

Hosoya Polynomial and Topological Indices of the Jahangir Graph $J_{7,m}$

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Abstract

The Hosoya polynomial of a graph was introduced by H. Hosoya in 1988, and the most interesting application of the Hosoya polynomial is that almost all distance-based graph invariants, which are used to predict physical, chemical and pharmacological properties of organic molecules, can be recovered from the Hosoya polynomial. In this article we not only give the general form of the Hosoya polynomial of the Jahangir graph $J_{7,m}$, $m \geq 3$, but also give the general forms of the topological indices, Wiener, hyper Wiener, Harary, and Tratch Stankevitch-Zefirov.

Keywords: Jahangir graph; Hosoya polynomial; Topological indices

Introduction

The Hosoya polynomial of a graph was introduced by H. Hosoya in 1988 as a counting polynomial; it actually counts the number of distances of paths of different lengths in a molecular graph [1].

Hosoya polynomial is very well studied. In 1993, Gutman introduced Hosoya polynomial for a vertex of a graph [2]; these polynomials are correlated. The most interesting application of the Hosoya polynomial is that almost all distance-based graph invariants, which are used to predict physical, chemical and pharmacological properties of organic molecules, can be recovered from the Hosoya polynomial [3-6].

Several people have computed the Hosoya polynomial and related indices of different classes of graphs. In 2002 Diudea computed the Hosoya polynomial of several classes of toroidal nets and recover their Wiener numbers [7-10]. In 2011 Ali gave the Hosoya polynomial of concatenated pentagonal rings [11]. In 2012 Kishori gave a recursive method for calculating the Hosoya polynomial of Hanoi graphs, and computed their sum distance-based invariants [12]. In 2013 Farahi computed the Hosoya polynomial of polycyclic aromatic hydrocarbons [13].

There are some useful topological indices which are related to Hosoya polynomial, and we are interested in Wiener, hyper Wiener, Tratch-StankevitchZefirov, and Harary indices as these can be recovered from it. The Wiener index was introduced by Harry Wiener in 1947 and was used to correlate with boiling points of alkanes [14]. Later it was observed that the Wiener index can be used to determine a number of physico-chemical properties of alkanes as heats of formation, heats of vaporization, molar volumes, and molar refractions [15]. Moreover, it can be used to correlate those physico-chemical properties which depend on the volume-surface ratio of molecules and to Gas chromatographic retention data for series of structurally related molecules. Another topological index whose mathematical properties are relatively well investigated is the hyper-Wiener index was introduced by Randic in 1993 [16]. It is also used to predict physico-chemical properties of organic compounds, particularly to pharmacology, agriculture, and environment protection [4]; for more details, see also [17-19]. In 1993 Plavsic et al. introduced a new topological index, known as Harary index, to characterize chemical graphs [15]. Tratch, Stankevitch and Zefirov introduced Tratch-Stankevitch-Zefirov index as expanded Wiener index in 1990 [18].

This article is concerned with the study of the Hosoya polynomial and its related topological indices of one class of the general Jahangir graph $J_{n,m}$.

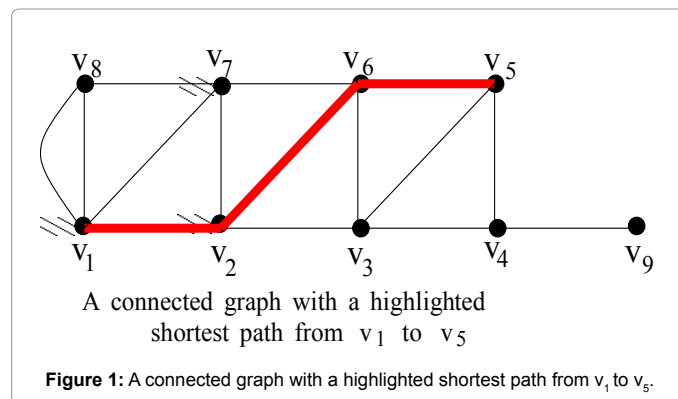
Basic Definitions

A graph G is a pair $(V(G), E(G))$, where V is the set of vertices and E is the set of edges. A path from a vertex v to a vertex w is a sequence of vertices and edges that starts from v and stops at w . The number of edges in a path is the length of that path. A graph is said to be connected if there is a path between any two of its vertices. The distance $d(u, v)$ between two vertices u, v of a connected graph G is the length of a shortest path between them. The diameter of G , denoted by $d(G)$, is the longest distance in G (Figure 1).

A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory. Specifically, molecular graph is a simple graph whose vertices correspond to atoms of the compound and whose edges correspond to chemical bonds; however, hydrogen atoms are often omitted. (In the present article all the graphs are molecular.)

Definition (1.1)

The Hosoya polynomial in variable x of a molecular graph $G=(V, E)$ is defined as



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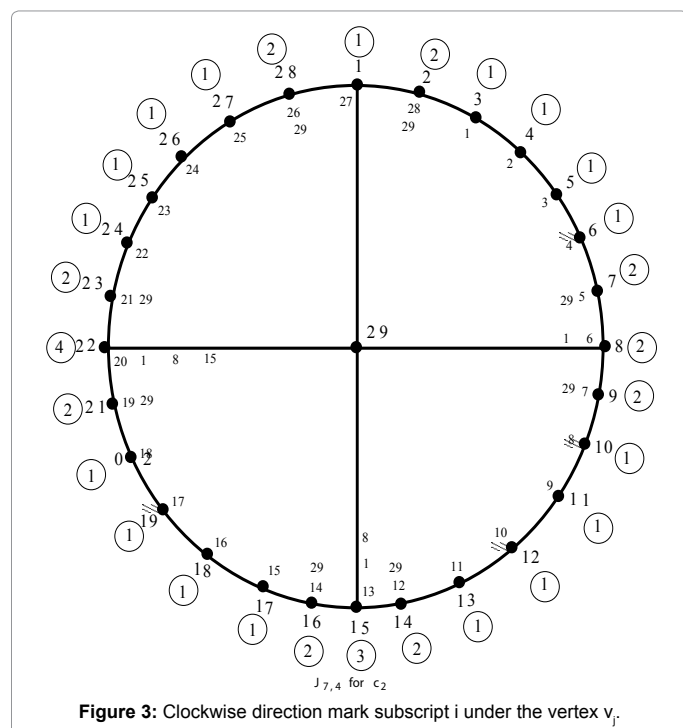


Figure 3: Clockwise direction mark subscript i under the vertex v_i .

$$\begin{aligned}
 c_2 &= \text{total number of vertices that lie at distance 2 from each other} \\
 &= \text{distances of vertices of } B_1 + \text{distances of vertices of } B_2 \\
 &+ \text{distances of vertices of } B_3 + \text{distances of vertices of } B_4 \\
 &= (1 + 2 + 3 + \dots + m) + (|B_2| \times 2) + (|B_3| \times 1) + (|B_4| \times 1) \\
 &= \frac{m(m+1)}{2} + (2m \times 2) + (2m \times 1) + (2m \times 1) \\
 &= \frac{m^2 + 17m}{2}
 \end{aligned}$$

3. c_3 is computed in four steps:

Step 1: Moving in clockwise direction mark subscript i of a vertex v_i under the vertex v_j lying at distance 3 from it; to handle the situation we mark such subscripts inside the main circle.

Step 2: Mark the subscript $7m+1$ of the central vertex v_{7m+1} under the vertices that lie at distance 3 from it.

Step 3: Now consider the m number of 3-degree vertices v_{7i-6} , $1 \leq i \leq m$. Starting from v_1 mark the subscript of v_1 under the vertices that lie at distance 3 from it via the central vertex v_{7m+1} .

Step 4: Now count the number of subscripts marked under each vertex and write that counted number over each vertex, outside the main circle; you can see in the figure where such numbers are encircled.

In order to count the total distances let B_1, B_2, B_3 , and B_4 be the sets that contain the vertices lying respectively at distances 1, 2, 3, and 4 from the central vertex. Observe that $|B_1|=m, |B_2|=2m, |B_3|=2m$, and $|B_4|=2m$.

$$\begin{aligned}
 c_3 &= \text{total number of vertices that lie at distance 3 from each other} \\
 &= \text{distances of vertices of } B_1 + \text{distances of vertices of } B_2 \\
 &+ \text{distances of vertices of } B_3 + \text{distances of vertices of } B_4 \\
 &= (|B_1| \times 1) + (|B_2| \times m) + (|B_3| \times 2) + (|B_4| \times 1) \\
 &= m + (2m \times m) + (2m \times 2) + (2m \times 1)
 \end{aligned}$$

$$= m(2m+7)$$

4. c_4 is computed in four steps:

Step 1: Moving in clockwise direction mark subscript i of a vertex v_i under the vertex v_j lying at distance 4 from it; to handle the situation we mark such subscripts inside the main circle.

Step 2: Mark the subscript $7m+1$ of the central vertex v_{7m+1} under the vertices that lie at distance 3 from it.

Step 3: Now consider the m number of 3-degree vertices v_{7i-6} , $1 \leq i \leq m$. Starting from v_1 mark the subscript of v_1 under the vertices that lie at distance 3 from it via the central vertex v_{7m+1} .

Step 4: Now count the number of subscripts marked under each vertex and write that counted number over each vertex, outside the main circle; you can see in the figure where such numbers are encircled.

In order to count the total distances let B_1, B_2, B_3 , and B_4 be the sets that contain the vertices lying respectively at distances 1, 2, 3, and 4 from the central vertex. Observe that $|B_1|=m, |B_2|=2m, |B_3|=2m$, and $|B_4|=2m$.

$$\begin{aligned}
 c_4 &= \text{total number of vertices that lie at distance 3 from each other} \\
 &= \text{distances of vertices of } B_1 + \text{distances of vertices of } B_2 \\
 &+ \text{distances of vertices of } B_3 + \text{distances of vertices of } B_4 \\
 &= (|B_1| \times 1) + (|B_2| \times m) + (|B_3| \times m) + (|B_4| \times 2) \\
 &= m + (2m \times m) + (2m \times m) + (2m \times 2) \\
 &= m(4m+5).
 \end{aligned}$$

5. c_5 is computed in five steps:

Step 1: Moving in clockwise direction mark subscript i of a vertex v_i under the vertex v_j lying at distance 5 from it; to handle the situation we mark such subscripts inside the main circle.

Step 2: Mark the subscript $7m+1$ of the central vertex v_{7m+1} under the vertices that lie at distance 5 from it.

Step 3: Now consider the m number of 3-degree vertices v_{7i-6} , $1 \leq i \leq m$. Starting from v_1 mark the subscript of v_1 under the vertices that lie at distance 5 from it via the central vertex v_{7m+1} .

Step 4: Now consider $2m$ number of 2-degree vertices which are adjacent to 3-degree vertices on the circle. Starting from v_2 mark its subscript under the vertices that lie at distance 5 from it via the central vertex and repetition not included.

Step 5: Now count the number of subscripts marked under each vertex and writes that counted number over each vertex, outside the main circle; you can see in the figure where such numbers are encircled.

In order to count the total distances let B_1, B_2, B_3 , and B_4 be the sets that contain the vertices lying respectively at distances 1, 2, 3, and 4 from the central vertex. Observe that $|B_1|=m, |B_2|=2m, |B_3|=2m$, and $|B_4|=2m$.

$$\begin{aligned}
 c_5 &= \text{total number of vertices that lie at distance 3 from each other} \\
 &= \text{distances of vertices of } B_1 + \text{distances of vertices of } B_2 \\
 &+ \text{distances of vertices of } B_3 + \text{distances of vertices of } B_4 \\
 &= (|B_1| \times 0) + (|B_2| - m) + m((2m - 3) + (2m - 2)) + (|B_4| \times (m - 1)) \\
 &= (|B_1| \times 0) + (|B_2| - m) + m((|B_3| - 3) + (|B_3| - 2)) + (|B_4| \times (m - 1)) \\
 &= 0 + (2m - m) + ((4m - 5) \times m) + (2m \times (m - 1)) \\
 &= 6m(m - 1)
 \end{aligned}$$

6. c_6 is computed in six steps:

Step 1: Moving in clockwise direction mark subscript i of a vertex v_i under the vertex v_j lying at distance 6 from it; to handle the situation we mark such subscripts inside the main circle.

Step 2: Now consider the m number of 3-degree vertices $v_{7i-6}, 1 \leq i \leq m$. Starting from v_1 mark the subscript of v_1 under the vertices that lie at distance 6 from it via the central vertex v_{7m+1} .

Step 3: Now consider $2m$ number of 2-degree vertices which are adjacent to 3-degree vertices on the circle. Starting from v_2 mark its subscript under the vertices that lie at distance 6 from it via the central vertex and repetition not included.

Step 4: Now consider $2m$ number of 2-degree vertices of the set B_2 on the circle. Starting from v_3 mark its subscript under the vertices that lie at distance 6 from it via the central vertex and repetition not included.

Step 5: Now count the number of subscripts marked under each vertex and writes that counted number over each vertex, outside the main circle; you can see in the figure where such numbers are encircled.

In order to count the total distances let B_1, B_2, B_3 , and B_4 be the sets that contain the vertices lying respectively at distances 1, 2, 3, and 4 from the central vertex. Observe that $|B_1|=m, |B_2|=2m, |B_3|=2m$, and $|B_4|=2m$.

$$\begin{aligned} c_6 &= \text{total number of vertices that lie at distance 6 from each other} \\ &= \text{distances of vertices of } B_{1+} \text{ distances of vertices of } B_2 \\ &+ \text{distances of vertices of } B_{3+} \text{ distances of vertices of } B_4 \\ &= (|B_1| \times 0) + (|B_2| \times 0) + [2(1+3+\dots+(m-1)) + 2(n-1)] + (|B_4| \times (2m-3)) \\ &= 0+0+((m-1)^2+(m-1) \times 2) + (2m \times (2m-3)) \\ &= 2m(3m-4). \end{aligned}$$

7. c_7 is computed in five steps:

Step 1: Moving in clockwise direction mark subscript i of a vertex v_i under the vertex v_j lying at distance 7 from it; to handle the situation we mark such subscripts inside the main circle.

Step 2: Now consider $2m$ number of 2-degree vertices of the set B_2 on the circle. Starting from v_3 mark its subscript under the vertices that lie at distance 7 from it via the central vertex and repetition not included.

Step 3: Now count the number of subscripts marked under each vertex and write that counted number over each vertex, outside the main circle; you can see in the figure where such numbers are encircled.

In order to count the total distances let B_1, B_2, B_3 , and B_4 be the sets that contain the vertices lying respectively at distances 1, 2, 3, and 4 from the central vertex. Observe that $|B_1|=m, |B_2|=2m, |B_3|=2m$, and $|B_4|=2m$.

$$\begin{aligned} c_7 &= \text{total number of vertices that lie at distance 3 from each other} \\ &= \text{distances of vertices of } B_{1+} \text{ distances of vertices of } B_2 \\ &+ \text{distances of vertices of } B_{3+} \text{ distances of vertices of } B_4 \\ &= (|B_1| \times 0) + (|B_2| \times 0) + (|B_3| \times 0) + (|B_4| \times (2m-3)) \\ &= 0+0+0+(2m \times (2m-3)) \\ &= 2m(2m-3). \end{aligned}$$

8. c_8 is computed in six steps:

Step 1: Moving in clockwise direction mark subscript i of a vertex v_i under the vertex v_j lying at distance 8 from it; to handle the situation we mark such subscripts inside the main circle.

Step 2: Now count the number of subscripts marked under each vertex and write that counted number over each vertex, outside the main circle; you can see in the figure where such numbers are encircled.

In order to count the total distances let B_1, B_2, B_3 , and B_4 be the sets that contain the vertices lying respectively at distances 1, 2, 3, and 4 from the central vertex. Observe that $|B_1|=m, |B_2|=2m, |B_3|=2m$, and $|B_4|=2m$.

$$\begin{aligned} c_8 &= \text{total number of vertices that lie at distance 6 from each other} \\ &= \text{distances of vertices of } B_{1+} \text{ distances of vertices of } B_2 \\ &+ \text{distances of vertices of } B_{3+} \text{ distances of vertices of } B_4 \\ &= (|B_1| \times 0) + (|B_2| \times 0) + (|B_3| \times 0) + ((2m-5) \times m) \\ &= 0+0+((m-1)^2+0) + ((2m-5) \times m) \\ &= m(2m-5). \end{aligned}$$

The topological indices, Wiener, hyper Wiener, Harary, and Tratch-StankevitchZefirovof (TSZ), of $J_{7,m}$ are given in the result

Proposition

The Wiener, hyper Wiener, Harary, and TSZ indices of $J_{7,m}$ are:

1. $W(J_{7,m}) = 87m^2 - 14m - 21$
2. $WW(J_{7,m}) = \frac{1}{2} [683m^2 - 513m - 168]$
3. $Ha(J_{7,m}) = \frac{131}{30}m^2 + \frac{3629}{280}m - \frac{3}{7}$
4. $TSZ(J_{7,m}) = \frac{2614}{3}m^2 - \frac{2584}{3}m - 252$

This completes the proof.

Proof: We prove these relations one by one using the above theorem and the relations given in Introduction section:

$$\begin{aligned} W(J_{7,m}) &= \frac{d}{dx} [H(J_{7,m})]_{x=1} \\ &= \frac{d}{dx} \left[8mx + \frac{m}{2} (m+17)x^2 + m(2m+7)x^3 + m(4m+5)x^4 + 6m(m-1)x^5 + 2m(3m-4)x^6 + (2m-3)x^7 + m(2m-5)x^8 \right]_{x=1} \\ &= [8m + m(m+17)x + 3m(2m+7)x^2 + 4m(4m+5)x^3 + 30m(m-1)x^4 + 6m(3m-4)x^5 + 7(2m-3)x^6 + 8m(2m-5)x^7]_{x=1} \\ &= 87m^2 - 14m - 21 \\ WW(J_{7,m}) &= \frac{1}{2} \frac{d^2}{dx^2} [xH(J_{7,m})]_{x=1} \\ &= \frac{1}{2} \frac{d^2}{dx^2} \left[x(8mx + \frac{m}{2} (m+17)x^2 + m(2m+7)x^3 + m(4m+5)x^4 + 6m(m-1)x^5 + 2m(3m-4)x^6 + (2m-3)x^7 + m(2m-5)x^8) \right]_{x=1} \\ &= \frac{1}{2} \frac{d^2}{dx^2} \left[8mx^2 + \frac{m}{2} (m+17)x^3 + m(2m+7)x^4 + m(4m+5)x^5 + 6m(m-1)x^6 + 2m(3m-4)x^7 + (2m-3)x^8 + m(2m-5)x^9 \right]_{x=1} \\ &= \frac{1}{2} \frac{d}{dx} \left[16mx + \frac{3m}{2} (m+17)x^2 + 4m(2m+7)x^3 + 5m(4m+5)x^4 + 36m(m-1)x^5 + 14m(3m-4)x^6 + 8(2m-3)x^7 + 9m(2m-5)x^8 \right]_{x=1} \\ &= \frac{1}{2} [16m + 3m(m+17)x + 12m(2m+7)x^2 + 20m(4m+5)x^3 + 180m(m-1)x^4 + 84m(3m-4)x^5 + 56(2m-3)x^6 + 72m(2m-5)x^7]_{x=1} \\ &= \frac{1}{2} [16m + 3m(m+17) + 12m(2m+7) + 20m(4m+5) + 180m(m-1) + 84m(3m-4) + 56(2m-3) + 72m(2m-5)] \\ &= \frac{1}{2} [683m^2 - 513m - 168] \end{aligned}$$

$$\begin{aligned} \text{Ha}(J_{7,m}) &= \int_0^1 \frac{H(J_{7,m})}{x} dx \\ &= \int_0^1 \frac{1}{x} \left[8mx + \frac{m}{2}(m+17)x^2 + m(2m+7)x^3 + m(4m+5)x^4 \right. \\ &\quad \left. + 6m(m-1)x^5 + 2m(3m-4)x^6 + (2m-3)x^7 + m(2m-5)x^8 \right] dx \\ &= \int_0^1 \left[8m + \frac{m}{2}(m+17)x + m(2m+7)x^2 + m(4m+5)x^3 \right. \\ &\quad \left. + 6m(m-1)x^4 + 2m(3m-4)x^5 + (2m-3)x^6 + m(2m-5)x^7 \right] dx \\ &= \int_0^1 \left[8mx + \frac{m}{4}(m+17)x^2 + \frac{m}{3}(2m+7)x^3 + \frac{m}{4}(4m+5)x^4 \right. \\ &\quad \left. + \frac{6m}{5}(m-1)x^5 + \frac{m}{3}(3m-4)x^6 + \frac{1}{7}(2m-3)x^7 + \frac{m}{8}(2m-5)x^8 \right] dx \\ &= \left[4mx^2 + \frac{m}{20}(m+17)x^3 + \frac{m}{12}(2m+7)x^4 + \frac{m}{20}(4m+5)x^5 \right. \\ &\quad \left. + \frac{6m}{35}(m-1)x^6 + \frac{m}{42}(3m-4)x^7 + \frac{1}{56}(2m-3)x^8 + \frac{m}{72}(2m-5)x^9 \right]_0^1 \\ &= \frac{131}{30}m^2 + \frac{3629}{280}m - \frac{3}{7} \end{aligned}$$

$$\begin{aligned} \text{TSZ}(J_{7,m}) &= \frac{1}{3!} \frac{d^3}{dx^3} [x^2 H(J_{7,m})]_{x=1} \\ &= \frac{1}{3!} \frac{d^3}{dx^3} \left[x^2 \left(8mx + \frac{m}{2}(m+17)x^2 + m(2m+7)x^3 + m(4m+5)x^4 \right. \right. \\ &\quad \left. \left. + 6m(m-1)x^5 + 2m(3m-4)x^6 + (2m-3)x^7 + m(2m-5)x^8 \right) \right]_{x=1} \\ &= \frac{1}{3!} \frac{d^3}{dx^3} \left[8mx^3 + \frac{m}{2}(m+17)x^4 + m(2m+7)x^5 + m(4m+5)x^6 \right. \\ &\quad \left. + 6m(m-1)x^7 + 2m(3m-4)x^8 + (2m-3)x^9 + m(2m-5)x^{10} \right]_{x=1} \\ &= \frac{1}{3!} \frac{d^2}{dx^2} \left[24mx^2 + 2m(m+17)x^3 + 5m(2m+7)x^4 + 6m(4m+5)x^5 \right. \\ &\quad \left. + 42m(m-1)x^6 + 16m(3m-4)x^7 + 9(2m-3)x^8 + 10m(2m-5)x^9 \right]_{x=1} \\ &= \frac{1}{3!} \frac{d}{dx} \left[48mx + 6m(m+17)x^2 + 20m(2m+7)x^3 + 30m(4m+5)x^4 \right. \\ &\quad \left. + 252m(m-1)x^5 + 112m(3m-4)x^6 + 72(2m-3)x^7 + 90m(2m-5)x^8 \right]_{x=1} \\ &= \frac{1}{3!} \left[48m + 12m(m+17)x + 60m(2m+7)x^2 + 120m(4m+5)x^3 \right. \\ &\quad \left. + 1160m(m-1)x^4 + 672m(3m-4)x^5 + 504(2m-3)x^6 + 720m(2m-5)x^7 \right]_{x=1} \\ &= \frac{1}{3!} \left[48m + 12m(m+17) + 60m(2m+7) + 120m(4m+5) \right. \\ &\quad \left. + 1160m(m-1) + 672m(3m-4) + 504(2m-3) + 720m(2m-5) \right] \\ &= \frac{2614}{3}m^2 - \frac{2584}{3}m - 252 \end{aligned}$$

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