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The Wiener and Schultz index of nanotubes covered by C_4

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Abstract

Formulas for calculating the Wiener index and Schultz index in nanotubes covered by C_4 are provided in this report.

1 Introduction

The information on the chemical constitution of molecule is conventionally represented by a molecular graph. In addition, graph theory was successfully provided the chemist with a variety of very useful tools, namely, topological index. Numbers reflecting certain structural features of organic molecules that are obtained from the molecular graph are usually called graph invariants or more commonly topological indices. The oldest and most thoroughly examined use of a topological index in chemistry was by Wiener [1] in the study of paraffin boiling points,and the topological index was called Wiener index or Wiener number. The conventional generalization of W for an arbitrary molecular graph

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is due to Hosoya [2]. 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 (or $d(i)$) 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. Then the Wiener index of the graph G, is equals to the sum of distances between all pairs of vertices of the respective molecular graph, i.e.,

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

The Schultz molecular topological index of a (chemical) graph G introduced by Schultz [3] in 1989 was a graph-theoretical descriptor for characterizing alkanes by an integer. He named this descriptor the molecular topological index and denoted it by MTI. Later, MTI became much better known under the name the *Schultz index*, defined as

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

where n is the number of vertices of G, A is the $n \times n$ adjacency matrix [3] of G and A_{ij} is the (i,j)-th entry of the adjacent matrix A. $d = (d_1, d_2, \cdots, d_n)$ is the $1 \times n$ vector of the degrees of the vertices of the molecular graph G. While Schultz in his initial paper only described MTI, von Knop and his group [4] gave the mathematical formulation of MTI in the same year (1989).

Let $D_i = \sum_{j=1}^{n} D_{ij}$ be the sum of distances between vertex i and all other vertices. Therefore, we can simplify the Schultz index in the following way.

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

which holds for all molecular graphs.

It has been demonstrated that MTI and W are closely mutually related for certain classes of molecular graphs [6-11]. Klein *et al* derived an explicit relation between MTI and W for trees [5]:

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

A. A. Dobrynin *et al* [6] get the explicit relation between the Wiener index and the Schultz index of Catacondensed Benzenoid graphs:

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

where G is an arbitrary catacondensed benzenoid graphs with h hexagons. A. A. Dobrynin *et al* [7] showed that the Schultz index has the same discriminating power with

the Wiener index, i.e., MTI(G_1)=MTI(G_2) if and only if W(G_1)=W(G_2) for an arbitrary catacondensed benzenoid graph pair.

Single walled carbon nanotubes as all-carbon molecules of tubular form exemplify modern nanometre scale material structures, where the number of atoms range from less than a million up to few millions. Such system are quite ideal for computational studies like Molecular Dynamics simulations because the studies can be done at the realistic limit, rendering them in a predictive way. This point of view we try to explore through simulations of novel ring-like carbon nanotubes, observed experimentally. Carbon nanotubes were discovered in 1992 by Iijima [11] as multi-walled structures. Two years later, two groups independently discovered the single-walled carbon nanotubes [12,13]. In 1996, Smalley's group synthesized the aligned single-wall nanotubes [14]. As pointed out by Smalley, a carbon nanotube is a carbon molecule with almost alien property of electrical conductivity and super-steel strength. It is expected that carbon nanotubes can be widely used in many fields. Nanotubes and fullerenes are promising candidates in the development of nanodevices and super-strong composites. They have aroused both theoretical and experimental interests either. The Wiener index of several nanotubes have been calculated [15–18]. In addition, in References [19–22] the formulas for computing the PI index of polyhex nanotubes were derived. In the present report, we shall get an explicit formula for computing the Wiener index and the Schultz index of nanotubes covered by C_4.

2 The Wiener index of nanotubes $TUC_4[p, q]$

In the following, our notation for nanotubes covered by C_4 will be denote by $G = TUC_4[p, q]$ (see figure 1). Let us denoted by p, q the number of squares at level 1 and the level number in the tube, respectively. *i.e*, the various levels (i.e. the length) of the tube.

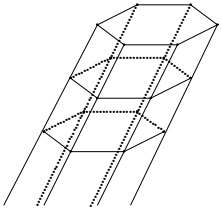

Figure 1. $TUC_4(6, q)$, a nanotube covered by C_4.

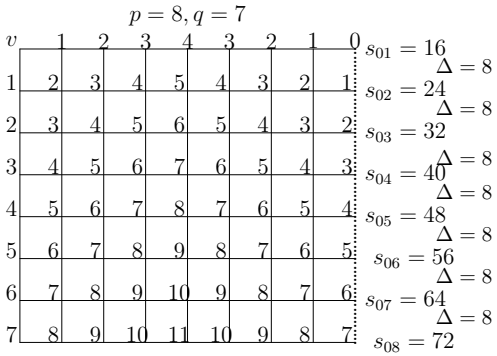

Figure 2. The distance sum from the vertex v to all other vertices

The sum from a vertex v lying at level 1 to all other vertices on the same level 1 is given by:

$$s_{1p} = \frac{p^2}{4} - \frac{1-(-1)^p}{8}. \tag{3}$$

Then the total distance from all vertices lying at level 1 to all other vertices is given by:

$$s_1(p) = \frac{p(q+1)[2p^2+4pq+(-1)^p-1]}{8} \tag{4}$$

The total distance from all vertices lying at level 2 to all other vertices is given by:

$$s_2(p) = \frac{p(q+1)[2p^2+4pq+(-1)^p-1]}{8} - p^2(q-1). \tag{5}$$

The total distance from all vertices lying at level i ($i \le \frac{q}{2}$ for i is even, and $i \le \frac{q+1}{2}$ for i is odd) to all other vertices is given by:

$$s_i(p) = \frac{p(q+1)[2p^2+4pq+(-1)^p-1]}{8} - p^2(i-1)(q+1-i). \tag{6}$$

By the symmetry of nanotubes, the total distance sums to all vertices can be divided into two cases:

Case 1. q is even.

From figure 2, we know $s_i = s_{q+2-i} (i = 1, 2, \cdots, \frac{q}{2})$. Now, the total distances in tube between vertices is given by:

$$\begin{aligned} st_1(p,q) &= 2\sum_{i=1}^{\frac{q}{2}}[s_1 - p^2(i-1)(q+1-i)] + s_{\frac{q}{2}+1} \\ &= \tfrac{p}{24}[6p^2q^2 + 8pq^3 + 12p^2q + 24pq^2 + 3(q+1)^2(-1)^p \\ &\quad +6p^2 - 3q^2 + 16pq - 6q - 3]. \end{aligned}$$

Case 2. q is odd.

From figure 2, we know $s_i = s_{q+2-i} (i = 1, 2, \cdots, \frac{q+1}{2})$. Now, the total distances in tube between vertices is given by:

$$\begin{aligned} st_2(p,q) &= 2\sum_{i=1}^{\frac{q+1}{2}}[s_1 - p^2(i-1)(q+1-i)] \\ &= \tfrac{p}{24}[6p^2q^2 + 8pq^3 + 12p^2q + 24pq^2 + 3(q+1)^2(-1)^p \\ &\quad +6p^2 - 3q^2 + 16pq - 6q - 3]. \end{aligned}$$

From two cases two, we get the total distances are the same when q is even or odd. Note that $W(G) = \sum\limits_{(i,j)} D_{i,j} = \frac{1}{2}\sum\limits_{i=1}^{n}\sum\limits_{j=1}^{n} D_{ij}$. Therefore, the Wiener index of nonatubes covered by C_4 is:

$$W(G) = \frac{p}{48}[6p^2q^2 + 8pq^3 + 12p^2q + 24pq^2 + 3(q+1)^2(-1)^p + 6p^2 - 3q^2 + 16pq - 6q - 3].$$

Theorem 1 *(i)*$W(G) = \frac{p}{48}[6p^2q^2 + 8pq^3 + 12p^2q + 24pq^2 + 3(q+1)^2 + 6p^2 + 16pq]$ *if p is even;*

(ii)$W(G) = \frac{p}{48}[6p^2q^2 + 8pq^3 + 12p^2q + 24pq^2 + 6p^2 - 6q^2 + 16pq - 12q - 6]$ *if p is odd.*

3 The Schultz index of nanotubes $TUC_4[p,q]$

Let $G = TUC_4[p,q]$ be the nanotubes covered by C_4 defined as above. In view of the fact that $TUC_4[p,q]$ have only degree three and degree four vertices, the Wiener index may be decomposed into two parts: $2W(G) = W_3(G) + W_4(G)$, where $W_3(G) = \sum\limits_{i,d_i=3} D_i$ and $W_4(G) = \sum\limits_{i,d_i=4} D_i$. The summation $\sum\limits_{d_i=k}$ goes over all vertices of G with degree k.

Note that the number of vertices with degree 3 and 4 in the graph $G = TUC_4[p,q]$ are $2p$, $p(q-1)$ respectively. The equation (2) can be further expressed as:

$$\begin{aligned} MTI &= \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i D_i \\ &= 9\times 2p + 16\times p(q-1) + 8W - \sum_{i,d_i=3} D_i \\ &= 16pq + 2p + 8W - \sum_{i,d_i=3} D_i. \end{aligned}$$

Let $s_k = \sum\limits_{x \text{ is at level } k} D_{vx}$ be the sum of distances from v to all other vertices at level k, where v is a vertex of degree 3 at level 1 (see Figure 2). By the symmetry of G,

$$W_3(G) = 2p\sum_{i=1}^{q} s_k.$$

From (4) we know that

$$p\sum_{i=1}^{q} s_k = \frac{p(q+1)[2p^2 + 4pq + (-1)^p - 1]}{8}.$$

Therefore,

$$\begin{aligned} W_3(G) &= 2\times \tfrac{p(q+1)[2p^2+4pq+(-1)^p-1]}{8} \\ &= \tfrac{p(q+1)[2p^2+4pq+(-1)^p-1]}{4}. \end{aligned}$$

Lemma 2 *(i)* $W_3(G) = \frac{p(q+1)(p^2+2pq)}{2}$ *if* p *is even;*
(ii) $W_3(G) = \frac{p(q+1)(p^2+2pq-1)}{2}$ *if* p *is odd.*

Now, we are ready to calculate the Schultz index of $G = TUC_4[p, q]$. By combining Theorem 1 and Lemma 2, we get

Theorem 3 *Let* $G = TUC_4[p, q]$ *be the nanotubes covered by* C_4*. Then the Schultz index of* G *is*
(i) $\frac{p}{6}[6p^2q^2 + 8pq^3 + 9p^2q + 18pq^2 + 3p^2 + 10pq + 90q + 12]$ *if* p *is even;*
(ii) $\frac{p}{6}[6p^2q^2 + 8pq^3 + 9p^2q + 18pq^2 + 3p^2 - 6q^2 + 10pq + 87q + 15]$ *if* p *is odd.*

The relationship between the Wiener index and the Schultz index has been explicated for several family of graphs. In this report, the Wiener index and the Schultz index are calculated by using the relationship between Wiener and Schultz index of nanotubes covered by C_4. In fact, we can utilize this relationship to calculate the Wiener and Schultz index for more graphs.

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