Schultz index of regular dendrimers

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The Schultz index of a connected graph G is defined as $MTI(G)=\sum_{i,j}\deg(i)[d(i,j)+A(i,j)]$ where $d(i, j)$ is the distance between vertices i and j, $deg(i)$ is the degree of vertex i, and $A(i, j)$ is the (i, j) entry of the adjacency matrix of G. In this paper computation of the Schultz index in regular dendrimers are proposed.

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1. Introduction

Let G be simple connected graph with vertex set $V(G)$. For vertices i and j in $V(G)$, we denote by $d(i, j)$ the topological distance i.e., the number of edges on the shortest path, joining the two vertices of G. The number of incident edges at vertex i is called degree of i and denoted by $deg(i)$. The Schultz index of a molecular graph G was introduced by Schultz [1] in 1989 for characterizing alkanes by an integer as follow

$$MTI(G)=\sum_{i,j}\deg(i)[d(i,j)+A(i,j)]. \qquad (1)$$

Where $A(i, j)$ is the (i, j) entry of the adjacency matrix of G. The Schultz index has been shown to be a useful molecular descriptor in the design of molecules with desired properties [2-7].

Dendrimers are hyperbranched molecules, synthesized by repeatable steps, either by adding branching blocks around a central *core* (thus obtaining a new, larger orbit or generation-the "divergent growth" approach) or by building large branched blocks starting from the periphery and then attaching them to the core (the "convergent growth" approach [8]). The vertices of a dendrimer, except the external end points, are considered as branching points. The number of edges emerging from each branching point is called progressive degree, (*i.e.*, the edges which enlarge the number of points of a newly added orbit). It equals the classical degree**.** If all the branching points have the same degree, the dendrimer is called regular.Otherwise it is irregular.

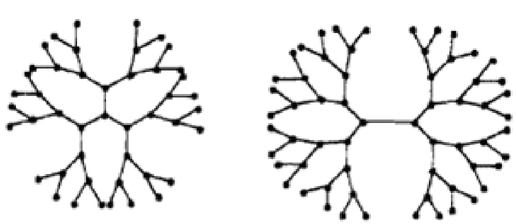

Fig. 1. Regular monocentric ($D_{3,4}$) and dicentric ($DD_{3,4}$) dendrimers.

It is well-known [9] that any graph of dendrimers has either a monocenter or a dicenter (i.e., two points joined by an edge). Accordingly, the dendrimers are called *monocentric* and *dicentric*, respectively (Fig. 1). The numbering of orbits starts with zero for the core and ends with r**,** which equals the radius of the dendrimer. A regular monocentric dendrimer, of progressive degree p and generation r is herein denoted by $D_{p,r}$, whereas the corresponding dicentric dendrimer, by $DD_{p,r}$ [10]. In this paper the Schultz index in regular monocentric and dicentric dendrimers are proposed.

Main results:

To compute the Schultz index of regular dendrimers the summation of distances between an arbitrary vertex and all of the other vertices of graph must be calculated. For this purpose we consider the graph of regular monocentric dendrimers as a rooted tree with $r+1$ levels where central core of this graph is the root of tree lying on the first level. Recall that a tree is a connected acyclic graph. In a tree, any vertex can be chosen as the root vertex. The level of a vertex on a tree is one more than its distance from the root vertex.

Now suppose x denotes the root vertex of the graph $G=D_{p,r}$. Let E_s denotes the set of vertices where are placed on the s-th level of G for $s=1,2,\ldots,r+1$. The summation of distances between x and all of the other vertices of G can be calculated by calculation distance between x and members of E_s for $s=1,2,\ldots,r+1$.

$$\sum_{i\in V(G)}d(x,i)=\sum_{s=1}^{r+1}\sum_{u\in E_s}d(x,i)=p+2p(p-1)+\ldots+rp(p-1)^{r-1}=p\frac{(p-1)^r(pr-2r-1)+1}{(p-2)^2}.$$

Now suppose i is an arbitrary vertex of G where is placed on s-th level of the graph and $d(i)$ denotes the summation of distances between i and all of the other vertices of G. By using of symmetry of the graph the value of $d(i)=d(s)$ is invariant for all of the vertices where are placed on s-th level of G for $s=1,2,\ldots,r+1$. Put $\lambda(s)=d(s+1)-d(s)$ for $s=1,2,\ldots,r$. If $n=|V(G)|$ then

$$\lambda(s)=n+1-2\sum_{t=0}^{r-s}(p-1)^t=\frac{(p-1)^r}{p-2}[p-2(p-1)^{1-s}].$$

And $s=2,3,\ldots,r+1$.

$$d(s)=d(1)+\lambda(1)+\ldots+\lambda(s-1)=d(1)+\sum_{t=1}^{s-1}\frac{(p-1)^r}{p-2}[p-2(p-1)^{1-t}]. \quad (2)$$

By using pervious computation the Schultz index of regular monocentric dendrimers can be computed.

Theorem 1. The Schultz index of monocentric dendrimers computed as

$$MTI(G)=p(d(1)+p)+p\sum_{s=1}^{r-1}p(p-1)^{s-1}(d(s+1)+p)+p(p-1)^{r-1}(d(r+1)+1).$$

Where

$$d(s)=p\frac{(p-1)^r(pr-2r-1)+1}{(p-2)^2}+\frac{(p-1)^r}{p-2}\sum_{t=1}^{s-1}(p-2(p-1)^{1-t}).$$

Proof: Let V^1 denote the set of pendent vertex of the graph. Thus if $i\in V^1$ then *deg(i)=1* other wise *deg(i)=p*. Therefore By using *(1)*

$$MTI(G)=\sum_{i,j\in V(G)}\deg(i)[d(i,j)+A(i,j)]=\sum_{j,i\in V^1}[d(i,j)+A(i,j)]+\sum_{j,i\notin V^1}p[d(i,j)+A(i,j)].$$

Since $|E_1|=1$ and $|E_s|=p(p-1)^{s-1}$ for $s=2,3\ldots,r+1$. Thus if x is the rooted vertex, $y\neq x$ is an nonpendent vertex on the s-th level and z is a pendent vertex of the graph then by using *(2)*

$$MTI(G)=p(d(1)+\sum_{i\in V(G)}A(x,i))+p\sum_{s=1}^{r-1}p(p-1)^{s-1}(d(s+1)+\sum_{i\in V(G)}A(y,i))+p(p-1)^{r-1}(d(r+1)$$
$$+\sum_{i\in V(G)}A(z,i))=p(d(1)+p)+p\sum_{s=1}^{r-1}p(p-1)^{s-1}(d(s+1)+p)+p(p-1)^{r-1}(d(r+1)+1).$$

Therefore proof is completed.

Example 1. Let $p=4$ and $r=3$. We compute the Schultz index of the graph $D_{4,3}$ by using Theorem *1*. The value of *d(s)* for $s=1,2,3,4$ can be calculated as

$$d(s)=4\frac{3^3(4.3-2.3-1)+1}{2^2}+\frac{3^3}{2}\sum_{t=1}^{s-1}(4-2.3^{1-t})=136+\frac{27}{2}\sum_{t=1}^{s-1}(4-\frac{6}{3^t}).$$

So *d(1)=136*, *d(2)=163*, *d(3)=208* and *d(4)=259*.

Therefore

$$MTI(D_{4,3})=4(136+4)+4(4.167+4.3.212)+4.9.260=22768.$$

In continue the Schultz index of dicentric dendrimers will be computed. For this purpose we consider the graph of $DD_{p,r}$ as two copy of $D_{p,r}$ where their rooted vertices (central vertices) are adjacent with one edge of the graph. Thus the Schultz index of $DD_{p,r}$ can be calculated similar method of calculation the Schultz index of $D_{p,r}$. Let x be one of the central vertices of $G=DD_{p,r}$ (located on the first level of rooted tree $D_{p,r}$). Thus

$$d(1)=\sum_{v\in V(G)}d(x,v)=\sum_{s=1}^{r}s(p-1)^s+\sum_{s=0}^{r}(s+1)(p-1)^s=\frac{(p-1)^{r+1}[2pr+p-4(r+1)]+p}{(p-2)^2}. \quad (3)$$

And for $s=1,2,\ldots,r$,

$$\lambda(s)=n-2\sum_{t=0}^{r-s}(p-1)^t=\frac{2(p-1)^{r+1}(1-(p-1)^{-s})}{p-2}.$$

Thus for $s=2,3,\ldots,r+1$,

$$d(s)=d(1)+\sum_{t=1}^{s}\frac{2(p-1)^{r+1}(1-(p-1)^{-t})}{p-2}. \quad (4)$$

Now the Schultz index of the graph of $DD_{p,r}$ can be computed by last computations.

Theorem 2. The Schultz index of regular dicentric dendrimers computed as

$$J(DD_{p,r})=2p(d(1)+p)+2p\sum_{s=1}^{r-1}(p-1)^s(d(s+1)+p)+2(p-1)^r(d(r+1)+1).$$

Where

$$d(s)=\frac{(p-1)^{r+1}[2pr+p-4(r+1)]+p}{(p-2)^2}+\sum_{t=1}^{s}\frac{2(p-1)^{r+1}(1-(p-1)^{-t})}{p-2}.$$

Proof: If i be a nonpendent vertex of the graph then *deg(i)=p* otherwise *deg(i)=1*. Therefore by using notation of Theorem *1* we have

$$MTI(G)=\sum_{i,j\in V(G)}\deg(i)[d(i,j)+A(i,j)]=\sum_{j,i\in V^1}[d(i,j)+A(i,j)]+\sum_{j,i\notin V^1}p[d(i,j)+A(i,j)].$$

Since $|E_1|=1$, $|E_s|=(p-1)^s$ for $s=2,3,\ldots,r+1$ and the graph of $DD_{p,r}$ obtained by connection rooted vertices of two copy of $D_{p,r}$ we have

$$MTI(DD_{p,r})=2[p(d(1)+\sum_{i\in V(G)}A(x,i))+p\sum_{s=1}^{r-1}(p-1)^s(d(s+1)+\sum_{i\in V(G)}A(y,i))+(p-1)^r(d(r+1)$$
$$+\sum_{i\in V(G)}A(z,i))]=2p(d(1)+p)+2p\sum_{s=1}^{r-1}(p-1)^s(d(s+1)+p)+2(p-1)^r(d(r+1)+1).$$

Therefore proof is completed.

Example 2. Let $p=4$ and $r=3$. By using *(3)* we have *d(1)=244*. So the value of *d(s)* for $s=2,3,4$ can be calculated as

$$d(s)=244+\sum_{t=1}^{s-1}\frac{2.3^4(1-3^{-t})}{2}.$$

So *d(1)=244, d(2)=298, d(3)=370 and d(4)=448*. Therefore by using Theorem *2*

$$MTI(DD_{3,4})=2[4.248+4(3.302+9.374)+27.449]=60406.$$

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