

## COMPUTATION OF HOSAYA POLYNOMIAL, WIENER AND HYPER WIENER INDEX OF JAHANGIR GRAPH $J_{6,m}$

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ABSTRACT. Let  $G = (V, E)$  be a simple connected graph with vertex set  $V$  and edge set  $E$ . For two vertices  $u$  and  $v$  in a graph  $G$ , the distance  $d(u, v)$  is the shortest path between  $u$  and  $v$  in  $G$ . Graph theory has much advancements in the field of theoretical chemistry. Recently, chemical graph theory is becoming very popular among researchers because of its wide applications of mathematics in chemistry. One of the important distance based topological index is the Wiener index, defined as the sum of distances between all pairs of vertices of  $G$ , defined as  $W(G) = \sum_{u,v \in V(G)} d(u, v)$ . The Hosaya polynomial is defined as  $H(G, x) = \sum_{u,v \in V(G)} x^{d(u,v)}$ . The hyper Wiener index is defined as  $WW(G) = \sum_{u,v \in V(G)} d(u, v) + \frac{1}{2} \sum_{u,v \in V(G)} d^2(u, v)$ . In this paper, we study and compute Hosaya polynomial, Wiener index and hyper Wiener index for Jahangir graph  $J_{6,m}$ ,  $m \geq 3$ . Furthermore, we give exact values of these topological indices..

*Key words* : Topological descriptors, Distance, Hosaya polynomial, Wiener index, Hyper Wiener index, Jahangir graph  $J_{6,m}$ .

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### 1. INTRODUCTION

Let a graph  $G = (V, E)$  be a simple connected graph with vertex set  $V$  and edge set  $E$ . A topological index is a numerical value which indicates some

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important information about the molecular graph. It is helpful in the study of *QSAR/QSPR* and also to correlate with physio-chemical properties and bioactivities of molecular graphs. Topological indices are classified as degree based, distance based, eccentric based and counting related indices etc. There is a remarkable advancements in the field of chemical graph theory.

Chemical graph theory is a branch of mathematical chemistry in which we apply tools of graph theory to model the chemical phenomenon mathematically. This theory contributes a prominent role in the fields of chemical sciences. The topological properties of molecular graphs and certain networks are studied by many researchers, see [9, 10, 11, 20, 21, 22, 27].

For a graph  $G$  with  $u$  and  $v$  be the vertices of  $G$ , the distance  $d(u, v)$  is the length of the shortest path between  $u$  and  $v$ . The concept of topological index came from the work done by Wiener in 1947 while he was working in boiling point of paraffin [34]. The Wiener index for a graph  $G$  is defined as:

$$W(G) = \frac{1}{2} \sum_{u,v \in V(G)} d(u, v) \quad (1)$$

The Hosoya polynomial is introduced in 1988 by Hosoya [28]. It is defined for a connected graph  $G$  as:

$$H(G, x) = \sum_{u,v \in V(G)} x^{d(u,v)} \quad (2)$$

The hyper Wiener index of acyclic graphs was introduced by Randić in 1993. Then, Klein et al. [29] generalized Randić's definition for all connected graphs, as a generalization of the Wiener index. The hyper Wiener index is defined as:

$$WW(G) = W(G) + \frac{1}{2} \sum_{u,v \in V(G)} d^2(u, v) \quad (3)$$

Where  $d^2(u, v) = (d(u, v))^2$ . Many chemical applications of Hosoya polynomial and Wiener index are given in detail [19, 25, 32]. In 1994, [36], Yeh and Gutman et al. computed the Wiener index of graph operations including product, join, composition, corona and cluster. Later on, Stevanović [33] generalized their results and computed Hosoya polynomial of product, join and composition of graphs. Recently, Eliasi et al. in [18] introduced four new sum of graphs called F-sums and computed the Wiener index. The Hosoya polynomial and Wiener index of some nanotorus and nanotubes and some molecular graphs are computed by many researchers. For more details, see [1, 12, 16, 17, 23, 24, 25, 26, 31, 35]. The mathematical properties and applications of hyper Wiener index in chemistry is discussed in [13, 14, 15, 30, 37]. The

Hosoya polynomial is useful for the calculation of Wiener index. The first derivative of the Hosoya polynomial at  $x = 1$  gives the Wiener index.

$$W(G) = \left. \frac{\partial H(G, x)}{\partial x} \right|_{x=1} \quad (4)$$

The topological diameter  $D(G)$  is the longest topological distance in a graph  $G$ .

$$D(G) = \max_{u, v \in V(G)} \{d(u, v) \mid \forall u, v \in V(G)\}$$

The hyper Wiener index can be calculated by using Hosoya polynomial [11]. It is defined as

$$WW(G) = H'(G, x)|_{x=1} + \frac{1}{2}H''(G, x)|_{x=1} \quad (5)$$

Where  $H'(G, x)$  and  $H''(G, x)$  are the first and second derivatives of Hosoya polynomial respectively.

The Jahangir graph  $J_{n,m}$ , where  $n \geq 2$ ,  $m \geq 3$  is defined below.

**Definition 1.** [1] Jahangir graph  $J_{n,m}$  is a graph on  $nm+1$  vertices i.e., a graph consisting of a cycle  $C_{nm}$  with one additional vertex which is adjacent to  $m$  vertices of  $C_{nm}$  at distance  $n$  to each other on  $C_{nm}$ .

The Jahangir graph  $J_{6,3}$ ,  $J_{6,4}$  and  $J_{6,m}$  are depicted in Fig. 1. For more information about the *Jahangir graph*, readers can see [2, 3, 4, 5, 6, 7, 8]

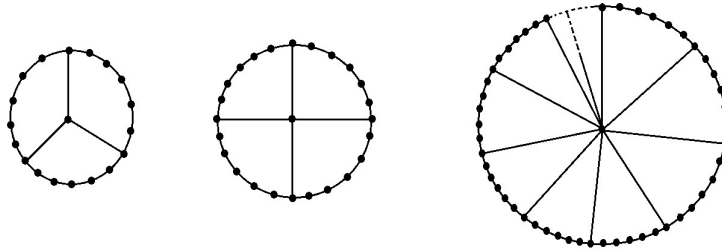


FIGURE 1. Jahangir graphs  $J_{6,3}$ ,  $J_{6,4}$  and  $J_{6,m}$

## 2. MAIN RESULTS

The aim of this section is to study the Jahangir graph  $J_{6,m}$  for  $m \geq 3$  and to compute exact values for Hosoya polynomial, Wiener index and hyper Wiener index of  $J_{6,m}$ . We, first of all, compute the Hosoya polynomial by finding distances of all pair of vertices of  $J_{6,m}$ . Then, as a result we use (4) to obtain the formula for Wiener index of  $J_{6,m}$ . Then, finally we compute hyper Wiener index by using (5). Here, we denote the number of unordered pairs of vertices  $u$  and  $v$  in a graph  $G$  at distance  $d(u, v) = k$  by  $d(G, k)$  for every number  $k$

up to  $D(G)$  (the topological diameter of  $G$ ). Thus, we redefine the Equations (1) and (2) as below:

$$W(G) = \sum_{k=1}^{D(G)} d(G, k)k \tag{6}$$

$$H(G, x) = \sum_{k=1}^{D(G)} d(G, k)x^k \tag{7}$$

In the following example, we compute Hosoya polynomial, Wiener index and hyper Wiener index for  $J_{6,3}$ .

**Example 1.** *The Hosoya polynomial, Wiener index and hyper Wiener index of Jahangir graph  $J_{6,3}$  is computed as below:*

$$H(G, x) = \sum_{k=1}^7 d(G, k)x^k$$

$$H(G, x) = d(G, 1)x + d(G, 2)x^2 + d(G, 3)x^3 + d(G, 4)x^4 + d(G, 5)x^5 + d(G, 6)x^6 + d(G, 7)x^7 + d(G, 8)x^8$$

The graph of  $J_{6,3}$  is depicted in Fig. 1. The topological diameter of  $J_{6,3}$  is seven. By using the definition of Jahangir graph and Hosoya polynomial, we compute distance  $d(G, k)$  for  $1 \leq k \leq 7$ . The Table 1 shows the distances  $d(G, k)$  for  $1 \leq k \leq 7$  and their frequency is mentioned. Using Table 1 in (7)

$d(G, k)$	frequency	$d(G, k)$	frequency
$d(G, 1)$	21	$d(G, 5)$	27
$d(G, 2)$	27	$d(G, 6)$	18
$d(G, 3)$	36	$d(G, 7)$	6
$d(G, 4)$	36		

TABLE 1. Distance  $d(G, k)$  for  $1 \leq k \leq D(G) = 7$  of each pair of vertices of  $J_{6,3}$ .

to compute Hosoya polynomial.

$$H(J_{6,3}, x) = d(J_{6,3}, 1)x + d(J_{6,3}, 2)x^2 + d(J_{6,3}, 3)x^3 + d(J_{6,3}, 4)x^4 + d(J_{6,3}, 5)x^5 + d(J_{6,3}, 6)x^6 + d(J_{6,3}, 7)x^7$$

$$H(J_{6,3}, x) = 21x + 27x^2 + 36x^3 + 36x^4 + 27x^5 + 18x^6 + 6x^7$$

The Wiener index of  $J_{6,3}$  can easily be calculated by taking the first derivative of  $H(J_{6,3}, x)$  at  $x = 1$ .

$$W(J_{6,3}) = 21 + 2(27)x|_{x=1} + 3(36)x^2|_{x=1} + 4(36)x^3|_{x=1} + 5(27)x^4|_{x=1} + 6(18)x^5|_{x=1} + 7(6)x^6|_{x=1}$$

$$W(J_{6,3}) = 612. \quad (8)$$

The hyper Wiener index of  $J_{6,3}$  can be calculated by using (5). Since  $W(J_{6,3}) = H'(J_{6,3}, x)|_{x=1}$ , we need to compute  $H''(J_{6,3}, x)$  at  $x = 1$ .

$$H''(J_{6,3}, x) = \frac{\partial H'(J_{6,3}, x)}{\partial x}$$

$$= 54 + 216x + 432x^2 + 540x^3 + 540x^4 + 252x^5$$

$$H''(J_{6,3}, x)|_{x=1} = 2034. \quad (9)$$

Now, for the computation of hyper Wiener index, we will use (8) and (9) in (5).

$$WW(G) = 612 + \frac{2034}{2}$$

$$WW(G) = 1629.$$

In the next example we will find the Hosoya polynomial, Wiener index and hyper Wiener index of  $J_{6,4}$ .

**Example 2.** The Hosoya polynomial, Wiener index and hyper Wiener index of Jahangir graph  $J_{6,4}$  is computed as below:

$$H(G, x) = \sum_{k=1}^8 d(G, k)x^k$$

$$H(G, x) = d(G, 1)x + d(G, 2)x^2 + d(G, 3)x^3 + d(G, 4)x^4 + d(G, 5)x^5 + d(G, 6)x^6 + d(G, 7)x^7 + d(G, 8)x^8$$

The graph of  $J_{6,4}$  is depicted in Fig. 1. The calculation is easy and simple. The topological diameter of  $J_{6,4}$  is eight. By using the definition of Jahangir graph and Hosoya polynomial, we compute distance  $d(G, k)$  for  $1 \leq k \leq 8$ . The Table 2 shows the distances  $d(G, k)$  for  $1 \leq k \leq 8$  and their frequency is mentioned. Using Table 2 in (7) to compute Hosoya polynomial.

$$H(J_{6,4}, x) = d(J_{6,4}, 1)x + d(J_{6,4}, 2)x^2 + d(J_{6,4}, 3)x^3 + d(J_{6,4}, 4)x^4 + d(J_{6,4}, 5)x^5 + d(J_{6,4}, 6)x^6 + d(J_{6,4}, 7)x^7 + d(J_{6,4}, 8)x^8$$

$$H(J_{6,4}, x) = 28x + 38x^2 + 56x^3 + 64x^4 + 56x^5 + 40x^6 + 16x^7 + 2x^8$$

$d(G, k)$	frequency	$d(G, k)$	frequency
$d(G, 1)$	28	$d(G, 5)$	56
$d(G, 2)$	38	$d(G, 6)$	40
$d(G, 3)$	56	$d(G, 7)$	16
$d(G, 4)$	64	$d(G, 8)$	2

TABLE 2. Distance  $d(G, k)$  for  $1 \leq k \leq D(G) = 8$  of each pair of vertices of  $J_{6,4}$ .

The Wiener index of  $J_{6,4}$  can easily be calculated by taking the first derivative of  $H(J_{6,4}, x)$  at  $x = 1$ .

$$W(J_{6,4}) = 28 + 2(38)x|_{x=1} + 3(56)x^2|_{x=1} + 4(64)x^3|_{x=1} + 5(56)x^4|_{x=1} + 6(40)x^5|_{x=1} + 7(16)x^6|_{x=1} + 8(2)x^7|_{x=1}$$

$$W(J_{6,4}) = 1176. \tag{10}$$

The hyper Wiener index of  $J_{6,4}$  can be calculated by using (5). Since  $W(J_{6,4}) = H'(J_{6,4}, x)|_{x=1}$ , we need to compute  $H''(J_{6,4}, x)$  at  $x = 1$ .

$$H''(J_{6,4}, x) = \frac{\partial H'(J_{6,4}, x)}{\partial x}$$

$$= 76 + 336x + 768x^2 + 1120x^3 + 1200x^4 + 672x^5 + 112x^6$$

$$H''(J_{6,4}, x)|_{x=1} = 4284. \tag{11}$$

Now, for the computation of hyper Wiener index of  $J_{6,4}$ , we will use (10) and (11) in (5).

$$WW(G) = 1176 + \frac{4284}{2}$$

$$WW(G) = 3318.$$

Our aim is to compute a close result of Hosoya polynomial, Wiener index and hyper Wiener index for Jahangir graph  $J_{6,m}$ , where  $m \geq 3$ . In the following theorem, we provide an exact result of Hosoya polynomial for  $H(J_{6,m}, x)$ .

**Theorem 1.** Consider the graph  $G \cong J_{6,m}$  for all integers  $m \geq 3$ , then its Hosoya polynomial is equal to

$$H(G, x) = 7mx + \left(\frac{m^2 + 15m}{2}\right)x^2 + (2m^2 + 6m)x^3 + 4m^2x^4 + (5m^2 - 6m)x^5 + (4m^2 - 6m)x^6 + (2m^2 - 4m)x^7 + \left(\frac{m^2 - 3m}{2}\right)x^8$$

$$\tag{12}$$

*Proof.* Let  $J_{6,m}$  be Jahangir graph with  $m \geq 3$ . The cardinality of vertices and edges of  $J_{6,m}$  are  $6m + 1$  and  $7m$ , respectively. We observe that the structure

$d(G, k)$	frequency	$d(G, k)$	frequency
$d(G, 1)$	$ E(J_{6,m}) $	$d(G, 5)$	$5m^2 - 6m$
$d(G, 2)$	$\frac{m^2+15m}{2}$	$d(G, 6)$	$4m^2 - 6m$
$d(G, 3)$	$2m^2 + 6m$	$d(G, 7)$	$2m^2 - 4m$
$d(G, 4)$	$4m^2$	$d(G, 8)$	$\frac{m^2-3m}{2}$

TABLE 3. Distance  $d(G, k)$  for  $1 \leq k \leq D(G) = 8$  of each pair of vertices of  $J_{6,m}$ .

of  $J_{6,m}$  that the topological diameter in  $J_{6,m}$  is eight. Thus  $D(J_{6,m}) = 8$  for  $m \geq 4$  and  $D(J_{6,m}) = 7$  for  $m = 3$ . In order to proof Hosoya polynomial of Jahangir graph, we will use Table 3 in (7). The computation of Hosoya polynomial is as follows:

$$H(G, x) = \sum_{k=1}^{D(G)} d(G, k)x^k$$

$$H(G, x) = d(G, 1)x + d(G, 2)x^2 + d(G, 3)x^3 + d(G, 4)x^4 + d(G, 5)x^5 + d(G, 6)x^6 + d(G, 7)x^7 + d(G, 8)x^8$$

After using Table 3, we get

$$H(G, x) = 7mx + \left(\frac{m^2+15m}{2}\right)x^2 + (2m^2 + 6m)x^3 + 4m^2x^4 + (5m^2 - 6m)x^5 + (4m^2 - 6m)x^6 + (2m^2 - 4m)x^7 + \left(\frac{m^2-3m}{2}\right)x^8. \quad \square$$

In the following theorem, we compute the formula of Wiener index for  $J_{6,m}$ .

**Theorem 2.** Consider the graph  $G \cong J_{6,m}$  for every integer  $m \geq 3$ , then its Wiener index is equal to

$$W(G) = 90m^2 - 66m. \quad (13)$$

*Proof.* Consider the Jahangir graph  $J_{6,m}$  where  $m \geq 3$ . By using the definition of Wiener index, Hosoya polynomial and (4), we can easily compute the Wiener index of  $J_{6,m}$  as follows:

$$W(G) = \left. \frac{\partial H(G, x)}{\partial x} \right|_{x=1}$$

$$\begin{aligned}
 &= 7m + \left(\frac{m^2+15m}{2}\right) \frac{\partial x^2}{\partial x} \Big|_{x=1} + (2m^2 + 6m) \frac{\partial x^3}{\partial x} \Big|_{x=1} + (4m^2) \frac{\partial x^4}{\partial x} \Big|_{x=1} + (5m^2 - \\
 &6m) \frac{\partial x^5}{\partial x} \Big|_{x=1} + (4m^2 - 6m) \frac{\partial x^6}{\partial x} \Big|_{x=1} + (2m^2 - 4m) \frac{\partial x^7}{\partial x} \Big|_{x=1} + \left(\frac{m^2-3m}{2}\right) \frac{\partial x^8}{\partial x} \Big|_{x=1} \\
 &= 7m + \left(\frac{m^2+15m}{2}\right) (2x) \Big|_{x=1} + (2m^2 + 6m) (3x^2) \Big|_{x=1} + 4m^2 (4x^3) \Big|_{x=1} + (5m^2 - \\
 &6m) (5x^4) \Big|_{x=1} + (4m^2 - 6m) (6x^5) \Big|_{x=1} + (2m^2 - 4m) (7x^6) \Big|_{x=1} + \left(\frac{m^2-3m}{2}\right) (8x^7) \Big|_{x=1}
 \end{aligned}$$

After an easy simplification, we get

$$W(G) = 90m^2 - 66m. \quad \square \quad \square$$

The hyper Wiener index  $WW(G)$  can be calculated by using (3). There is an alternative and easy way to compute hyper Wiener index from Hosoya polynomial as mentioned above in (5). In the next theorem, we provide the formula of hyper Wiener index for  $J_{6,m}$ .

**Theorem 3.** Consider the graph  $G \cong J_{6,m}$  for all integers  $m \geq 3$ , then its hyper Wiener index is equal to

$$WW(G) = \frac{1}{2}(573m^2 - 633m). \quad (14)$$

*Proof.* Consider the Jahangir graph  $J_{6,m}$  where  $m \geq 3$ . By using the definition of Wiener index, hyper Wiener index, hosoya polynomial and (5), we can easily compute the hyper Wiener index of  $J_{6,m}$  as follows:

Since it is proved in Theorem 2.2., that Wiener index is equal to  $W(G) = 90m^2 - 66m$ . We compute  $H''(G, x)$  at  $x = 1$ , where  $G \cong J_{6,m}$ . The computation is given below:

$$\begin{aligned}
 H''(G, x) &= \frac{\partial H'(G, x)}{\partial x} \\
 &= \frac{\partial(m^2+15m)x}{\partial x} + \frac{\partial 3(2m^2+6m)x^2}{\partial x} + \frac{\partial 16m^2x^3}{\partial x} + \frac{\partial 5(5m^2-6m)x^4}{\partial x} + \frac{\partial 6(4m^2-6m)x^5}{\partial x} + \frac{\partial 7(2m^2-4m)x^6}{\partial x} + \\
 &\frac{\partial 7m}{\partial x} + \frac{\partial 4(m^2-3m)x^7}{\partial x} \\
 &= (m^2 + 15m) + 6(2m^2 + 6m)x + 48m^2x^2 + 20(5m^2 - 6m)x^3 + 30(4m^2 - \\
 &6m)x^4 + 42(2m^2 - 4m)x^5 + 28(m^2 - 3m)x^6
 \end{aligned}$$

At  $x = 1$  and after an easy simplification, we get

$$H''(G, x) \Big|_{x=1} = 393m^2 - 501m. \quad (15)$$

The hyper Wiener index for  $J_{6,m}$  is obtained by using (13) and (15) in (5).

$$WW(G) = H'(G, x) \Big|_{x=1} + \frac{1}{2}H''(G, x) \Big|_{x=1}$$



$$\begin{aligned}
&= (90m^2 - 66m) + \frac{1}{2}(393m^2 - 501m) \\
&= \frac{1}{2}(573m^2 - 633m). \quad \square
\end{aligned}$$

### 3. CONCLUSION

Graph theory is a useful area of mathematics that has wide range of applications in many areas of science such as chemistry, computer science, biology, electrical engineering and medicines etc. Graph theory has made it possible to study complex structures and networks by transforming it into molecular graph.

In this paper, we have studied Jahangir graph and computed exact values of Hosoya polynomial, Wiener index and hyper Wiener index for the Jahangir graph  $J_{6,m}$ , where  $m \geq 3$ . In future, we will explore some new graphs (or molecular graphs) of our interest and compute Hosoya polynomial and Wiener index to better understand their underlying topologies.

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