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Schultz Polynomials and Their Topological Indices of Jahangir Graphs $J_{2,m}$

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Abstract

Let $G = (V; E)$ be a simple connected graph. The Wiener index $W(G)=\sum_{\{v,u\}\in V(G)} d(u,v)$ is the sum of distances between all pairs of vertices of a connected graph. The Schultz topological index is equal to $Sc(G)=\frac{1}{2}\sum_{u,v\in V(G)}(d_u+d_v)d(u,v)$ and the Modified Schultz topological index is $Sc^*(G)=\sum_{u,v\in V(G)}\frac{1}{2}(d_u\times d_v)d(u,v)$. In this paper, the Schultz, Modified Schultz polynomials and their topological indices of *Jahangir graphs* $J_{2,m}$ for all integer number $m \geq 3$ are calculated.

Keywords

Molecular Topological Index, Schultz Index, Schultz Polynomials, Jahangir Graphs $J_{2,m}$

1. Introduction

Let $G = (V; E)$ be an undirected connected graph without loops or multiple edges. The sets of vertices and edges of G are denoted by $V(G)$ and $E(G)$, respectively. A topological index is a numerical quantity derived in an unambiguous manner from the structure graph of a molecule. As a graph structural invariant, *i.e.* it does not depend on the labelling or the pictorial representation of a graph. Various topological indices usually reflect molecular

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size and shape. An oldest topological index in chemistry is the Wiener index, that first introduced by *Harold Wiener* in 1947 to study the boiling points of paraffin. It plays an important role in the so-called inverse structure-property relationship problems. The Wiener index of a molecular graph G was defined as [1]:

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

where the summation goes over all pairs of vertices of G and $d(u, v)$ denotes the distance of the two vertices u and v in the graph G (the number of edges in a shortest path connecting u and v). For details of mathematical properties and applications, the readers are suggested to refer to [2]-[4] and the references therein. Other properties and applications of Wiener index can be found in [5]-[12].

In 1989, *H.P. Schultz* [13] has introduced a graph theoretical descriptor for characterizing alkanes by an integer number as follow:

$$Sc(G) = \sum_{\{u,v\} \subset V(G)} \frac{1}{2}(d_u + d_v) d(u,v) \tag{2}$$

where d_u and d_v are degrees of vertices u and v. Schultz named this descriptor the "*molecular topological index*" and denoted it by MTI. Later MTI became much better known under the name the Schultz index.

In 1997, S. Klavžar and I. Gutman [14] defined another based structure descriptors the Modified Schultz index of G is defined as:

$$Sc^*(G) = \sum_{\{u,v\} \subset V(G)} \frac{1}{2}(d_u \times d_v) d(u,v) \tag{3}$$

Now, there are two topological polynomials of a graph G as follow:

$$Sc(G,x) = \sum_{\{u,v\} \subset V(G)} \frac{1}{2}(d_u + d_v) x^{d(u,v)} \tag{4}$$

and

$$Sc^*(G,x) = \sum_{\{u,v\} \subset V(G)} \frac{1}{2}(d_u \times d_v) x^{d(u,v)} \tag{5}$$

For more details about the Schultz, Modified Schultz polynomials and their topological indices and other molecular topological polynomials and indices reader can see the paper series [13]-[29].

In this paper we study the Schultz, Modified Schultz polynomials and their topological indices of *Jahangir graphs* $J_{2,m}$ for all integer number $m \geq 3$.

2. Main Results

In this section we compute the Schultz, Modified Schultz polynomials and their topological indices for Jahangir graphs $J_{2,m}$ $\forall m \geq 3$. The general form of *Jahangir graphs* $J_{n,m}$ is defined as follows:

Definition 1. [30]-[35] Jahangir graphs $J_{n,m}$ for $m \geq 3$, 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}.

Theorem 1. Let $J_{2,m}$ be the Jahangir graphs ($\forall m \geq 3$). Then,

The Schultz polynomial of $J_{2,m}$ is equal to

$$Sc(J_{2,m}, x) = m(m+13)x^1 + (4m^2 + 3m)x^2 + 5m(m-2)x^3 + 2m(m-3)x^4$$

The Modified Schultz polynomial of $J_{2,m}$ is equal to

$$Sc^*(J_{2,m}, x) = 3m(m+4)x^1 + \frac{1}{2}m(13m-1)x^2 + 6m(m-2)x^3 + 2m(m-3)x^4$$

Proof. $\forall m \geq 3$ consider Jahangir graph $J_{2,m}$. By using Definition 1 and [29]-[32], one can see that the number of vertices in Jahangir graph $J_{2,m}$ is equal to $|V(J_{2,m})| = m + m + 1$ $(\forall m \geq 3)$. And the number of edges of Jahangir graph $J_{2,m}$ is equal to $|E(J_{2,m})| = \frac{2 \times m + 3 \times m + m \times 1}{2} = 3m.$ Because, there is only Center vertex with degree m and there are m vertices with degree 2 and m vertices with degree. In this paper, we denote the sets of all vertices with degree two by A, all vertices with degree three by B and only Center vertex *c* by C.

From the structure of Jahangir graph $J_{2,m}$ (**Figure 1**), we see that there are distances from one to four, for every vertices $u, v \in V(J_{2,m})$. In other words, $\forall u, v \in V(J_{2,m}), \exists d(u,v) \in \{1,2,3,4\}$ and the Diameter D of Jahangir graph $J_{2,m}$ is equal to $D(J_{2,m}) = 4$.

I. If $\forall v, u \in V(J_{2,m})$, $d(u,v) = 1$, we have two case for first sentences of the Schultz, Modified Schultz polynomials of $J_{2,m}$.

I-1. For a vertex $v \in A \subset V(J_{2,m})$, there are two path with length one until a vertex $u \in B \subset V(J_{2,m})$, thus there are $2m$ edges $uv \in E(J_{2,m})$, such that $d_u + d_v = 5$, $d_u \times d_v = 6$. Therefore, we have two terms $5 \times 2mx^1$, $6 \times 2mx^1$ of the Schultz and Modified Schultz polynomials of Jahangir graph $J_{2,m}$, respectively.

I-2. For only vertex $c \in C \subset V(J_{2,m})$, there are m path with length one until a vertex $u \in B \subset V(J_{2,m})$, thus there are m edges $uv \in E(J_{2,m})$, such that $d_u + d_v = m+3$, $d_u \times d_v = 3m$. So, we have two terms $(m+3) \times mx^1$ and $3m \times mx^1$ of the Schultz and Modified Schultz polynomials of $J_{2,m}$, respectively.

Thus, the first sentences of the Schultz and Modified Schultz polynomials of Jahangir graph $J_{2,m}$ are equal to $m(m+13)x^1$ and $3m(m+4)x^1$, respectively.

II. If $\forall v, u \in V(J_{2,m})$, $d(u,v) = 2$, we have three case for first sentences of the Schultz, Modified Schultz polynomials of $J_{2,m}$.

II-1. For a vertex $v \in A \subset V(J_{2,m})$, there are two path with length two until other vertices *A*, so there are (1/2) × $2m$ 2-edge-path in $J_{2,m}$, such that $d_u + d_v = d_u \times d_v = 4$. Therefore, we have a terms $4 \times mx^2$ of the Schultz and Modified Schultz polynomials of $J_{2,m}$.

II-2. For every vertex $v \in A \subset V(J_{2,m})$, there are only 2-edge-path until the Center vertex *c*, and there are m 2-edge-path in $J_{2,m}$ with $d_u + d_v = m+2$ and $d_u \times d_v = 2m$. Therefore, we have two terms $(m+2) \times mx^2$, $2m \times mx^2$ of the Schultz and Modified Schultz polynomials of $J_{2,m}$, respectively.

II-3. For a vertex $v \in B \subset V(J_{2,m})$, there are $m - 1$ path with length two until other vertices $u \in B \subset V(J_{2,m})$, so there are $1/2(m-1)m$ 2-edge-path in $J_{2,m}$, such that $d_u + d_v = 6$, $d_u \times d_v = 9$. So, we have two terms $6 \times 1/2(m-1)mx^2$ and $9 \times 1/2(m-1)mx^2$ of the Schultz and Modified Schultz polynomials of $J_{2,m}$, respectively.

Thus, the second sentences of the Schultz and Modified Schultz polynomials of Jahangir graph $J_{2,m}$ are equal to $(4m^2 + 3m)x^2$ and $\left(\frac{13}{2}m^2 - \frac{1}{2}m\right)x^2$, respectively.

III. If $\forall v, u \in V(J_{2,m})$, $d(u,v) = 3$, for a vertex $v \in A \subset V(J_{2,m})$, there are $(m - 2)m$ path with length three until vertices of *B*, such that $d_u + d_v = 5$, $d_u \times d_v = 6$. Therefore, we have two sentences $5 \times (m-2)mx^3$ and $6 \times (m-2)mx^3$ of the Schultz and Modified Schultz polynomials of Jahangir graph $J_{2,m}$, respectively.

IV. If $\forall v, u \in V(J_{2,m})$, $d(u,v) = 4$, for a vertex $v \in A \subset V(J_{2,m})$, there are $m - 3$ path with length 4 = $D(J_{2,m})$, between *v* and other vertices *u* of *A*. Thus by $d_u + d_v = d_u \times d_v = 4$, the fourth sentence of the Schultz and Modified Schultz polynomials of Jahangir graph $J_{2,m}$ is equal to $4 \times 1/2(m-3)mx^4$.

From the definition of the Schultz, Modified Schultz polynomials and above mentions, we have following results $\forall m \in \mathbb{N} - \{2\}$.

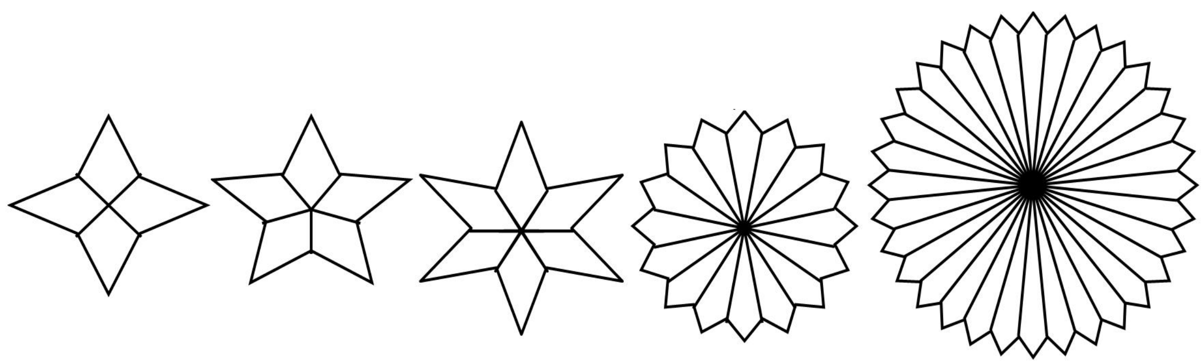

Figure 1. Jahangir graphs $J_{2,4}$, $J_{2,5}$, $J_{2,6}$, $J_{2,16}$ and $J_{2,32}$ [32].

$$Sc\left(J_{2,m},x\right)=\sum_{\{u,v\}\subset V\left(J_{2,m}\right)}\frac{1}{2}\left(d_u+d_v\right)x^{d(u,v)}=m\left(m+13\right)x^1+\left(4m^2+3m\right)x^2+5m\left(m-2\right)x^3+2m\left(m-3\right)x^4 \quad (6)$$

and

$$Sc^*\left(J_{2,m},x\right)=\sum_{\{u,v\}\subset V\left(J_{2,m}\right)}\frac{1}{2}\left(d_ud_v\right)x^{d(u,v)}=3m\left(m+4\right)x^1+\frac{1}{2}m\left(13m-1\right)x^2+6m\left(m-2\right)x^3+2m\left(m-3\right)x^4 \quad (7)$$

And these complete the proof. □

Theorem 2. Let $J_{2,m}$ be the Jahangir graphs ($\forall m \geq 3$). Then, the Schultz, Modified Schultz indices of $J_{2,m}$ are equal to

$$Sc\left(J_{2,m}\right)=32m^2-35m$$

$$\text{and } S^{c*}\left(J_{2,m}\right)=42m^2-49m.$$

Proof. Consider the Jahangir graph $J_{2,m}$ ($\forall m \geq 3$) that presented in above proof. Now, by using the results from proof of Theorem 1 and according to the definitions of the Schultz, Modified Schultz indices of the graph G, one can see that these indices are the first derivative of their polynomials (evaluated at $x = 1$). Thus we have following computations $\forall m \in \mathbb{N} - \{2\}$.

$$\begin{aligned}Sc\left(J_{2,m}\right)&=\left.\frac{\partial Sc\left(J_{2,m},x\right)}{\partial x}\right|_{x=1}\\&=\left.\left[m\left(m+13\right)x^1+m\left(4m+3\right)x^2+5m\left(m-2\right)x^3+2m\left(m-3\right)x^4\right]'\right|_{x=1}\\&=\left[m\left(m+13\right)\times1+m\left(4m+3\right)\times2+5m\left(m-2\right)\times3+2m\left(m-3\right)\times4\right]\\&=32m^2-35m.\end{aligned} \quad (8)$$

And

$$\begin{aligned}Sc^*\left(J_{2,m}\right)&=\left.\frac{\partial Sc^*\left(J_{2,m},x\right)}{\partial x}\right|_{x=1}\\&=\left.\left[3m\left(m+4\right)x^1+\frac{1}{2}m\left(13m-1\right)x^2+6m\left(m-2\right)x^3+2m\left(m-3\right)x^4\right]'\right|_{x=1}\\&=\left[3m\left(m+4\right)\times1+\frac{1}{2}m\left(13m-1\right)\times2+6m\left(m-2\right)\times3+2m\left(m-3\right)\times4\right]\\&=42m^2-49m.\end{aligned} \quad (9)$$

Here the proof of theorem is completed. □

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