Int. J. Mol. Sci. **2008**, *9*, 2016-2026; DOI: 10.3390/ijms9102016

OPEN ACCESS

International Journal of Molecular Sciences
ISSN 1422-0067
www.mdpi.com/journal/ijms

Article

Schultz Index of Armchair Polyhex Nanotubes

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Received: 3 July 2008; in revised form: 23 August 2008 / Accepted: 14 October 2008 / Published: 29 October 2008

Abstract: The study of topological indices – graph invariants that can be used for describing and predicting physicochemical or pharmacological properties of organic compounds – is currently one of the most active research fields in chemical graph theory. In this paper we study the Schultz index and find a relation with the Wiener index of the armchair polyhex nanotubes $TUVC_6[2p, q]$. An exact expression for Schultz index of this molecule is also found.

Keywords: Topological index; Wiener index; Schultz index; Armchair nanotube; Molecular graph; Distance; Carbon Nanotube.

1. Introduction

Topological indices are a convenient method of translating chemical constitution into numerical values that can be used for correlations with physical, chemical or biological properties. This method has been introduced by Harold Wiener as a descriptor for explaining the boiling points of paraffins [1–3]. If $d(u, v)$ is the distance of the vertices u and v of the undirected connected graph G (*i.e.*, the number of edges in the shortest path that connects u and v) and $V(G)$ is the vertex set of G, then the Wiener index of G is the half sum of distances over all its vertex pairs (u, v):

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

A unified approach to the Wiener topological index and its various recent modifications is presented. Among these modifications particular attention is paid to the Hyper-Wiener, Harary, Szeged, Cluj and

Schultz indices as well as their numerous variants and generalizations [4–10]. The Schultz index of the graph G was introduced by Schultz [14] in 1989 and is defined as follows:

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

where $\deg(u)$ is the degree of the vertex u.
The main chemical applications and mathematical properties of this index were established in a series of studies [12–15]. Also a comparative study of molecular descriptors showed that the Schultz index and Wiener index are mutually related [16–18].
Carbon nanotubes, the one-dimensional carbon allotropes, are intensively studied with respect to their promise to exhibit unique physical properties: mechanical, optical electronic etc. [19–21]. In [19], Diudea *et al.* obtained the Wiener index of $TUVC_6[2p, q]$, the armchair polyhex nanotube (see Figure 1). Here we find a relation between the Schultz index and Wiener index of this molecule. By using this relation we find an exact expression for the Schultz index of the same. The Appendix includes a Maple program [22] to produce the graph of $TUVC_6[2p, q]$, and to compute the Schultz index of the graph.

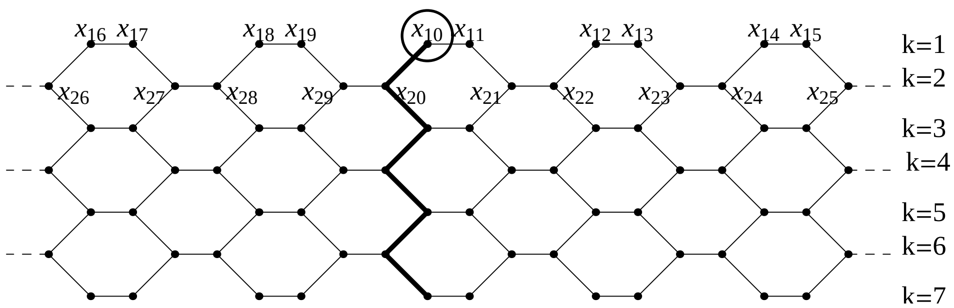
2. Schultz index of armchair polyhex nanotubes

Throughout this paper $G := TUVC_6[2p, q]$ denotes an arbitrary armchair polyhex nanotube in terms of its circumference $2p$ and their length q, see Figure 2. At first we consider an armchair lattice and choose a coordinate label for it, as illustrated in Figure 2. The distance of a vertex u of G is defined as

$$d(u) = \sum_{x \in V(G)} d(u, x),$$

the summation of distances between v and all vertices of G. By considering this notation the following lemma gives us a relation between the Schultz and Wiener index of G.

Figure 1. A $TUVC_6[2p, q]$ Lattice with $p = 5$ and $q = 7$.



Lemma 1. For the graph $G = TUVC_6[2p, q]$ we have

$$S(G) = 6W(G) - 2 \sum_{u \in level\ 1} d(u).$$

Figure 2. An armchair polyhex nanotube [19].

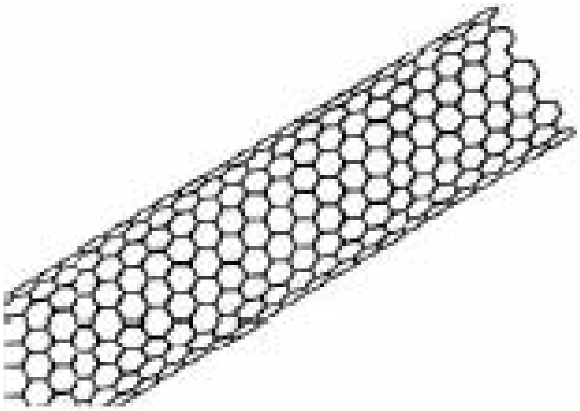
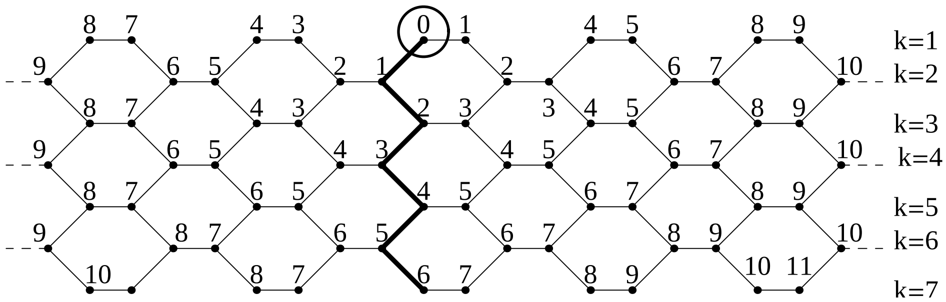


Figure 3. Distances from x_{01} to all vertices of $TUVC_6[2p, q]$ with $p = 5$ and $q = 7$.



Proof: For each k such that $1 \leq k \leq q$ put $A_k := \{u \in V(G) \mid u \in \ level\ k\}$(see Figure 2). Then

$$\begin{aligned}
S(G) &= \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}(\deg(u)+\deg(v))d(u,v)\\
&= \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}\deg(u)d(u,v)+\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}\deg(v)d(u,v)\\
&= \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}\deg(u)d(u,v)+\frac{1}{2}\sum_{v\in V(G)}\sum_{u\in V(G)}\deg(v)d(u,v)\\
&= \frac{1}{2}\sum_{u\in V(G)}\deg(u)\sum_{v\in V(G)}d(u,v)+\frac{1}{2}\sum_{v\in V(G)}\deg(v)\sum_{u\in V(G)}d(u,v)\\
&= \frac{1}{2}\sum_{u\in V(G)}\deg(u)d(u)+\frac{1}{2}\sum_{v\in V(G)}\deg(v)d(v)\\
&= \sum_{u\in V(G)}\deg(u)d(u)
\end{aligned}$$

But

$$\deg(u) \;=\; \begin{cases} 2 & \text{if} \;\; u \in A_1 \cup A_q \\ \\ 3 & \text{if} \;\; otherwise. \end{cases}$$

Also in the graph G it is clear that $\sum_{u\in A_1} d(u) = \sum_{u\in A_q} d(u)$. Therefore

$$\begin{aligned} S(G) &= \sum_{u\in V(G)} \deg(u)d(u) = \sum_{u\in A_1\cup A_q} \deg(u)d(u) + \sum_{u\in V(G)\setminus(A_1\cup A_q)} deg(u)d(u) \\ &= \sum_{u\in A_1\cup A_q} 2d(u) + \sum_{u\in V(G)\setminus(A_1\cup A_q)} 3d(u) \\ &= 3\sum_{u\in V(G)} d(u) - 2\sum_{u\in A_1} d(u) \\ &= \;6W(G) - 2\sum_{u\in A_1} d(u). \end{aligned}$$

This completes the proof.

To compute the $d(u)$ in the graph G, when u is a vertex in level 1, we first prove the following lemma.

Lemma 2. The sum of distances of one vertex of level 1 to all vertices of level k is given by

$$\begin{aligned} w_k := \sum_{x\in \; level \; k} d(x_{10}, x) \;&=\; \sum_{x\in \; level \; k} d(x_{11}, x) \\ &\;\vdots \\ &=\; \begin{cases} 2p^2 + k^2 - 2k - 2p + 1 + H(p,k) & \text{if} \;\; 1 \le k < p \\ \\ p(p + 2k - 2) & \text{if} \;\; k \ge p, \end{cases} \end{aligned}$$

where

$$H(p,k) = \begin{cases} 2p - 1 & \text{if} \;\; k + p \;\; \text{is even} \\ \\ 2p & \text{if} \;\; k + p \;\; \text{is odd.} \end{cases}$$

Proof: We calculate the value of w_k. We consider that the tube can be built up from two halves collapsing at the polygon line joining x_{10} to $x_{q,0}$ (see Figure 2). The right part is the graph G_1 which consists of vertical polygon lines $0, 1, \ldots, p$ and x_{10} is one of the vertices in the first row of the graph G_1. The left part is the graph G_2 which consists of vertical polygon lines $(p+1), (p+2), \ldots, 2p-1$. We change the indices of the vertices of G_2 in the following way:

$$V(G_2) = \{\hat{x}_{ji} \mid \hat{x}_{j,i} = x_{j,2p-i} \in V(G)\}$$

(See Figure 3)

We must consider two cases:

Case 1: If $\;k \ge p$. In the graphs G_1 and for $0 \le \; i < k$ we have

$$d(x_{10}, x_{k,i}) = k + i - 1.$$

Also in the graphs G_2 and for $1 \leq \ i < k$ we have

$$d(x_{10}, \hat{x}_{k,i}) = k + i - 1.$$

So

$$\sum_{x \in \ level \ k} d(x_{10}, x) = 2\sum_{i=1}^{p-1}(k + i - 1) + (0 + k - 1) + (p + k - 1) = p(p + 2k - 2).$$

Case 2: If $k < p$. First suppose that $1 \leq \ i < k$. In the graphs G_1 and G_2 we have

$$d(x_{10}, x_{k,i}) = k + i - 1 = d(x_{10}, \hat{x}_{k,i}) = k + i - 1.$$

Now suppose that $k \leq \ i \leq p$. Then in the graph G_1 we can see that if k is odd, then

$$d(x_{10}, x_{k,i}) = \begin{cases} 2i & \text{if } \ i \ \text{ is even} \\ \\ 2i - 1 & \text{if } \ i \ \text{ is odd} \end{cases}$$

and if k is even, then

$$d(x_{10}, x_{k,i}) = \begin{cases} 2i - 1 & \text{if } \ i \ \text{ is even} \\ \\ 2i & \text{if } \ i \ \text{ is odd.} \end{cases}$$

Also in G_2 we have

$$d(x_{10}, \hat{x}_{k,i}) = \begin{cases} 2i & \text{if } \ i \ \text{ is even} \\ \\ 2i + 1 & \text{if } \ i \ \text{ is odd} \end{cases}$$

if k is odd and

$$d(x_{10}, \hat{x}_{k,i}) = \begin{cases} 2i + 1 & \text{if } \ i \ \text{ is even} \\ \\ 2i & \text{if } \ i \ \text{ is odd} \end{cases}$$

if k is even.
All of this distances give us

$$\sum_{x \in \ level \ k} d(x_{10}, x) = 2p^2 + k^2 - 2k - 2p + 1 + H(p, k).$$

For other vertices we can convert those to x_{10} by changing transfer vertices and apply a similar argument by choosing suitable G_1 and G_2 and compute w_k.

By a straightforward computation (if irem means the positive integer remainder) we can see:

$$\begin{aligned} H(p, k) &= 2p - 1 + \mathrm{irem(k + p, 2)} \\ &= 2p - 1 + \frac{1}{2} + \frac{1}{2}(-1)^{k - \mathrm{irem(p,2)} + 1}, \end{aligned}$$

where

$$\text{irem}(\text{p}, 2) = \begin{cases} 0 & \text{if } \ p \ \text{ is even} \\ \\ 1 & \text{if } \ p \ \text{ is odd.} \end{cases}$$

So, by Lemma 1, when $1 \le k \le p$, we have

$$w_k \;=\; 2p^2 + k^2 - 2k + \frac{1}{2} + \frac{1}{2}(-1)^{k-\text{irem}(\text{p},2)+1}. \tag{1}$$

Also in the graph G,

$$\begin{aligned} d(x_{10}) &= \sum_{x \in level\ 0} d(x_{10}, x) + \sum_{x \in level\ 1} d(x_{10}, x) + \cdots + \sum_{x \in level\ q} d(x_{10}, x) \\ &= w_1 + w_2 + \cdots + w_q. \end{aligned}$$

So

$$d(x_{10}) = d(x_{11}) = \cdots = d(x_{2p-1,1}) = w_1 + w_2 + \cdots + w_q.$$

This leads us to the following corollary:

Corollary 1. For each vertex u on level 1 we have

$$d(u) = w_1 + w_2 + \cdots + w_q.$$

Now suppose that $p > q$. Then by lemma 2 and equation (1) we have

$$\begin{aligned} d(u) &= \sum_{k=1}^{q} \left(2p^2 + k^2 - 2k + \frac{1}{2} + \frac{1}{2}(-1)^{k-\text{irem}(\text{p},2)+1} \right) \\ &= 2p^2q + \frac{q^3}{3} - \frac{q^2}{2} - \frac{q}{3} + \frac{1}{4}(-1)^{-irem(p,2)+1+q} + \frac{1}{4}(-1)^{-irem(p,2)}. \end{aligned}$$

Also if $p \le q$, then by Lemma 1 and equation (1) we have

$$\begin{aligned} d(u) &= w_1 + w_2 + \cdots + w_{p-1} + w_p + w_{p+1} + \cdots + w_q \\ &= \sum_{k=1}^{p-1} \left(2p^2 + k^2 - 2k + \frac{1}{2} + \frac{1}{2}(-1)^{k-\text{irem}(\text{p},2)+1} \right) + \\ &\qquad \sum_{k=p}^{q} p(p + 2k - 2) \\ &= \frac{p^3}{3} + \frac{p^2}{2} - \frac{p}{3} - \frac{1}{4}(-1)^{-irem(p,2)+1+p} - \frac{1}{2} - \frac{1}{4}(-1)^{-irem(p,2)+1} + p^2q - pq + pq^2 \end{aligned}$$

We summarize the above results in the following proposition

Corollary 2. For each vertex u on level 1, $d(u)$ is given by

Case 1: p is even

$$d(u) = \begin{cases} 2p^2q + \frac{q^3}{3} - \frac{q^2}{2} - \frac{q}{3} + \frac{1}{4} + \frac{1}{4}(-1)^{q+1} & \text{if } \ p > q \\ \\ \frac{p}{6}[2p^2 + 3p - 2 + 6pq - 6q + 6q^2] & \text{if } \ p \le q \end{cases}$$

Case 2: p is odd

$$d(u) = \begin{cases} 2p^2q + \frac{q^3}{3} - \frac{q^2}{2} - \frac{q}{3} - \frac{1}{4} + \frac{1}{4}(-1)^q & \text{if } \ p > q \\ \\ \frac{p^3}{3} + \frac{p^2}{2} - \frac{p}{3} - \frac{1}{2} + p^2q - pq + pq^2 & \text{if } \ p \leq q \end{cases}$$

Theorem 1. The Wiener index of $G := TUVC_6[2p, q]$ nanotubes is given by

Case 1: p is even

$$W(G) = \begin{cases} \frac{p}{12}[3(-1)^{q+1} + 3 + 24q^2p^2 - 8q^2 + 2q^4] & \text{if } \ p > q \\ \\ \frac{-p^2}{6}[8q - 4p + p^3 - 4qp^2 - 4q^3 - 6q^2p] & \text{if } \ p \leq q \end{cases}$$

Case 2: p is odd

$$W(G) = \begin{cases} \frac{p}{12}[3(-1)^{q} - 3 + 24q^2p^2 - 8q^2 + 2q^4] & \text{if } \ p > q \\ \\ \frac{-p}{6}[-4p^3q - 4pq^3 - 6q^2p^2 + 3 + 8qp - 4p^2 + p^4] & \text{if } \ p \leq q \end{cases}$$

Proof: See [19].

Now we are in the position to prove the main result of this section.

Theorem 2. The Schultz index of $G := TUVC_6[2p, q]$ nanotubes is given by

Case 1: p is even

$$S(G) = \begin{cases} \frac{p}{6}[-48p^2q + 72p^2q^2 + 3(-1)^{q+1} + 3 - 8q^3 - 12q^2 + 6q^4 + 8q] & \text{if } \ p > q \\ \\ \frac{-p^2}{3}[-18q^2p + 3p^3 - 6p - 12p^2q - 12q^3 + 12q + 4p^2 - 4 + 12pq + 12q^2] & \text{if } \ p \leq q \end{cases}$$

Case 2: p is odd

$$S(G) = \begin{cases} \frac{p}{6}[72q^2p^2 + 6q^4 - 12q^2 - 3 + 3(-1)^q - 48p^2q - 8q^3 + 8q] & \text{if } \ p > q \\ \\ \frac{-p}{3}[-12p^3q - 12pq^3 - 18p^2q^2 + 3 + 12pq - 6p^2 + 3p^4 + \\ \quad 4p^3 - 4p + 12p^2q + 12pq^2] & \text{if } \ p \leq q \end{cases}$$

Proof: According to Lemma 1 we must calculate $6W(G) - \sum_{u \in level\ 1} d(u)$. But by corollary 1 we have

$$d(u) = w_1 + w_2 + \cdots + w_q.$$

Since there are $2p$ vertices on level 1 therefore

$$S(G) \quad = \quad 6W(G) - 4pd(u) \tag{2}$$

Finally by replacing $d(u)$ from corollary 1 in the equation (2) the result obtains.

Table 1. Schultz index of short tubes, $p > q$.

p	q	$S(G)$	p	q	$S(G)$
6	2	6912	5	2	4000
6	3	18366	5	3	10650
6	4	35424	5	4	20720
6	5	58656	9	5	193266
10	2	32000	9	6	288432
10	5	264160	9	7	404514
10	6	393440	9	8	542880
10	7	550560	15	8	2425440
10	8	736960	15	7	1823310
10	9	954400	15	6	1310160

Table 2. Schultz index of long tubes, $p \leq q$.

p	q	$S(G)$	p	q	$S(G)$
4	4	10816	3	4	4752
4	5	18304	3	5	8262
4	6	28352	3	6	13104
4	7	41344	3	7	19494
4	8	57664	3	8	27648
10	21	6810400	11	11	1954502
10	22	7641600	11	12	2371952
10	23	8536800	11	13	2839524
10	24	9498400	11	14	3359312
10	25	10528800	11	15	3935030

3. Experimental Section

Tables 1 and 2 show the numerical data for the Schultz index in tubes $TUVC_6[2p, q]$ of various dimensions.

Acknowledgements

This work was supported by a grant from the Center of Research of Islamic Azad University, Najafabad Branch, Isfahan, Iran.

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4. Appendix

The following code is the MAPLE program [22] used to produce the graph of $TUHC_6[2p, q]$ and to compute the Schultz index of the graph.

```
> restart;with(networks):
> l:=proc(p,q) (*generating the graph *)
 local G,i,j,k,ff,cc;G:=new();
  for i from 0 to (2*p-1) do
          for j from 1 to q do
          addvertex(a[i,j],G);
          end do;
  end do;
  for i from 0 to (2*p-1) do
          for j from 1 to (q-1) do
            addedge ({a[i,j],a[i,j+1]},G);
          end do;
  end do;
         for i from 0 to (2*p-2)/2 do
                   for k from 1 to iquo(q,2) do
                         addedge({a[2*i,2*k-1],a[2*i+1,2*k-1]},G);
                   end do;
              end do;
     for i from 0 to (2*p-4)/2 do
             for k from 1 to iquo(q,2) do
                   addedge({a[2*i+1,2*k],a[2*i+2,2*k]},G);
             end do;
     end do;
 for ff from 1 to iquo(q,2) do
 addedge({a[2*p-1,2*ff],a[0,2*ff]},G);
 end do;
 if irem(q,2)=1 then
 for cc from 0 to 2*p/2-1 do
 addedge({a[2*cc,q],a[2*cc+1,q]},G);end do;
 end if ;return(G);
 end proc:
```

```
> m:=l(3,8):(#Graph G:=TUVC_6[2*3,8]#)
> t :=edges(m):
> ii:=vertices(m):
> T := allpairs(m,p):
> Sch:=proc(u)
  local b,o,pp;
  b:=0;
 for o in ii do
   for pp in ii do
       b:=b+ T[(pp,o)]*(vdegree(o,m)+vdegree(pp,m));
   end do;
 end do;
 return(b/2);
 end proc:
> Sch(u); 27648(#The Schultz index of the graph #)
```