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The Schultz Molecular Topological Index of Polyhex Nanotubes[1]

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Abstract

Formulas for calculating the Schultz molecular topological index in polyhex nanotubes are given in this report.

1 Introduction

Carbon nanotubes were discovered in 1991 by Iijima [1] as multi walled structures. Two years later, two groups independently discovered the single-wall carbon nanotubes [2,3]. In 1996, Smalley's group synthesized the aligned single-wall nanotubes [4]. As point out by Smalley, a carbon nanotube is a carbon molecule with the almost alien property of electrical conductivity, and super-steel strength. It is expected that carbon nanotubes can be widely used in many fields. Due to this reason, carbon nanotubes have attracted

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great attention in different research communities such as chemistry physics and artificial materials. For the details, see [5,6].

In fact, polyhex nanotubes or tubules (the graphs of open-end nanotubes) are the basis for many researches in physics and chemistry. For example, the problem of recognizing the metallic carbon nanotubes and semicondicting nanotubes has been shown to be dependent on the size and geometry of the tubule [6]. Most nanotubes discussed in the literature have closed caps, open-ended tubules have also been reported [7-10]. Sachs, Hansen and Zheng [11] discussed the enumeration of the number of Kekule structures (perfect matchings) of tubules. Zhang and Wang [12] considers the k-resonant theory of tubules. [13,14] gave a method for evaluating the Wiener index of polyhex nanotubes. Ashrafi and Loghman [15] and Deng [16] derived the formulas for computing the PI index of polyhex nanotubes. In this line, we consider the Schultz molecular topological index (MTI) and derive the formulas for calculating the Schultz molecular topological index in polyhex nanotubes.

Let $G = (V, E)$ be a simple connected graph with the vertex set V and the edge set E. For any $i, j \in V$, d_i and D_{ij} denote the degree of i and the distance (i.e., the number of edges on the shortest path) between i and j, respectively.

The Schultz molecular topological index (MTI) of a (chemical) graph G introduced by Schultz [17] in 1989 is defined as

$$MTI = MTI(G) = \sum_{i=1}^{n}\sum_{j=1}^{n} d_i(A_{ij} + D_{ij})$$

where n is the number of vertices of G, $d = (d_1, d_2, \cdots, d_n)$ is the degree vector of vertices of G. A_{ij} is the (i, j)-th entry of the adjacency matrix A of G and A_{ij} is 1 if vertices i and j are adjacent and 0 otherwise.

Let $D_i = \sum_{j=1}^{n} D_{ij}$ be the sum of distances between vertex i and all other vertices. The Schultz molecular topological index can be expressed in the following manner [18]:

$$MTI(G) = \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i D_i \tag{1}$$

It has been demonstrated that the MTI and the Wiener index W are closely mutually related for certain classes of molecular graphs [18-24], where the Wiener index [25] of a connected graph G is the sum of distances between all pairs of vertices of G, i.e.

$$W(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} D_{ij} \tag{2}$$

[24] derived an explicit relation between MTI and W for a tree T with n vertices

$$MTI(T) = 4W(T) + \sum_{i=1}^{n} d_i^2 - n(n-1).$$

Dobrynin [22,23] gave the explicit relation between the Wiener index and the Schultz molecular topological index of a catacondensed benzenoid graph with h hexagons

$$MTI(G) = 5W(G) - (12h^2 - 14h + 5).$$

Here, we will find a relation between the Schultz molecular topological index MTI and the Wiener index W for the polyhex nanotubes, and calculate the Schultz molecular topological indices of polyhex nanotubes by using their Wiener indices.

2 The Schultz molecular topological index of armchair polyhex nanotubes

Note that the degrees of vertices in an arbitrary polyhex nanotube G are two or three. The Wiener index $W(G)$ can be written as

$$W(G) = \frac{1}{2}(W_2(G) + W_3(G)),$$

where $W_2(G) = \sum_{d_i=2} D_i$ and $W_3(G) = \sum_{d_i=3} D_i$, the summation $\sum_{d_i=k}$ goes over all vertices of G with degree k.

Let $G = TUVC_6[p,q]$ be the armchair nanotube with $2p$ vertices at each level and q levels (see Figure 1). Then the Wiener index of G is as follows:

Lemma 1([13]).
(i)$W(G) = \frac{1}{12}p[24p^2q^2 + 2q^4 - 8q^2 + 3(-1)^p(1-(-1)^q)]$ for $q \leq p$ (i.e., short tubes);
(ii)$W(G) = \frac{1}{12}p[p^2(12q^2 - 2p^2 + 8) + 8pq(p^2 + q^2 - 2) + 3(-1 + (-1)^p)]$ for $q \geq p$ (i.e., long tubes).

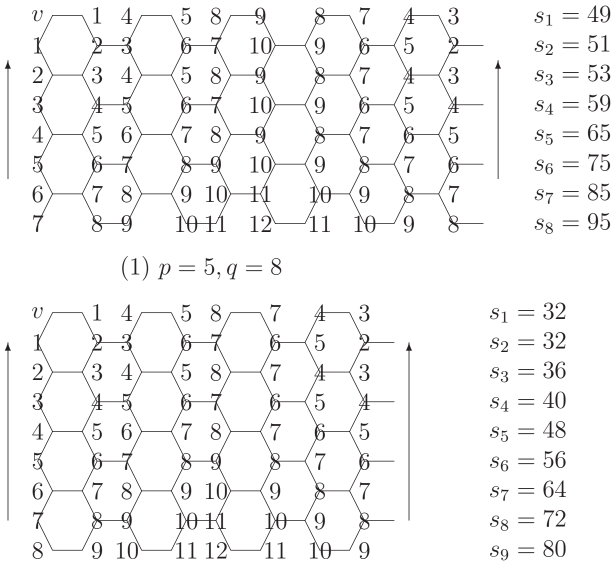
Now, we derive a formula for calculating the Schultz molecular topological index of $TUVC_6[p,q]$.

Note that the numbers of vertices with degree 2 and 3 in the graph $G = TUVC_6[p,q]$ are $4p$ and $2p(q-2)$, respectively. The equation (1) can be further expressed as:

$$\begin{aligned} MTI(G) &= \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i D_i \\ &= 4 \cdot 4p + 9 \cdot 2p(q-2) + 6W(G) - \sum_{d_i=2} D_i \\ &= 6W(G) + 18pq - 20p - W_2(G) \end{aligned} \tag{3}$$

Let $s_k = \sum_{x \text{ is at level } k} D_{vx}$ be the sum of distances from v to all other vertices at level k, where v is a vertex of degree 2 at level 1 (see Figure 1). By the symmetry of G,

$$W_2(G) = 4p \sum_{k=1}^{q} s_k.$$



(1) $p = 5, q = 8$

(2) $p = 4, q = 9$

Figure 1. Two armchair polyhex nanotubes.

From [13,16], we know that

$$\begin{cases} s_1 = 2p^2 - z; \\ s_k = s_{k-1} + (2k - 3 - (-1)^{k-z}), & 2 \le k \le p; \\ s_k = s_p + 2p(k-p), & p \le k \le q. \end{cases}$$

where $z \equiv p(mod 2)$. Therefore,

(i)$W_2(G) = p - (-1)^q p - \frac{4}{3}pq + 8p^3 q - 2pq^2 + \frac{4}{3}pq^3$ for $q \le p$ and p is even;

(ii)$W_2(G) = -p + (-1)^q p - \frac{4}{3}pq + 8p^3 q - 2pq^2 + \frac{4}{3}pq^3$ for $q \le p$ and p is odd;

(iii)$W_2(G) = -\frac{4}{3}p^2 + 2p^3 + \frac{4}{3}p^4 - 4p^2 q + 4p^3 q + 4p^2 q^2$ for $q \ge p+1$ and p is even;

(iv)$W_2(G) = -2p - \frac{4}{3}p^2 + 2p^3 + \frac{4}{3}p^4 - 4p^2q + 4p^3q + 4p^2q^2$ for $q \geq p+1$ and p is odd.

Combining the equation (3) with Lemma 1, we have

Theorem 2. The Schultz molecular topological index of the armchair polyhex nanotube $G = TUVC_6[p,q]$ is

(i)$-\frac{39}{2}p - \frac{1}{2}(-1)^q p + \frac{58}{3}pq - 8p^3q - 2pq^2 + 12p^3q^2 - \frac{4}{3}pq^3 + pq^4$ for $q \leq p$ and p is even;

(ii)$-\frac{41}{2} + \frac{1}{2}(-1)^q p + \frac{58}{3}pq - 8p^3q - 2pq^2 + 12p^3q^2 - \frac{4}{3}pq^3 + pq^4$ for $q \leq p$ and p is odd;

(iii)$-20p + \frac{4}{3}p^2 + 2p^3 - \frac{4}{3}p^4 - p^5 + 18pq - 4p^2q - 4p^3q + 4p^4q - 4p^2q^2 + 6p^3q^2 + 4p^2q^3$ for $q \geq p+1$ and p is even;

(iv)$-21p + \frac{4}{3}p^2 + 2p^3 - \frac{4}{3}p^4 - p^5 + 18pq - 4p^2q - 4p^3q + 4p^4q - 4p^2q^2 + 6p^3q^2 + 4p^2q^3$ for $q \geq p+1$ and p is odd.

3 The Schultz molecular topological index of zig-zag nanotubes

Let $G = TUHC_6[p,q]$ be the zig-zag polyhex nanotube with $2p$ vertices at each level and q levels (see Figure 2). Then the Wiener index of G was given in [14]:

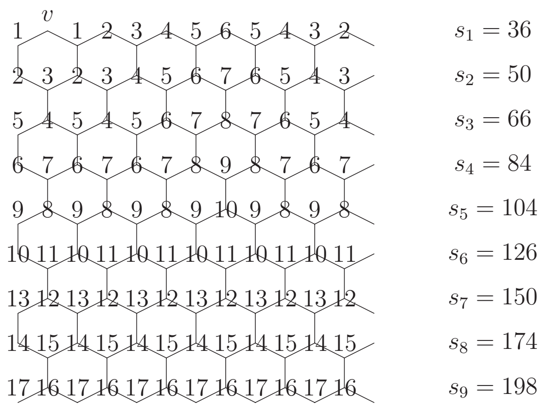


Figure 2. The zig-zag polyhex nanotube $TUHC_6[6,9]$.

Lemma 3([14]).
(i)$W(G) = \frac{1}{6}pq[q^3 + 4pq^2 + 6p^2q - q - 4p]$ for $q \le p$ (i.e., short tubes);
(ii)$W(G) = \frac{1}{6}p^2[8q^3 + 4p^2q - 6q - p^3 + p]$ for $q \ge p$ (i.e., long tubes).

As in the section two, we derive a formula for calculating the Schultz molecular topological index of the zig-zag polyhex nanotube $TUHC_6[p,q]$.

Note that the numbers of vertices with degree 2 and 3 in the graph $G = TUHC_6[p,q]$ are $4p$ and $2p(q-2)$, respectively. The equation (1) can be further expressed as:

$$MTI(G) = \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i D_i = 6W(G) + 18pq - 20p - W_2(G) \qquad (4)$$

Let $s_k = \sum_{x \text{ is at level } k} D_{vx}$ be the sum of distances from v to all other vertices at level k, where v is a vertex of degree 2 at level 1 (see Figure 2). By the symmetry of G,

$$W_2(G) = 4p \sum_{k=1}^{q} s_k.$$

In addition,

$$\begin{cases} s_1 = p^2; \\ s_k = s_{k-1} + 2(p+k-1), & 2 \le k \le p; \\ s_k = s_p + 4p(k-p), & p \le k \le q. \end{cases}$$

Therefore,

$$W_2(G) = \begin{cases} -\frac{4}{3}pq - 4p^2q + 4p^3q + 4p^2q^2 + \frac{4}{3}pq^3, & q \le p; \\ -\frac{4}{3}p^2 + \frac{4}{3}p^4 - 4p^2q + 8p^2q^2, & q \ge p+1. \end{cases}$$

Combining the equation (4) and Lemma 3, we have

Theorem 4. The Schultz molecular topological index of the zig-zag polyhex nanotube $TUHC_6[p,q]$ is
(i)$-20p + \frac{58}{3}pq - 4p^3q - pq^2 - 4p^2q^2 + 6p^3q^2 - \frac{4}{3}pq^3 + 4p^2q^3 + pq^4$ for $q \le p$;
(ii)$-20p + \frac{4}{3}p^2 + p^3 - \frac{4}{3}p^4 - p^5 + 18pq - 2p^2q + 4p^4q - 8p^2q^2 + 8p^2q^3$ for $q \ge p+1$.

Conclusions

Using the summation of the sum of distances between a vertex with degree 2 and all other vertices, formulas for calculating the Schultz molecular topological index in armchair polyhex nanotubes and zig-zag nanotubes are given.

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