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 $TUV C_6[2p, q]$, 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 $TUV C_6[2p, q]$, and to compute the Schultz index of the graph.

2. Schultz index of armchair polyhex nanotubes

Throughout this paper $G := TUV C_6[2p, q]$ 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 $TUV C_6[2p, q]$ Lattice with $p = 5$ and $q = 7$.

**Lemma 1.** For the graph $G = TUV C_6[2p, q]$ we have

$$S(G) = 6W(G) - 2 \sum_{u \in \text{level 1}} d(u).$$
Figure 2. An armchair polyhex nanotube [19].

Figure 3. Distances from \( x_{01} \) to all vertices of \( TUV C_6[2p, q] \) with \( p = 5 \) and \( q = 7 \).

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

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

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

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

\[
= \frac{1}{2} \sum_{u \in V(G)} \deg(u)d(u) + \frac{1}{2} \sum_{v \in V(G)} \deg(v)d(v)
\]

\[
= \sum_{u \in V(G)} \deg(u)d(u)
\]
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
\[
S(G) = \sum_{u \in V(G)} \deg(u)d(u) = \sum_{u \in A_1 \cup A_q} \deg(u)d(u) + \sum_{u \in (A_1 \cup A_q)^c} \deg(u)d(u)
\]
\[
= \sum_{u \in A_1 \cup A_q} 2d(u) + \sum_{u \in (A_1 \cup A_q)^c} 3d(u)
\]
\[
= 3 \sum_{u \in V(G)} d(u) - 2 \sum_{u \in A_1} d(u)
\]
\[
= 6W(G) - 2 \sum_{u \in A_1} d(u).
\]

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
\[
w_k := \sum_{x \in \text{level } k} d(x_{10}, x) = \sum_{x \in \text{level } k} d(x_{11}, x)
\]
\[
\vdots
\]
\[
= \begin{cases} 
2p^2 + k^2 - 2k - 2p + 1 + H(p, k) & \text{if } 1 \leq k < p \\
p(p + 2k - 2) & \text{if } k \geq p,
\end{cases}
\]

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:
\[
V(G_2) = \{ \hat{x}_{ji} : \hat{x}_{j,i} = x_{j,2p-i} \in V(G) \}
\]
(See Figure 3)

We must consider two cases:

**Case 1:** If \(k \geq p\). In the graphs \(G_1\) and for \(0 \leq i < k\) 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
\[
\sum_{x \in \text{level } k} d(x_{10}, x) = 2 \sum_{i=1}^{p-1} (k + i - 1) + (0 + k - 1) + (p + k - 1) = p(p + 2k - 2).
\]

**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 these distances give us
\[
\sum_{x \in \text{level } k} d(x_{10}, x) = 2p^2 + k^2 - 2k - 2p + 1 + H(p, k).
\]

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:
\[
H(p, k) = 2p - 1 + \text{irem}(k + p, 2)
= 2p - 1 + \frac{1}{2} + \frac{1}{2}(-1)^{k - \text{irem}(p, 2) + 1},
\]
where
\[
\text{irem}(p, 2) = \begin{cases} 
0 & \text{if } p \text{ is even} \\
1 & \text{if } p \text{ is odd.}
\end{cases}
\]

So, by Lemma 1, when \(1 \leq k \leq p\), we have
\[
w_k = 2p^2 + k^2 - 2k + \frac{1}{2} + \frac{1}{2}(-1)^{k-\text{irem}(p,2)+1}.
\]  

(1)

Also in the graph \(G\),
\[
d(x_{10}) = \sum_{x \in \text{level } 0} d(x_{10}, x) + \sum_{x \in \text{level } 1} d(x_{10}, x) + \cdots + \sum_{x \in \text{level } q} d(x_{10}, x) = w_1 + w_2 + \cdots + w_q.
\]

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
\[
d(u) = \sum_{k=1}^{q} \left(2p^2 + k^2 - 2k + \frac{1}{2} + \frac{1}{2}(-1)^{k-\text{irem}(p,2)+1}\right) = 2p^2q + \frac{q^3}{3} - \frac{q^2}{2} - \frac{q}{3} + \frac{1}{4}(-1)^{\text{irem}(p,2)+1+q} + \frac{1}{4}(-1)^{\text{irem}(p,2)}.
\]

Also if \(p \leq q\), then by Lemma 1 and equation (1) we have
\[
d(u) = w_1 + w_2 + \cdots + w_{p-1} + w_p + w_{p+1} + \cdots + w_q
\]
\[
= \sum_{k=p}^{p-1} \left(2p^2 + k^2 - 2k + \frac{1}{2} + \frac{1}{2}(-1)^{k-\text{irem}(p,2)+1}\right) + \sum_{k=p}^{q} p(p + 2k - 2)
\]
\[
= \frac{p^3}{3} + \frac{p^2}{2} - \frac{p}{3} - \frac{1}{4}(-1)^{\text{irem}(p,2)+1+p} - \frac{1}{2} - \frac{1}{4}(-1)^{\text{irem}(p,2)+1} + p^2q - pq + pq^2
\]

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
\[
d(u) = \begin{cases} 
2p^2q + \frac{q^3}{3} - \frac{q^2}{2} - \frac{q}{3} + \frac{1}{4}(-1)^{q+1} & \text{if } p > q \\
\frac{q}{8}[2p^2 + 3p - 2 + 6pq - 6q + 6q^2] & \text{if } p \leq q
\end{cases}
\]
Case 2: $p$ is odd
\[
d(u) = \begin{cases} 
2p^2q + \frac{q^3}{3} - \frac{q^2}{2} - \frac{q}{4} + \frac{1}{4}(-1)^q & \text{if } p > q \\
\frac{q^3}{3} + \frac{p^2}{2} - \frac{p}{4} + p^2q - pq + pq^2 & \text{if } p \leq q
\end{cases}
\]

Theorem 1. The Wiener index of $G := TUV C_6[2p, q]$ nanotubes is given by

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

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

Proof: See [19].

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

Theorem 2. The Schultz index of $G := TUV C_6[2p, q]$ nanotubes is given by

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

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

Proof: According to Lemma 1 we must calculate $6W(G) - \sum_{u \in \text{level 1}} d(u)$. But by corollary 1 we have
\[
d(u) = w_1 + w_2 + \cdots + w_q.
\]

Since there are $2p$ vertices on level 1 therefore
\[
S(G) = 6W(G) - 4pd(u)
\]
(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.

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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.

```maple
> 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 #)