

## Chemical Bonding and Valencies using $\mathcal{H}$ -HW Index of HM Graphs

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### Abstract

The *Wiener Index* of a connected graph  $G$ , denoted by  $\mathcal{W}(G)$  has been proposed independently by *Wiener* in 1947. The *Wiener Index* and *HW Index* are graph characters that are distance based, which are used as structure labels for forecasting physiochemical attributes of organic compounds. The *HW Index* is a abstraction proposed by Milan Randic from the notion of the *Wiener Index*, proposed by Harary Wiener. The *HW Index* is a kind of extension of the *Wiener Index*, which is the topological value assigned to  $G=(\mathcal{V},\mathcal{E})$  with set of vertices  $\mathcal{V}$  and Edges  $\mathcal{E}$  is based on the distance function. The *HW Index* of a connected graph  $G$  is denoted by  $HW(G)$  and is defined as,  $HW(G) = \frac{1}{2} \sum_{u,v \in V(G)} [d_G(x,y) + d_G^2(x,y)]$ . Where  $d_G(x,y)$  is the distance between the vertices  $x$  and  $y$  in the graph  $G$  and the summations run over all (unordered) pairs of vertices of  $G$ . The distance  $d_G(x)$  of a vertex  $x$  is the sum of all distances between  $x$  and all other vertices of  $G$ .

In the present research article, we attained the  $\mathcal{H}$ -HW Index of Path, Comb and Cycle graphs that are HM graphs. We have investigated for graphs that are HM graphs and we have generalized that the  $\mathcal{H}$ -HW Index of all the standard HM graphs are polynomials in  $m$  ( $m \leq 3$ ) with degree  $\leq 3$ . In this manner, we can calculate the Chemical Bonding of various Organic Compounds and also evaluate the Valencies of each Compound.

**Keywords:** Graph, Path, Comb, Cycle, Distance of a graph, HM graphs, *HW Index*,

Chemical Bonding, Valency.

### Introduction

In this article, the graphs considered to be are simple, undirected graphs without loops or multiple edges. For the graph theoretical characters and functions not described here, we refer to [1]. We consider  $Q$  be a simple graph of order  $h$  with vertex set  $V(Q)$  and edge set  $E(Q)$ . The distance between two vertices  $s, t \in Q$ , denoted by  $dd_Q(s, t)$  or  $d_Q(s, t)$  is defined as the shortest distance connecting  $s$  and  $t$  in  $Q$ . The exploration of the distance-related graph unvarying were first done by Harold Wiener in 1947 [2]. He realized that there exist correlation between boiling point and molecular structure. Mathematicians study *Wiener Index* since the 1970s. For a graph to be traceable from every vertex on the *Wiener Index* and *HW Index* conditions are noted[3-4].

For acyclic graphs, the *HW Index* was proposed by Milan Randic in 1993. For connected graphs, Klein et al extended the definition as a notion of the *Wiener Index* [5]. For trees with given parameters, Yuet.al considered the *HW Index*[6]. In particular, *Wiener index* of edge version was suggested by Iranmanesh et.al [7]. Randic's definition for connected graphs was generalized by Klein et.al, as a notion of the *Wiener Index*. The *Wiener Index* and its mathematical attributes, *HW Index* and its utilization in chemistry are noted [8].

HM Labeling of graphs was introduced by S.D.Deepa et.al. Motivated by the work done in *HW Index*, we have investigated the *H-HW Index* of HM graphs. In the present research article, *H-HW Index* of Path, Comb and Cycle graphs that are HM graphs are explored. We have investigated for graphs that are HM graphs and we have generalized that the *H-HW Index* of all the standard HM graphs are polynomials with degree  $\leq 3$ . The formulation of Chemical bonding between two or more atoms and molecules and also the Valencies of electrons and molecules can be calculated using *H-HW Index* of Path, Comb and Cycle graphs that are HM graphs.

## Literature Review:

There is no established method for determining the *H-HW Index* of HM graphs [9]. However the growth of Graph Theory has highlighted the importance of finding the proofs and thus there is a body of literature that attempts to address the efficacy of *HW Index* of Heronian graphs in various standard graphs. Theory of *Wiener Index* and intermolecular forces were studied in [10-11]. Before finding the results of *H-HW Index* on HM Graphs, the difference between *Wiener Index*, *Hyper-Wiener* and Harary indices were noted [12-15]. This review will outline the method of calculation that have been used for the proofs. The current study is closely

modeled on the graphs that are HM Graphs. In Graph Theory, Distance is one of the important notion [16-18]. Distance of Graphs and Weighted Graphs is studied in [19-22]. Mean Distance of graphs is studied in [23]. Sum of all distances of graphs and Average distance of graphs were studied in [24-26]. By finding the distances between vertices, we cast the  $\mathcal{H}$ -HW Index of HM Graphs. Several variations such as decomposition and subdivision of HM Graphs have also been proved [27-30]. HW Index of bicyclic graphs and unicyclic graphs were studied in [31-32].

$\mathcal{HW}$  Index of extended hydrocarbons leads to Polynomial expressions and is noted [33]. Of particular relevance to the evaluation of  $\mathcal{HW}$  Index of graphs [34], we have discussed and calculated the  $\mathcal{H}$ -HW Index of HM graphs.  $\mathcal{HW}$  Index of several standard graphs have been discussed in various research papers and they were polynomials in  $n$  with degree  $\leq n$ . We have discussed and generalized the  $\mathcal{H}$ -HW Index of HM graphs and attained polynomials in  $h$  ( $h \leq 3$ ) with degree  $\leq 3$ . We can easily calculate the Chemical bonding between two or more atoms and molecules and also the Valencies of electrons and molecules using  $\mathcal{H}$ -HW Index of Path, Comb and Cycle graphs that are HM graphs.

If  $Q$  is a  $r$ -regular graph (with  $r > 4$ ) then  $Q$  is not a HM graph. Also, if  $k > l+1$ , then the graph  $Q(k,l)$ , where  $k$  is the number of vertices and  $l$  is the number of edges, is not a HM graph. In our present article, we restrict our discussions to certain graphs that satisfies these conditions and are only HM graphs. Since HM graphs are  $k$ -regular graphs (with  $k \leq 3$ ), in our present paper we attained polynomials in  $h$  ( $h \leq 3$ ) with degree  $\leq 3$ . We have generalized the proofs through deductive method. We have attained polynomials in  $h$  ( $h \leq 3$ ) with degree  $\leq 3$  for every standard graphs that are HM graphs

## Objectives :

In the present research article, we have argued the  $\mathcal{H}$ -HW Index of HM graphs and attained polynomials in  $h$  ( $h \leq 3$ ) with degree  $\leq 3$ . . In our present article, we discussed for certain graphs that are only HM graphs. We have generalized the proofs and attained polynomials in  $h$  ( $h \leq 3$ ) with degree  $\leq 3$  for every standard graphs that are HM graphs. Accordingly, we can calculate the Chemical Bonding of various Organic Compounds and also evaluate the Valencies of each Compound in Organic Chemistry.

## Basic Definitions:

Motivated by the work done in  $\mathcal{HW}$  Index, we introduced  $\mathcal{H}$ -HW Index of HM graphs and it is defined as below.

**Definition: 1**

The  $\mathcal{H}$ -HW Index of a connected graph  $Q$  which is HM is defined as,

$$HW(Q) = \frac{1}{2} \sum_{s,t \in V(Q)} [dd_Q(s, t) + dd_Q^2(s, t)]. \quad \text{----- (1)}$$

Where  $dd_Q(s, t)$  is the distance between two vertices  $s, t \in Q$ .

$$\text{Then, } HW(Q) = \frac{1}{2} \{P(Q) + T(Q)\} \quad \text{----- (2)}$$

Where,  $P(Q) = \frac{1}{2} \sum_{s,t \in V(Q)} dd_Q(s, t)$ .

$$T(Q) = \frac{1}{2} \sum_{s,t \in V(Q)} dd_Q^2(s, t)$$

HM of graphs was introduced by S.D.Deepa et.al in 2016

We have already proved that Path, Comb and Cycle are HM Graphs.

**Results and Discussions:**

We have discussed for  $r$ -regular graphs (with  $r > 4$ ) and for graphs that satisfies  $k > l + 1$  (Where  $k$  is the number of vertices and  $l$  is the number of edges). We have generalized the proofs and attained the results in polynomials of  $h$  ( $h \leq 3$ ) with degree  $\leq 3$  for every standard graphs that are HM graphs, which is used to calculate the Chemical Bonding of various Organic Compounds and also evaluate the Valencies of each Compound in Organic Chemistry.

We attain the outcome for  $\mathcal{H}$ -HW Index of a Path graph first.

**Theorem: 1**

$$\mathcal{H}\text{-HW Index of Path is } HW(Q) = \frac{1}{2} \sum_{e=1}^{(h-1)} [e^2(e^2 - 1) + h(e + he^2 - 2e^3)]$$

**Proof:**

Let  $Q$  be a Path. Path is a HMgraph. We first calculate the distance from the first vertex to the last vertex. We use the distance formula for calculating this. We give the value of distance from each vertex as  $1, 2, 3, \dots, h$ .

$$\begin{aligned} dd_Q(s, t) = & [1 + 2 + 3 + 4 + \dots + (h-1)] + [1 + 2 + 3 + 4 + \dots + (h-2)] \\ & + [1 + 2 + 3 + 4 + \dots + (h-3)] + \dots + (1 + 2 + 3 + 4) + (1 + 2 + 3) \\ & + (1 + 2) + 1 \end{aligned}$$

$$dd_Q(s, t) = \sum_{e=1}^{(h-1)} (h-e) \times e \quad \text{----- (3)}$$

$$dd_Q^2(s, t) = \sum_{e=1}^{(h-1)} (h-e)^2 \times e^2 \quad \text{----- (4)}$$

After calculating the distance between the vertices, we now calculate the value of  $P$  and  $T$  using the formulae given below.

$$P(Q) = \frac{1}{2} \sum_{s, t \in V(Q)} dd_Q(s, t).$$

$$T(Q) = \frac{1}{2} \sum_{s, t \in V(Q)} dd_Q^2(s, t)$$

$$\text{From (3) \& (4),} \quad P(Q) = \frac{1}{2} \sum_{e=1}^{h-1} (h-e) \times e \quad \text{----- (5)}$$

$$T(Q) = \sum_{e=1}^{(h-1)} (h-e)^2 \times e^2 \quad \text{----- (6)}$$

After evaluating the value of  $P$  and  $T$ , we now calculate the HW index of the given graph using the below formulae.

$$\text{Now by (1), } HW(Q) = \frac{1}{2} \sum_{s, t \in V(Q)} [dd_Q(s, t) + dd_Q^2(s, t)].$$

$$HW(Q) = \frac{1}{2} \left[ \sum_{e=1}^{h-1} (h-e) \times e + \sum_{e=1}^{(h-1)} (h-e)^2 \times e^2 \right]$$

$$= \frac{1}{2} \sum_{e=1}^{(h-1)} [(h-e) \times e + (h-e)^2 \times e^2]$$

$$\begin{aligned}
&= \frac{1}{2} \sum_{e=1}^{(h-1)} [he - e^2 + (h + e^2 - 2he) \times e^2] \\
&= \frac{1}{2} \sum_{e=1}^{(h-1)} [he - e^2 + h^2e^2 + 2he^3 + e^4] \\
&= \frac{1}{2} \sum_{e=1}^{(h-1)} [e^2(e^2 - 1) + h(e + he^2 - 2e^3)] \quad \text{----- (7)}
\end{aligned}$$

Hence we complete the proof.

From (7), We observe that the  $\mathcal{H}$ -HW Index of a Path graph is a polynomial in  $h$  ( $h \leq 3$ ) of degree 2. This is used to calculate the Chemical Bonding of various compounds that are visibly seen in the shape of a path graph easily.

The illustration of a Path graph is given below.



Next, we prove the  $\mathcal{H}$ -HW Index of a Comb graph.

### Theorem: 2

$\mathcal{H}$ -HW Index of Comb is  $HW(Q) = \frac{1}{2}(13h^2 - 23h + 12) + \sum_{e=3}^{h-2} [4h - 6e^2 - 8e^3 - 4e^4 - 2e - 16h^2 + 16e^2h + 16eh + 48e^3h]$

### Proof:

Let  $Q$  be a Comb. Comb is a HM graph. We first calculate the distance from the first vertex to the last vertex. We use the distance formula for calculating this. We give the value of distance from each vertex as 1,2,3,.....,  $h$ .

$$\begin{aligned}
dd_Q(s, t) &= [1 + 2 + 2 + \cdots + (h-1) + (h-1) + h] + [2 + 3 + 3 + \cdots + h + h + (h+1)] \\
&\quad + [1 + 1 + 2 + 2 + \cdots + (h-2) + (h-2) + (h-1)] \\
&\quad + [2 + 3 + 3 + 4 + 4 + \cdots + (h-1) + (h-1) + h] \\
&\quad + [1 + 1 + 2 + 2 + \cdots + (h-3) + (h-3) + (h-2)] \\
&\quad + [2 + 3 + 3 + \cdots + (h-2) + (h-2) + (h-1)] + \cdots + [1 + 1 + 2] + [2 + 3] \\
&\quad + 1 \\
&= (2h-1) + (3h-4) + \sum_{e=3}^{h-2} [4h - 2(e+1) \times e]
\end{aligned}$$

$$dd_Q(s, t) = (2h-1) + (3h-4) + \sum_{e=3}^{h-2} [4h - 2e^2 - 2e] \quad \text{----- (8)}$$

$$dd_Q^2(s, t) = (2h-1)^2 + (3h-4)^2 + \sum_{e=3}^{h-2} [4h - 2e^2 - 2e]^2 \quad \text{----- (9)}$$

After calculating the distance between the vertices, we now calculate the value of P and T using the formulae given below.

$$P(Q) = \frac{1}{2} \sum_{s,t \in V(Q)} dd_Q(s, t).$$

$$T(Q) = \frac{1}{2} \sum_{s,t \in V(Q)} dd_Q^2(s, t)$$

$$\text{From (8) \& (9), } P(Q) = \frac{1}{2} [(2h-1) + (3h-4) + \sum_{e=3}^{h-2} [4h - 2(e+1) \times e]] \quad \text{----- (10)}$$

$$T(Q) = \frac{1}{2} [(2h-1)^2 + (3h-4)^2 + \sum_{e=3}^{h-2} [4h - 2(e+1) \times e]^2] \quad \text{----- (11)}$$

After evaluating the value of P and T, we now calculate the HW index of the given graph using the below formulae.

$$\text{Now by (1), } HW(Q) = \frac{1}{2} \sum_{s,t \in V(Q)} [dd_Q(s, t) + dd_Q^2(s, t)].$$

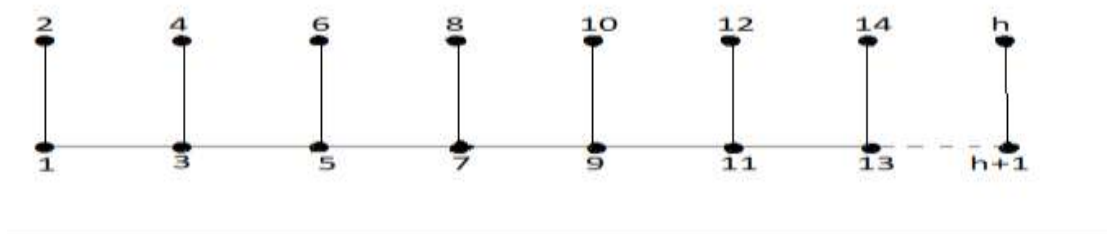
$$\begin{aligned}
HW(Q) &= \frac{1}{2} [(2h-1) + (2h-1)^2 + (3h-4) + (3h-4)^2] \\
&\quad + \frac{1}{2} \sum_{e=3}^{h-2} [(4h - 2e^2 - 2e) - (4h - 2e^2 - 2e)^2]
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{2} [(2h - 1) + (4h^2 - 4h + 1) + (3h - 4) + (9h^2 - 24h + 16)] \\
&\quad + \frac{1}{2} \sum_{e=3}^{h-2} [(4h - 2e^2 - 2e) - (4h - 2e^2 - 2e)^2] \\
&= \frac{1}{2} [2h - 1 + 4h^2 - 4h + 1 + 3h - 4 + 9h^2 - 24h + 16] \\
&\quad + \frac{1}{2} \sum_{e=3}^{h-2} [(4h - 2e^2 - 2e) - (4h - 2e^2 - 2e)^2] \\
&= \frac{1}{2} [13h^2 - 23h + 12] \\
&\quad + \frac{1}{2} \sum_{e=3}^{h-2} [4h - 2e^2 - 2e - 16h^2 - 4e^4 - 4e^2 + 16e^2h + 16eh - 8e^3 + 48e^3h] \\
&= \frac{1}{2} (13h^2 - 23h + 12) \\
&\quad + \sum_{e=3}^{h-2} [4h - 6e^2 - 8e^3 - 4e^4 - 2e - 16h^2 + 16e^2h + 16eh + 48e^3h] \text{ -----(12)}
\end{aligned}$$

Hence we complete the proof.

From (12), We observe that the  $\mathcal{H}$ -HW Index of a comb graph is also a polynomial in  $h$  ( $h \leq 3$ ) of degree 2. This is used to calculate the Chemical Bonding of various compounds that are visibly seen in the shape of a comb graph easily.

The illustration of a Comb graph is given below.



Next, we prove the  $\mathcal{H}$ -HW Index of a Cycle graph. For a cycle graph the  $\mathcal{H}$ -HW Index is attained for  $h$  is odd and  $h$  is even.

**Theorem: 3**

$\mathcal{H}$ -HW Index of Cycle is  $\text{HW}(Q)=$

$$\begin{cases} \frac{1}{2} \sum_{e=1}^{\frac{h-1}{2}} [h^2 + 3eh + e^2] & \text{if } h \text{ is odd.} \\ \frac{1}{2} \left[ \sum_{e=1}^{\frac{h-2}{2}} (h^2 + 3eh + e^2) + \sum_{e=h} \frac{1}{4} (h^2 + eh + e^2) \right] & \text{if } h \text{ is even} \end{cases}$$

**Proof:**

Let  $Q$  be a Cycle. Cycle is a HM graph. We first calculate the distance from the first vertex to the last vertex. We use the distance formula for calculating this. We give the value of distance from each vertex as  $1, 2, 3, \dots, h$ . Since Cycles with odd and even number of vertices have different values while calculating distance, We calculate the HW Index for odd and even number of vertices in a Cycle graph

First, We calculate the HW Index for cycle graph with odd number of vertices.

If  $h$  is odd,

$$\begin{aligned}
dd_Q(s, t) &= \left[ 1 + 2 + 3 + \dots + \left( h - \frac{h}{2} \right) + \left( h - \left( \frac{h}{2} + 1 \right) \right) + \left( h - \left( \frac{h}{2} + 1 \right) \right) \right. \\
&\quad \left. + \left( h - \left( \frac{h}{2} + 2 \right) \right) + \dots + \left( h - \left( \frac{h}{2} + (h - 5) \right) \right) \right] \\
&\quad + \left[ 1 + 2 + 3 + \dots + \left( h - \frac{h}{2} \right) + \left( h - \left( \frac{h}{2} + 1 \right) \right) + \left( h - \left( \frac{h}{2} + 1 \right) \right) \right. \\
&\quad \left. + \left( h - \left( \frac{h}{2} + 2 \right) \right) + \dots + \left( h - \left( \frac{h}{2} + (h - 6) \right) \right) \right] \\
&\quad + \left[ 1 + 2 + 3 + \dots + \left( h - \frac{h}{2} \right) + \left( h - \left( \frac{h}{2} + 1 \right) \right) + \left( h - \left( \frac{h}{2} + 1 \right) \right) \right. \\
&\quad \left. + \left( h - \left( \frac{h}{2} + 2 \right) \right) + \dots + \left( h - \left( \frac{h}{2} + (h - 3) \right) \right) \right] \\
&\quad + \left[ 1 + 2 + 3 + \dots + \left( h - \frac{h}{2} \right) + \left( h - \left( \frac{h}{2} + 1 \right) \right) + \left( h - \left( \frac{h}{2} + 1 \right) \right) \right. \\
&\quad \left. + \left( h - \left( \frac{h}{2} + 2 \right) \right) + \dots + \left( h - \left( \frac{h}{2} + (h - 2) \right) \right) \right] + \dots + (1 + 2 + 3) \\
&\quad + (1 + 2) + 1 \\
&= (h \times 1) + (h \times 2) + (h \times 3) + \dots + \left( h \times \left( \frac{h-1}{2} \right) \right) \\
&= \sum_{e=1}^{\frac{h-1}{2}} (h \times e)
\end{aligned}$$

$$dd_Q(s, t) = \sum_{e=1}^{\frac{h-1}{2}} (h \times e) \quad \text{----- (13)}$$

$$dd_Q^2(s, t) = \sum_{e=1}^{\frac{h-1}{2}} (h \times e)^2 \text{----- (14)}$$

After calculating the distance between the vertices, we now calculate the value of P and T using the formulae given below.

$$P(Q) = \frac{1}{2} \sum_{s, t \in V(Q)} dd_Q(s, t).$$

$$T(Q) = \frac{1}{2} \sum_{s,t \in V(Q)} dd_Q^2(s, t)$$

From (13) & (14),

$$P(Q) = \frac{1}{2} \sum_{e=1}^{\frac{h-1}{2}} (h \times e) \text{-----} (15)$$

$$T(Q) = \frac{1}{2} \sum_{e=1}^{\frac{h-1}{2}} (h \times e)^2 \text{-----} (16)$$

After evaluating the value of P and T, we now calculate the HW index of the given graph using the below formulae.

Now by (1),  $HW(Q) = \frac{1}{2} \sum_{s,t \in V(Q)} [dd_Q(s, t) + dd_Q^2(s, t)]$ .

$$\begin{aligned} HW(Q) &= \frac{1}{2} \left[ \sum_{e=1}^{\frac{h-1}{2}} (h \times e) \right] + \frac{1}{2} \sum_{e=3}^{h-2} \left[ \sum_{e=1}^{\frac{h-1}{2}} (h \times e)^2 \right] \\ &= \frac{1}{2} \sum_{e=1}^{\frac{h-1}{2}} [he + h^2 + 2eh + e^2] \\ &= \frac{1}{2} \sum_{e=1}^{\frac{h-1}{2}} [h^2 + 3eh + e^2], \text{if } h \text{ is odd.} \quad \text{-----} (17) \end{aligned}$$

Now, We calculate the HW Index for cycle graph with even number of vertices.

If  $h$  is even,

$$\begin{aligned}
dd_Q(s, t) = & \left[ 1 + 2 + 3 + \dots + \left( h - \left( \frac{h+1}{2} \right) \right) + \left( h - \left( \frac{h+1}{2} \right) \right) + \left( h - \left( \frac{h+3}{2} \right) \right) + \dots \right. \\
& \left. + \left( h - \left( \frac{h+7}{2} \right) \right) \right] \\
& + \left[ 1 + 2 + 3 + \dots + \left( h - \left( \frac{h+1}{2} \right) \right) + \left( h - \left( \frac{h+1}{2} \right) \right) + \left( h - \left( \frac{h+3}{2} \right) \right) \right. \\
& \left. + \dots + \left( h - \left( \frac{h+5}{2} \right) \right) \right] \\
& + \left[ 1 + 2 + 3 + \dots + \left( h - \left( \frac{h+1}{2} \right) \right) + \left( h - \left( \frac{h+1}{2} \right) \right) + \left( h - \left( \frac{h+3}{2} \right) \right) \right. \\
& \left. + \dots + \left( h - \left( \frac{h+3}{2} \right) \right) \right] \\
& + \left[ 1 + 2 + 3 + \dots + \left( h - \left( \frac{h+1}{2} \right) \right) + \left( h - \left( \frac{h+1}{2} \right) \right) + \left( h - \left( \frac{h+3}{2} \right) \right) \right. \\
& \left. + \dots + \left( h - \left( \frac{h+1}{2} \right) \right) \right] + \dots + (1 + 2 + 3) + (1 + 2) + 1
\end{aligned}$$

$$= (h \times 1) + (h \times 2) + (h \times 3) + \dots + \left( h \times \left( \frac{h-2}{2} \right) \right) + \left( \frac{h}{2} \times \frac{h}{2} \right)$$

$$= \sum_{e=1}^{\frac{h-2}{2}} (h \times e) + \sum_{e=h} \left( \frac{h}{2} \times \frac{e}{2} \right)$$

$$dd_Q(s, t) = \sum_{e=1}^{\frac{h-2}{2}} (h \times e) + \sum_{e=h} \left( \frac{h}{2} \times \frac{e}{2} \right) \quad \text{----- (18)}$$

$$dd_Q^2(s, t) = \sum_{e=1}^{\frac{h-2}{2}} (h \times e)^2 + \sum_{e=h} \left( \frac{h}{2} \right)^2 \times \left( \frac{e}{2} \right)^2 \quad \text{----- (19)}$$

After calculating the distance between the vertices, we now calculate the value of P and T using the formulae given below.

$$P(Q) = \frac{1}{2} \sum_{s, t \in V(Q)} dd_Q(s, t).$$

$$T(Q) = \frac{1}{2} \sum_{s,t \in V(Q)} dd_Q^2(s, t)$$

$$\text{From (18) \& (19), } P(Q) = \frac{1}{2} \left[ \sum_{e=1}^{\frac{h-2}{2}} (h \times e) + \sum_{e=h} \left( \frac{h}{2} \times \frac{e}{2} \right) \right] \text{----- (20)}$$

$$T(Q) = \frac{1}{2} \left[ \sum_{e=1}^{\frac{h-2}{2}} (h \times e)^2 + \sum_{e=h} \left( \frac{h}{2} \right)^2 \times \left( \frac{e}{2} \right)^2 \right] \text{----- (21)}$$

After evaluating the value of  $P$  and  $T$ , we now calculate the  $HW$  index of the given graph using the below formulae.

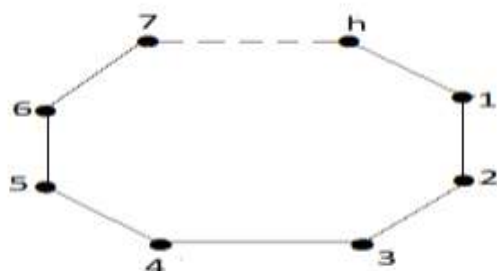
$$\text{Now by (1), } HW(Q) = \frac{1}{2} \sum_{s,t \in V(Q)} [dd_Q(s, t) + dd_Q^2(s, t)].$$

$$\begin{aligned} HW(Q) &= \frac{1}{2} \left[ \sum_{e=1}^{\frac{h-2}{2}} ((h \times e) + (h \times e)^2) + \sum_{e=h} \left( \frac{h}{2} \times \frac{e}{2} \right) + \left( \frac{h}{2} \right)^2 \times \left( \frac{e}{2} \right)^2 \right] \\ &= \frac{1}{2} \left[ \sum_{e=1}^{\frac{h-2}{2}} (he + h^2 + 2eh + e^2) + \sum_{e=h} \left( \frac{eh}{4} + \frac{h^2}{4} + \frac{e^2}{4} \right) \right] \\ &= \frac{1}{2} \left[ \sum_{e=1}^{\frac{h-2}{2}} (h^2 + 3eh + e^2) + \sum_{e=h} \frac{1}{4} (h^2 + eh + e^2) \right], \text{ if } h \text{ is even ----- (22)} \end{aligned}$$

Hence We complete the proof.

From (17) & (22), We observe that the  $\mathcal{H}$ -HW Index of a Cycle graph is also a polynomial in  $h$  ( $h \leq 3$ ) of degree 2. This is used to calculate the Chemical Bonding of various compounds that are visibly seen in the shape of a cycle graph easily.

The illustration of a Cycle graph is given below.



From the abovediscussions, We observe that  $\mathcal{H}$ -HW Index of some standard graphs that are HM graphs are polynomials in  $h$  ( $h \leq 3$ ) with degree  $\leq 3$ .

Now we discuss for some Special graphs that are HM graphs.

### Comparative Study on $\mathcal{H}$ -HW Index on HM graphs :

$\mathcal{H}$ -HW Index of standard graphs and Special graphs that are HM graphs are polynomials in  $h$  ( $h \leq 3$ ) of degree  $\leq 3$ . In Standard graphs we calculate for  $h$  number of vertices. It is found that in every graphs we obtain polynomials in  $h$  ( $h \leq 3$ ) of degree  $\leq 3$ . If the total number of vertices is known or if it is not known, we can calculate the HW Index and it will be are polynomials in  $h$  ( $h \leq 3$ ) of degree  $\leq 3$ , since HM graphs are regular graphs with  $r < 4$ . In the same manner, we can calculate the Chemical Bonding and Valencies of Organic Compounds very easily. Each vertex of a graph represents an element or molecule. Each bond connecting two elements or molecule is represented as straight line in the graph.

### Future Scope:

Graph Theory has a wide scope in Applied Mathematics than other subjects.  $\mathcal{H}$ -HW Index of HM Graphs has a broad scope in various areas such as Chemical Graph Theory in evaluating the Chemical Bonding and Valencies of various compounds. It has also been used for enhancing the lattice hardware security and also for the representation of various computer networks. It has a wide scope in limiting the structure of a particle in electronic structures. Evaluation of  $\mathcal{H}$ -HW Index of HM graphs is applicable in the electric engineering to find the false electric flow of current. There is also a scope for evaluating the Fuzzy  $\mathcal{H}$ -HW Index of HM Graphs.

### Conclusion:

The attributes and benefits of the  $\mathcal{H}$ -HW Index have received considerable attention recently in Chemical graph theory and in applied mathematics. We can calculate the Chemical Bonding of various Organic Compounds and also evaluate the Valencies of each Compound in Organic Chemistry very easily. The study of  $\mathcal{H}$ -HW Index is significant due to its varied functions. All graphs are not HM graphs. It is very appealing to explore the  $\mathcal{H}$ -HW Index of graphs that reveals HM Labeling. We have explored the  $\mathcal{H}$ -HW Index of Path, Comb and Cycle graph. By means of sufficient illustrations, the derived results are demonstrated which provides better understanding. We have generalized the proofs through deductive method. We have attained polynomials in  $h$  ( $h \leq 3$ ) with degree  $\leq 3$  for every those standard graphs that are HM graphs.

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