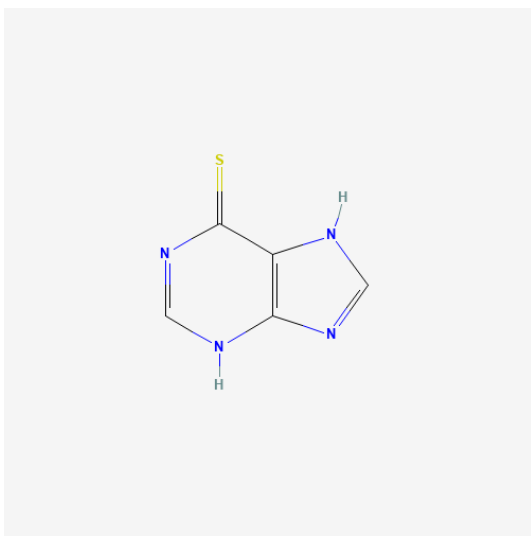
The Banana Graph, $B_{3,8}$

Banana Graph

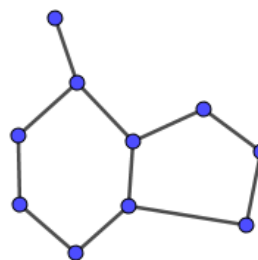
Some of the examples of pendant regular graph and their corresponding chemical graphs are given below;

1. Example for Trivial Pendant Graph

In Chemical graphs only hydrogen suppressed graphs are considered. The chemical graph of anticancer drug Mercaptopurine has exactly one pendant vertex.



Mercaptopurine

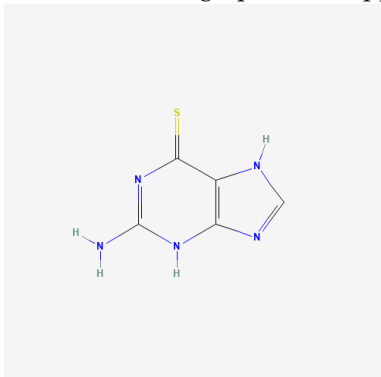


Chemical graph of Mercaptopurine

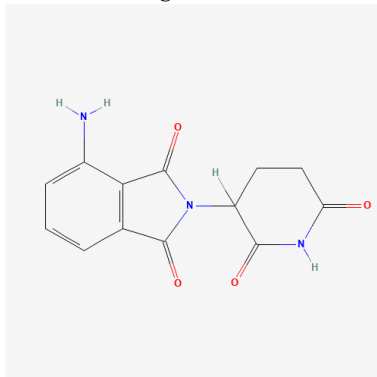
Chemical Graph of Mercaptopurine

2. Example for PR Graph

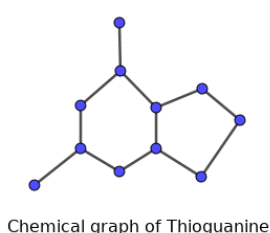
Both Pomalidomide and Thioguanine are anticancer drugs. The hydrogen suppressed chemical graphs of both of them are PR graph with support vertices degree 3.



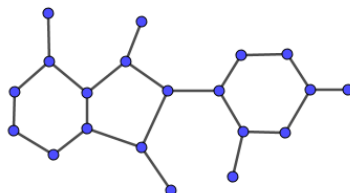
Pomalidomide



Thioguanine



Chemical graph of Thioguanine



Chemical graph of Pomalidomide

Chemical Graph of Pomalidomide and Thioguanine

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