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The Schultz Index and Schultz Polynomial of the Jahangir Graphs $J_{5,m}$

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Abstract

Let G be simple connected graph with the vertex and edge sets $V(G)$ and $E(G)$, respectively. The Schultz and Modified Schultz indices of a connected graph G are defined as $Sc(G)=\frac{1}{2}\sum_{u,v\in V(G)}(d_u+d_v)d(u,v)$ and $Sc^*(G)=\frac{1}{2}\sum_{u,v\in V(G)}(d_u\times d_v)d(u,v)$, where $d(u, v)$ is the distance between vertices u and v; d_v is the degree of vertex v of G. In this paper, computation of the Schultz and Modified Schultz indices of the Jahangir *graphs* $J_{5,m}$ is proposed.

Keywords

Wiener Index, Schultz Index, Modified Schultz Index, Distance, Jahangir Graphs

1. Introduction

Let G be simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. For vertices u and v in $V(G)$, we denote by $d(u, v)$ the topological distance *i.e.*, the number of edges on the shortest path, joining the two vertices of G.

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 size and shape.

As an oldest topological index in chemistry, the Wiener index was first introduced by *Harold Wiener* [1] 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 G is defined as [1]-[7]:

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

The Hosoya polynomial was introduced by *Haruo Hosoya*, in 1988 [8] and defined as follows:

$$H(G,x)=\frac{1}{2}\sum_{v\in V(G)}\sum_{u\in V(G)}x^{d(v,u)}$$

The number of incident edges at vertex *v* is called degree of *v* and denoted by d_v.

The Schultz index of a molecular graph *G* was introduced by *Schultz* [9] in 1989 for characterizing alkanes by an integer as follow:

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

The Modified Schultz index of a graph *G* was introduced by *S. Klavžar* and *I. Gutman* in 1996 as follow [10]:

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

Also the Schultz and Modified Schultz polynomials of *G* are defined as:

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

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

where d_u and d_v are degrees of vertices *u* and *v*.

The Schultz indices have been shown to be a useful molecular descriptors in the design of molecules with desired properties, reader can see the paper series [11]-[29].

In this paper computation of the Schultz and Modified Schultz indices of the Jahangir *graphs* $J_{5,m}$ are proposed. The *Jahangir graphs* $J_{5,m}$ $\forall m\geq 3$ is defined as a graph on 5*m* + 1 vertices and 6 *m* edges *i.e.*, a graph consisting of a cycle C_{5m} with one additional vertex (Center vertex *c*) which is adjacent to *m* vertices of C_{5m} at distance 5 to each other on C_{5m}. Some example of the Jahangir graphs and the general form of this graph are shown in **Figure 1** and **Figure 2** and the paper series [30]-[35].

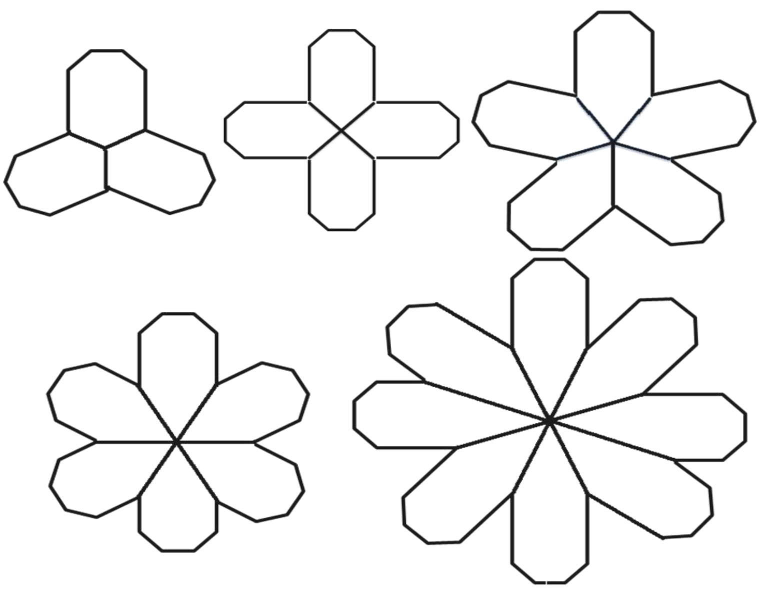

Figure 1. Some examples of the Jahangir graphs $J_{5,3}$, $J_{5,4}$, $J_{5,5}$, $J_{5,6}$ and $J_{5,8}$.

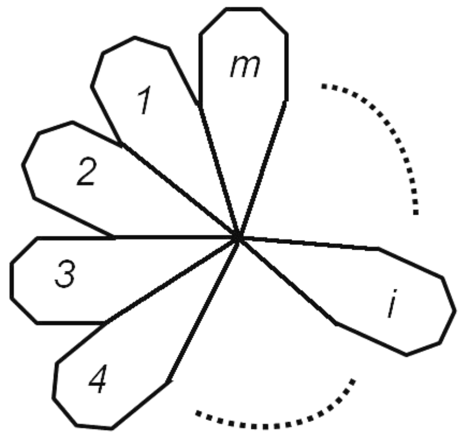

Figure 2. A general representation of the Jahangir graphs $J_{n,m}$ $n = 5$, $\forall m \ge 3$.

2. Results and Discussion

In this present section, we compute the Schultz and Modified Schultz indices and the Schultz and Modified Schultz polynomials of the Jahangir graphs $J_{n,m}$ $n = 5$, $\forall m \ge 3$ as.

Theorem 1. Let $J_{5,m}$ be the Jahangir graphs for all integer numbers $\forall m \ge 3$. Then, the Schultz, Modified Schultz polynomials and indices are as:

The Schultz index and polynomial are equal to

- $$Sc(J_{5,m},x) = [m^2 + 27m]x^1 + [7m^2 + 23m]x^2 + [12m^2 + 16m]x^3 + [20m^2 - 24m]x^4 + [16m^2 - 24m]x^5 + [8m^2 - 20m]x^6,$$
- $Sc(J_{5,m}) = 259m^2 - 215m$.

The Modified Schultz index and polynomial are equal to:

- $$Sc^*(J_{5,m},x) = [3m^2 + 24m]x^1 + \left[\frac{17m^2 + 19m}{2}\right]x^2 + [16m^2 + 12m]x^3 + [24m^2 - 32m]x^4 + [16m^2 - 24m]x^5 + [8m^2 - 20m]x^6,$$
- $Sc^*(J_{5,m}) = 292m^2 - 289m.$

Proof. Let $J_{5,m}$ be Jahangir graphs $\forall m \ge 3$ with $5m + 1$ vertices and $6m$ edges. From **Figure 1** and **Figure 2**, we see that $4m$ vertices of $J_{5,m}$ have degree two and m vertices of $J_{5,m}$ have degree three and one additional vertex (Center vertex) of $J_{5,m}$ has degree m. Thus we have three partitions of the vertex set $V(J_{5,m})$ as follow

$$V_2 = \{v \in V(J_{5,m}) | d_v = 2\} \to |V_2| = 4m$$

$$V_3 = \{v \in V(J_{5,m}) | d_v = 3\} \to |V_3| = m$$

$$V_m = \{c \in V(J_{5,m}) | d_c = m\} \to |V_m| = 1$$

Obviously, $V(J_{5,m}) = V_2 \cup V_3 \cup V_m$ and $V_2 \cap V_3 \cap V_m = \varnothing$, thus

$$|E(J_{5,m})| = \frac{1}{2}[2 \times |V_2| + 3 \times |V_3| + m \times |V_m|] = 6m.$$

Now, for compute the Schultz and Modified Schultz indices and the Schultz and Modified Schultz polynomials of the Jahangir graphs $J_{n,m}$, we see that for all vertices u, v in $V(J_{5,m}), \exists d(u,v) \in \{1, 2, \cdots, 6\}$ and the diameter of the Jahangir graph $J_{5,m}$ is equal to $d(J_{5,m}) = 6$.

Now, we compute all cases of $d(u,v)$-edge-paths $d(u,v) = 1, 2, \cdots, 6$ of $J_{5,m}$ in **Table 1**.

Table 1. All cases of $d(u,v)$-edge-paths $d(u,v)=1,2,\cdots,6$ of the Jahangir graph $J_{5,m}$.

The distance $d(u,v)=i$	degrees of d_u & d_v	Number of i-edges paths	Term of Schultz polynomial	Term of Modified Schultz polynomial
1	2 & 2	$3m=2\|V_3\|+\|V_3\|$	$12m$	$12m$
1	2 & 3	$2m=2\|V_3\|$	$10m$	$12m$
1	3 & 3	0	0	0
1	2 & m	0	0	0
1	3 & m	$m=\|V_3\|$	$(m+3)m$	$3m^2$
2	2 & 2	$2\|V_3\|+\|V_3\|$	$12m$	$12m$
2	2 & 3	$2\|V_3\|$	$10m$	$12m$
2	3 & 3	$\frac{1}{2}\|V_3\|(\|V_3\|-1)$	$3m(m-1)$	$\frac{9}{2}m(m-1)$
2	2 & m	$2m=2\|V_3\|$	$2m(m+2)$	$4m^2$
2	3 & m	0	0	0
3	2 & 2	$2\|V_3\|+\|V_3\|$	$12m$	$12m$
3	2 & 3	$2\|V_3\|+2\|V_3\|(m-1)$	$10m^2$	$12m^2$
3	3 & 3	0	0	0
3	2 & m	$2m=\|V_3\|$	$2m(m+2)$	$4m^2$
3	3 & m	0	0	0
4	2 & 2	$m+\|V_3\|(2\|V_3\|-3)$	$8m(m-1)$	$8m(m-1)$
4	2 & 3	$\|V_3\|(2\|V_3\|-4)$	$10m(m-2)$	$12m(m-2)$
4	3 & 3	0	0	0
4	2 & m	$2m=2\|V_3\|$	$2m(m+2)$	$4m^2$
4	3 & m	0	0	0
5	2 & 2	$2m+\frac{1}{2}\|V_2\|(2\|V_3\|-4)$	$8m(2m-3)$	$8m(2m-3)$
5	2 & 3	0	0	0
5	3 & 3	0	0	0
5	2 & m	0	0	0
5	3 & m	0	0	0
6	2 & 2	$\frac{1}{2}\|V_3\|(2\|V_3\|-5)$	$4m(2m-5)$	$4m(2m-5)$
6	2 & 3	0	0	0
6	3 & 3	0	0	0
6	2 & m	0	0	0
6	3 & m	0	0	0

For example, in case $d(u,v)=1,\forall v,u\in V(J_{5,m})$; one can see that there are $|V_3|=m$ 1-edges paths between the vertex c and vertices from V_3 (where $d_c+d_v=m+3, d_c\times d_v=3m$). There exist two 1-edges paths starts every vertex $u\in V_3$ until $v\in V_2$ (where $d_u+d_v=5, d_u\times d_v=6$). There are 3 m 1-edges paths between two vertices $u,v\in V_2\subset V(J_{5,m})$ (two adjacent vertices or edges), such that $d_u+d_v=d_u\times d_v=4$. Thus, the first terms of the Schultz and Modified Schultz polynomials of $J_{5,m}$ are equal to $(12m+10m+(m+3)m)x^1=(m^2+27m)x^1$ and $(12m+12m+3m^2)x=(3m^2+24m)x$ respectively.

Also, in case $d(u,v)=2,\forall v,u\in V(J_{5,m})$; there are two 2-edges paths between Center vertex $c\in V(J_{5,m})$ and other vertices of vertex set $V_2\subset V(J_{5,m})$. $\frac{1}{2}|V_3|(m-1)$ 2-edges paths between all vertices of $u,v\in V_3\subset V(J_{5,m})$ and $2|V_3|+|V_3|$ 2-edges paths start from vertices of V_2 until vertices of V_3 and $V_2\subset V(J_{5,m})$. Thus, the second terms of the Schultz and Modified Schultz polynomials of $J_{5,m}$ are equal to $(12m+10m+3m(m-1)+2m(m+2))x^2$ and $(12m+12m+m(m-1)+4m^2)x^2$, respectively.

By using the definition of the Jahangir graphs and **Figure 1** and **Figure 2**, we can compute other terms of the Schultz and Modified Schultz polynomials of $J_{5,m}$. We compute and present all necessary results on based the degrees of d_u & d_v for all cases of $d(u,v)$-edge-paths $d(u,v)=1,2,\cdots,6$ in following table.

Now, we can compute all coefficients of the Schultz $Sc(J_{5,m},x)$ and Modified Schultz $Sc^*(J_{5,m},x)$ polynomials and indices of $J_{5,m}$ by using all cases of the $d(u,v)$-edge-paths $(d(u,v)=1,2,\cdots,6)$ of the Jahangir graph $J_{5,m}$ in **Table 1** and alternatively

$$\begin{aligned}
Sc(J_{5,m},x)&=\frac{1}{2}\sum_{u,v\in V(J_{5,m})}(d_u+d_v)x^{d(u,v)}=\left[12m+12m+0+0+m(m+3)\right]x^1\\
&\quad+\left[12m+10m+3m(m-1)+2m(m+2)+0\right]x^2+\left[12m+10m^2+0+2m(m+2)+0\right]x^3\\
&\quad+\left[8m(m-1)+10m(m-2)+0+2m(m+2)+0\right]x^4+\left[8m(2m-3)\right]x^5+\left[4m(2m-5)\right]x^6\\
&=\left[m^2+27m\right]x^1+\left[7m^2+23m\right]x^2+\left[12m^2+16m\right]x^3+\left[20m^2-24m\right]x^4\\
&\quad+\left[16m^2-24m\right]x^5+\left[8m^2-20m\right]x^6.
\end{aligned}$$

From the definition of Schultz index and the Schultz Polynomial of G, we can compute the Schultz index of the Jahangir graph $J_{5,m}$ by the first derivative of Schultz polynomial of $J_{5,m}$ (evaluated at $x = 1$) as follow:

$$\begin{aligned}
Sc(J_{5,m})&=\left.\frac{\partial Sc(J_{5,m},x)}{\partial x}\right|_{x=1}=\frac{\partial}{\partial x}\Big((m^2+27m)x^1+(7m^2+23m)x^2+(12m^2+16m)x^3\\
&\quad+(20m^2-24m)x^4+(16m^2-24m)x^5+(8m^2-20m)x^6\Big)_{x=1}\\
&=\Big[(m^2+27m)\times1+(7m^2+23m)\times2+(12m^2+16m)\times3+(20m^2-24m)\times4\\
&\quad+(16m^2-24m)\times5+(8m^2-20m)\times6\Big]\\
&=259m^2-215m.
\end{aligned}$$

And also Modified Schultz polynomial of $J_{5,m}$ is equal to

$$\begin{aligned}
Sc^*(J_{5,m},x)&=\frac{1}{2}\sum_{u,v\in V(J_{5,m})}(d_u\times d_v)x^{d(u,v)}=\left[12m+12m+0+0+3m^2\right]x^1\\
&\quad+\left[12m+12m+m(m-1)+4m^2+0\right]x^2+\left[12m+12m^2+0+4m^2+0\right]x^3\\
&\quad+\left[8m(m-1)+12m(m-2)+0+4m^2+0\right]x^4+\left[8m(2m-3)\right]x^5+\left[4m(2m-5)\right]x^6\\
&=\left[3m^2+24m\right]x^1+\left[\frac{17}{2}m^2+\frac{19}{2}m\right]x^2+\left[16m^2+12m\right]x^3+\left[24m^2-32m\right]x^4\\
&\quad+\left[16m^2-24m\right]x^5+\left[8m^2-20m\right]x^6.
\end{aligned}$$

And from the first derivative of Schultz Modified polynomial of the Jahangir graph $J_{5,m}$ (evaluated at $x = 1$), the Modified Schultz index of $J_{5,m}$ is equal to:

$$Sc^*\left(J_{5,m}\right)=\left.\frac{\partial Sc^*\left(J_{5,m},x\right)}{\partial x}\right|_{x=1}$$

$$=\frac{\partial}{\partial x}\Big(3m^2+24m)x^1+(m^2+m)x^2+\left(16m^2+12m\right)x^3+\left(24m^2-32m\right)x^4$$

$$+\left(16m^2-24m\right)x^5+\left(8m^2-20m\right)x^6\Big)_{x=1}$$

$$=292m^2-289m.$$

Here these completed the proof of Theorem 1. ■

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Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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