Wiener and Schultz Indices of $TUC_4C_8(S)$ Nanotubes

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Abstract
The Wiener index of a graph $G$ is defined as $W(G) = \frac{1}{2} \sum_{\{i,j\}\subseteq V(G)} d(i,j)$, where $V(G)$ is the set of all vertices of $G$ and for $i,j \in V(G)$, $d(i,j)$ is the minimum distance between $i$ and $j$. The Schultz index of $G$ is defined by $MTI(G) = \sum_{\{i,j\}\subseteq V(G)} v(i)(d(i,j) + A(i,j))$, where for $v(i)$ is the vertex degree of $i$ and $A_{ij}$ is the $(i,j)$ entry of adjacency matrix of $G$. Stefu and Diudea (see Monica Stefu and Mircea V. Diudea, MATCH Commun. Math. Comput. Chem. 50 (2004) 133-144) computed the Wiener index of $TUC_4C_8(S)$ nanotubes. In this paper we use a new method to compute the Wiener index of these nanotubes. As a corollary of this method we also compute the Schultz (Molecular topological) index of $TUC_4C_8(S)$.

1. Introduction

A topological index is a real number related to a structural graph of a molecule. It does not depend on the labelling or pictorial representation of a graph. Wiener index is one of the most studied topological indices and is connected to the problem of distances in graph. Harold Wiener [3] in 1947 introduced the notion of path number of a graph as the sum of the distances between two carbon atoms in the molecules, in terms of carbo-carbon bound.
Let $G$ be a connected graph, the set of vertices and edges of will be denoted by $V(G)$ and $E(G)$, respectively. If $e$ is an edge of $G$ connecting the vertices $i$ and $j$ of $G$, then we write $e = ij$. The distance between a pair of vertices $i$ and $j$ of $G$ is denoted by $d(i, j)$. The degree of a vertex $i \in V(G)$ is the number of vertices joining to $i$ and denoted by $v(i)$. The $(i, j)$ entry of the adjacency matrix of $G$ is denoted by $A(i, j)$.

The Wiener index of the graph $G$ is the half sum of distances over all its vertex pairs $(i, j)$:

$$W(G) = \frac{1}{2} \sum_{i,j} d(i, j).$$

The distance of a vertex $u$ of $G$ is defined as

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

So we have

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

Another topological index is the molecular topological index or Schultz index, which is defined by

$$MTI(G) = \sum_{\{i,j\} \subseteq V(G)} v(i)(d(i, j) + A(i, j)).$$

The molecular topological index has been defined by Schultz [21] and studied in many papers, see for example [22]-[25].

Diudea and coauthors computed the Wiener index of some nanotubes (see for example [11]-[20]). Stefu and Diudea in [20] computed the Wiener index of $TUC_4C_8(S)$ nanotubes. In this paper we use a new method to compute the Wiener index of these nanotubes. As a corollary of this method we also compute the Schultz index of $TUC_4C_8(S)$.

### 2. Main results

In this section we derive an exact formula for the Wiener index of graph $T(p, q) := TUC_4C_8(S)$. Then we compute the Schultz index of $T(p, q)$, by using the Wiener index and some equations which obtained in computing the Wiener index. For this purpose first we choose a coordinate label for vertices of $T(p, q)$ as shown in Figure 1. In Appendix we include a MATHEMATICA [4] program to produce the graph of $T(p, q)$ and computing the Wiener and Schultz indices of the graph, using the definitions. If $q \leq p$ the graph of $T(p, q)$ is called short and if $q > p$, then the graph is called long. Let $a_{0p} \in \{x_{0p}, y_{0p}\}$ in first row of the graph. In Lemma 1 and Lemma 2, below we compute the subtraction of the summation of distances between $a_{0p}$ and $(k - 1)$th row of graph from the summation of the distances between $y_{0p}$ and $k$th row of the graph. In the following Lemma, referring to Figure 1, we prove that the subtraction of the summation of distances between $x_{0p}$ (in Figure 1 we have $p = 4$) and $(k - 1)$th row of graph from the summation of the distances between $y_{0p}$ and $k$th row of the graph is 4, if the vertices that are considered are below the black edges; and is 2, if the vertices are above the black edges. For example, as shown in Figure 1, $(d(x_{35}, x_{04}) + d(y_{35}, x_{04})) - (d(x_{25}, x_{04}) + d(y_{25}, x_{04})) = 4$. 


Lemma 1. Let $1 \leq k < q$, $0 \leq t < 2p$ and $R_x(k) = (d(x_{kt}, x_{0p}) + d(y_{kt}, x_{0p})) - (d(x_{k-1,t}, x_{0p}) + d(y_{k-1,t}, x_{0p}))$. If $p$ is an even integer then

$$R_x(k) = \begin{cases} 4 & \text{if } p - k + 1 \leq t \leq p + k \\ 2 & \text{otherwise.} \end{cases}$$

If $p$ is an odd integer then

$$R_x(k) = \begin{cases} 4 & \text{if } p - k \leq t \leq p + k - 1 \\ 2 & \text{otherwise.} \end{cases}$$

Proof: We prove the assertion when, $p$ is an even integer. If $p$ is an odd integer proof is similar. Suppose for $1 \leq k < q$, $p - k + 1 \leq t \leq p + k$, i.e. the vertices $x_{kt}$, $y_{kt}$, $x_{k-1,t}$, and $y_{k-1,t}$ are below the black edges (see Figure 1). A shortest path from $x_{kt}$ or $y_{kt}$ to $x_{0p}$ contain vertices $x_{k-1,t}$ and $y_{k-1,t}$. So if $k$ is an even integer, then

$$d(x_{kt}, x_{0p}) = d(x_{k-1,t}, x_{0p}) + 1 \quad \text{and} \quad d(y_{kt}, x_{0p}) = d(y_{k-1,t}, x_{0p}) + 3.$$  

If $k$ is an odd integer, then

$$d(x_{kt}, x_{0p}) = d(x_{k-1,t}, x_{0p}) + 3 \quad \text{and} \quad d(y_{kt}, x_{0p}) = d(y_{k-1,t}, x_{0p}) + 1.$$  

Therefore in any case $R_x(k) = 4$.

Figure 1: A $TUC_4C_8(S)$ Lattice with $p = 4$ and $q = 6$. 
Now suppose \( t > p + k \) or \( t < p - k + 1 \), i.e. the vertices \( x_{kt}, y_{kt}, x_{k-1,t} \) and \( y_{k-1,t} \) are above the black edges. Suppose that \( k \) is even. Then a shortest path from \( x_{k-1,t} \) and \( y_{k-1,t} \) to \( x_{0p} \), and also a shortest path from \( x_{kt} \) and \( y_{kt} \) to \( x_{0p} \), both contain vertex \( x_{k-1,t} \), if \( t \) is odd and contain \( x_{k-1,t+1} \), if \( t \) is even. So \( d(x_{kt}, x_{0p}) = d(y_{k-1,t}, x_{0p}) \) and \( d(y_{kt}, x_{0p}) = d(x_{k-1,t}, x_{0p}) + 2 \). Now let \( k \) be an odd integer. Then a shortest path from \( x_{k-1,t} \) and \( y_{k-1,t} \) to \( x_{0p} \) and also a shortest path from \( x_{kt} \) and \( y_{kt} \) to \( x_{0p} \), both contain vertex \( y_{k-1,t} \), if \( t \) is odd, and contain \( y_{k-1,t+1} \), if \( t \) is even. Therefore \( d(x_{k-1,t}, x_{0p}) = d(y_{kt}, x_{0p}) \) and \( d(y_{k-1,t}, x_{0p}) = d(x_{kt}, x_{0p}) + 2 \). Thus \( R_y(k) = 2 \). \( \square \)

As in Lemma 1, we can compute the subtraction of the summation of distances between \( y_{0p} \) and \( k \) th row of graph from the summation of the distances between \( y_{0p} \) and \( (k-1) \)th row of the graph.

**Lemma 2.** Let \( 2 \leq k < q \), \( 0 \leq t < 2p \) and \( R_y(k) = (d(x_{kt}, y_{0p}) + d(y_{kt}, y_{0p})) - (d(x_{k-1,t}, y_{0p}) + d(y_{k-1,t}, y_{0p})) \). If \( p \) is an even integer then

\[
R_y(k) = \begin{cases} 
4 & \text{if } p - k + 1 \leq t \leq p + k - 2 \\
2 & \text{otherwise.}
\end{cases}
\]

If \( p \) is an odd integer then

\[
R_y(k) = \begin{cases} 
4 & \text{if } p - k + 2 \leq t \leq p + k - 1 \\
2 & \text{otherwise.}
\end{cases}
\]

**Proof:** The proof is similar to that of Lemma 1. \( \square \)

For all \( 0 \leq r < q \) and \( 0 \leq t < 2p \), let \( a_{rt} \in \{x_{rt}, y_{rt}\} \) and let \( d_{a_{rt}}(k) \) denotes the sum of distances between \( a_{rt} \) and vertices on \( k \)th row of the graph. By symmetry of the graph for all \( 0 \leq t < 2p \), \( d_{x_{rt}}(k) \) are equal and \( d_{y_{rt}}(k) \) are equal. So we may compute this summation for \( x_{0p} \) and \( y_{0p} \) in the 0th row of the graph, which is denoted by \( d_x(k) \) \( d_y(k) \), respectively. For \( x_{rp} \) and \( y_{rp} \) we can compute \( d_{a_{rt}}(k) \) similarly.

**Lemma 3.** Let \( 0 \leq k < q \), then

\[
d_x(k) = \begin{cases} 
4p^2 + 4kp + 2(k^2 + k) & \text{if } k \leq p \\
2p^2 + 8kp + 2p & \text{if } k > p
\end{cases}
\]

and

\[
d_y(k) = \begin{cases} 
4p^2 + 4kp + 2(k^2 - k) & \text{if } k \leq p \\
2p^2 + 8kp - 2p & \text{if } k > p
\end{cases}
\]
Proof: Let \( k = 0 \). Then for vertices \( a_{0t} \in \{x_{0t}, y_{0t} \} \) in the first row of the graph, we have

\[
\sum_{t=0}^{2p-1} d(a_{0t}, x_{0p}) = \sum_{t=0}^{2p-1} d(a_{0t}, y_{0p}) = (1 + 2 + \cdots + 2p) + (1 + 2 + \cdots + 2p - 1) = 4p^2.
\]

So \( d_x(0) = d_y(0) = 4p^2 \).

Now suppose that \( k \leq p \). Then

\[
d_x(k) = d_x(0) + (d_x(1) - d_x(0)) + (d_x(2) - d_x(1)) + \cdots + (d_x(k) - d_x(k - 1))
\]

By Lemma 1, the number of vertices satisfying the condition \( p - i + 1 \leq t \leq p + i \), is \( 2i \) and for those vertices, \( R_x(k) = 4 \) and for other \( 2p - 2i \) remaining vertices of this row we have \( R_x(k) = 2 \).

So

\[
d_x(k) = 4p^2 + 8 \sum_{i=1}^{k} i + 4 \sum_{i=1}^{k} (p - i)
\]

With a similar argument, using Lemma 2, we have

\[
d_y(k) = d_y(0) + (d_y(1) - d_y(0)) + (d_y(2) - d_y(1)) + \cdots + (d_y(k) - d_y(k - 1))
\]

\[
d_y(k) = 4p^2 + 8 \sum_{i=1}^{k-1} i + 4 \sum_{i=1}^{k-1} (p - i)
\]

Now let \( k > p \). Then all of vertices satisfy the condition \( p - i + 1 \leq t \leq p + i \). So by Lemma 1, we have

\[
d_x(k) = d_x(p) + (d_x(p + 1) - d_x(p)) + (d_x(p + 2) - d_x(p + 1)) + \cdots + (d_x(p + k) - d_x(p + k - 1))
\]

\[
d_x(k) = (10p^2 + 2p) + 4(2p)(k - p)
\]

Similarly we have

\[
d_y(k) = d_y(p) + (d_y(p + 1) - d_y(p)) + (d_y(p + 2) - d_y(p + 1)) + \cdots + (d_y(p + k) - d_y(p + k - 1))
\]

\[
d_y(k) = (10p^2 - 2p) + 4(2p)(k - p)
\]
This completes the proof. \[
\]

Now we use Lemma 3 and compute the Wiener index of short and long \(TUC_4C_8(S)\) nanotubes.

**Theorem 1.** The Wiener index of \(G := TUC_4C_8(S)\) nanotubes given by

\[
W(G) = \begin{cases} 
\frac{pq}{3} \left(2q^3 + 8pq(3p + q) - 2q - 8p\right) & \text{if } q \leq p \\
\frac{p^2}{3} \left(-2p^3 + 8pq^2 + (12q^2 + 2)p + 16q^3 - 12q\right) & \text{if } q > p.
\end{cases}
\]

**Proof:** Let \(S(l) = \sum_{k=0}^{l} (d_x(k) + d_y(k))\). First suppose that \(q \leq p\). By Lemma 3, we have

\[
S(l) = \sum_{k=0}^{l} (4p^2 + 4kp + 2(k^2 + k) + 4p^2 + 4kp + 2(k^2 - k))
\]

\[
= \frac{4}{3} l^3 + (4p + 2)l^2 + \left(8p^2 + 4p + \frac{2}{3}\right)l + 8p^2.
\]

Therefore, by definition of the Wiener index we have

\[
W(G) = \frac{1}{2} \sum_{\{i, j\} \subseteq V(G)} d(i, j)
\]

\[
= 2p \left(\frac{q-1}{q} \left(S(k) + S(q - k - 1) - S(0)\right)\right)
\]

\[
= 2p \left(\frac{2}{3} \sum_{k=0}^{q-1} S(k) - qS(0)\right)
\]

\[
= \frac{pq}{3} \left(2q^3 + 8pq(3p + q) - 2q - 8p\right).
\]

Now suppose that \(q > p\). If \(l \geq p\), then

\[
S(l) = \sum_{k=0}^{p} (4p^2 + 4kp + 2(k^2 + k) + 4p^2 + 4kp + 2(k^2 - k))
\]

\[
+ \sum_{k=p+1}^{l} ((2p^2 + 8kp + 2p) + (2p^2 + 8kp - 2p))
\]

\[
= 8pl^2 + (4p^2 + 8)l + \frac{4}{3} p^3 + 6p^2 + \frac{2}{3} p.
\]

Hence, by definition of Wiener index we have

\[
W(G) = \frac{1}{2} \sum_{\{i, j\} \subseteq V(G)} d(i, j)
\]
Proof. Put 

\[
\text{MTI}(G) = 6W(G) - 4p \sum_{k=0}^{q-1} d_x(k) + (6p(6q - 2) - 8p
\]

= 6\left(\frac{pq}{3} \left(2q^3 + 8pq(3p + q) - 2q - 8p\right)\right)

- 4p\left(2pq(2p + q - 1) + \frac{2}{3}q(q^2 - 1)\right) + (36pq - 20p)

= pq\left(16pq(3p + q) + 4q(q^2 - 1) - 8p(2p + 1) - 8q(p + \frac{q}{3}) + \frac{116}{3}\right) - 20p.

Now if \(q > p\), then

\[
\text{MTI}(G) = 6W(G) - 4p\left(\sum_{k=0}^{q-1} d_x(k) + \sum_{k=p+1}^{q-1} d_x(k)\right) + (6p(6q - 2) - 8p
\]
\[
6 \left( \frac{p^2}{3} \left( -2p^3 + 8qp^2 + (12q^2 + 2)p + 16q^3 - 12q \right) \right) \\
-4p \left( 2pq(2q + p - 1) + \frac{2}{3}p(p^2 - 1) \right) + (36pq - 20p) \\
= pq \left( 8pq(3p + 4q - 2) + 8p(2p^2 - p - 2) + 36 \right) - p \left( 4p^2(p^2 + 1) + \frac{8}{3}p(p^2 - 1) - 20 \right).
\]

Therefore the proof is complete. \[\Box\]

In Tables (1) and (2) the numerical data for Wiener and Schultz indices of \(TUC_4C_8(S)\) nanotubes of various dimensions are given.

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<th>(q)</th>
<th>(W(G))</th>
<th>(MTI(G))</th>
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<th>(q)</th>
<th>(W(G))</th>
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Table 1. Wiener and Schultz indices in short tubes, \(TUC_4C_8(S)\), \(q \leq p\)

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<th>(W(G))</th>
<th>(MTI(G))</th>
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Table 2. Wiener and Schultz indices in long tubes, \(TUC_4C_8(S)\), \(q > p\)
Appen
dix

In this appendix we include a MATHEMATICA program to produce the graph of $T(p, q)$ and computing the Wiener and Schultz indices of the graph.

```
<< Graphics'Arrow'
<< DiscreteMath'Combinatorica'

horlin[x_, y_] := {{x, y}, {x+1, y}}
verlin[x_, y_] := {{x, y}, {x, y+1}}

pos[x_, y_] := {{x, y}, {x+1/2, y+1/2}}

neg[x_, y_] := {{x, y}, {x+1/2, y-1/2}}

sq[x_, y_] := {{x, y}, {x+1, y}, {x+1, y-1}, {x, y-1}, {x, y}}

pts[x_, y_] := {{x, y}, {x+1, y}, {x+1, y-1}, {x+1, y-1}, {x, y-1}}

c4c8s[p_, q_] := If[EvenQ[q], (* generating the coordinates *)
    Join[Flatten[Table[sq[x, y], {y, 3q/2-2, 0, -3}, {x, 3, 3p-3, 3}], 2],
        Flatten[Table[sq[x, y], {y, 3q/2-7/2, 0, -3}, {x, 3/2, 3p, 3}], 2],
        Flatten[Table[verlin[1, y], {y, 3q/2-3, 0, -3}],
            Table[{{1, y}, {3p, y}}, {y, 3q/2-2, 0, -3}],
            Table[{{1, y}, {3p, y}}, {y, 3q/2-3, 0, -3}],
            Flatten[Table[pos[x, y], {y, 3q/2-2, 0, -3}, {x, 1, 3p, 3}], 1],
            Flatten[Table[verlin[1, y], {y, 3q/2-3/2, 0, -3}, {x, 5/2, 3p, 3}], 1],
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        ],
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        Flatten[Table[pos[x, y], {y, 3q/2-2, 0, -3}, {x, 1, 3p, 3}], 1], (**)
        Flatten[Table[pos[x, y], {y, 3q/2-7/2, 0, -3}, {x, 5/2, 3p, 3}], 1], (**)
        Flatten[Table[neg[x, y], {y, 3q/2-3/2, 3, -3}, {x, 5/2, 3p, 3}], 1], (**)
        Flatten[Table[neg[x, 0], {y, 3q/2-3, 0, -3}, {x, 1, 3p, 3}], 1],
        Table[neg[x, 0], {y, 5/2, 3p, 3}], (**)
        Table[pos[x, -1/2], {x, 1, 3p, 3}], (**)
    ]
```

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Table[verlin[3p,y],{y,3q/2-3,0,-3}] (*last piece of column*)
Table[horlin[x,3q/2-3/2],{x,3/2,3p,3}] (*last piece of row*)
Table[horlin[x,-1/2],{x,3,3p-3,3}] (*last piece of row*) (**)

p=4; q=6;(*for example *)
pic=c4c8s[p,q]; (* Show the figure *)
Show[Graphics[Map[Line,pic]],AspectRatio ->Automatic];
drawgraph[edges_] := Module[{vert,G,n,t,e,vv},
    vert=Union[Flatten[edges,1]];
    n=Length[vert]; t=Length[edges];
    e={}; vv=Table[{vert[[t]],VertexLabel -> t},{t,1,n}];
    For[i=1,i <= t,
        z=edges[[i]];
        AppendTo[e,{{Position[vert,z[[1]]]}[[1,1]],
            Position[vert,z[[2]]]}[[1,1]]} ];
        i++ ];
    G=Graph[e,vv];
    ShowGraph[G];
    Return[G];]
K=drawgraph[pic]; (* Show the graph*)

(* computing the Wiener index *)
wiener[G_] := Module[{vert,t,i,j},
    vert=Union[Flatten[Edges[G],1]];
    t=Sum[Length[ShortestPath[G,vert[[i]],vert[[j]] ] ]-1,{i,1,Length[vert]},
        {j,1,Length[vert]}];
    Return[t/2]
]

wiener[K] (* computing the Schultz index *)

schultz[G_] := Module[{v,t,i,j, dist},
    adjac[r_,s_]:=If[Length[ShortestPath[G,r,s ] ]-1\[Equal]1, 1 ,0];
    v=Union[Flatten[Edges[G],1]];
    t=Sum[(InDegree[G,v[[i]]]+OutDegree[G,v[[i]]])*
        (Length[ShortestPath[G,v[[i]],v[[j]] ] ]-1+
            adjac[v[[i]],v[[j]]]),{i,1,Length[v]},{j,1,Length[v]}];
    Return[t]
]

schultz[K]
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References


