MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **57** (2007) 665-676

ISSN 0340 - 6253

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

Abbass Heydari and **Bijan Taeri***

Department of Mathematics, Isfahan University of Technology, Isfahan, Iran

(Received October 10, 2006)

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 matrice 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.

*E-mail: b.taeri@cc.iut.ac.ir (Author to whom correspondence should be addressed.)

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 kth row of the graph.

In the following Lemma, refereing 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 kth 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, $(d(x_{35}, x_{04}) + d(y_{35}, x_{04})) - (d(x_{25}, x_{04}) + d(y_{25}, x_{04})) = 4$.

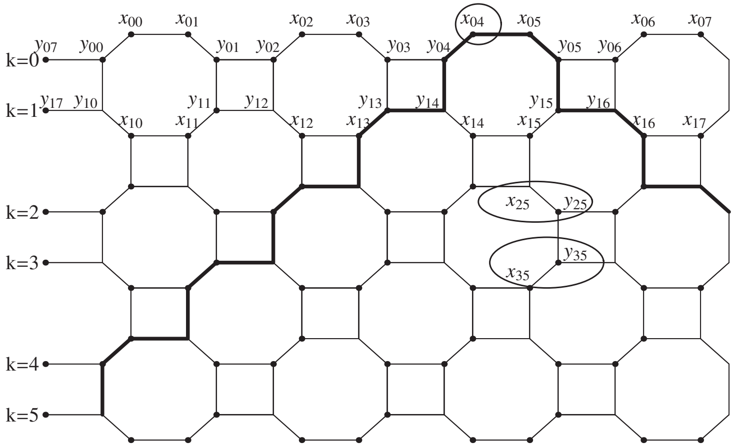

Figure 1: A $TUC_4C_8(S)$ Lattice with $p = 4$ and $q = 6$.

Lemma 1. Let $1 \le k < q$, $0 \le t < 2p$ 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

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

If p is an odd integer then

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

Proof: We prove the assertion when, p is an even integer. If p is an odd integer proof is similar. Suppose for $1 \le k < q$, $p - k + 1 \le t \le p + k$, 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 $R_x(k) = 4$.

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 $d(x_{k-1,t}, x_{0p}) = d(y_{k,t}, x_{0p})$ and $d(y_{k-1,t}, x_{0p}) = d(x_{kt}, x_{0p}) + 2$. Thus $R_x(k) = 2$. □

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 $2 \le k < q$, $0 \le t < 2p$ 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

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

If p is an odd integer then

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

Proof: The proof is similar to that of Lemma 1. □

For all $0 \le r < q$ and $0 \le t < 2p$, 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 kth row of the graph. By symmetry of the graph for all $0 \le t < 2p$, $d_{x_{rt}}(k)$ 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 $d_x(k)$ and $d_y(k)$, respectively. For x_{rp} and y_{rp} we can compute $d_{a_{rt}}(k)$ similarly.

Lemma 3. Let $0 \le k < q$, then

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

and

$$d_y(k) = \begin{cases} 4p^2 + 4kp + 2(k^2-k) & \text{if } k \le p \\ 2p^2 + 8kp - 2p & \text{if } k > p. \end{cases}$$

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

$$\begin{aligned} d_x(k) &= 4p^2 + (4 \times 2 + 2(2p-2) + (4 \times 4 + 2(2p-4)) + \cdots + (4 \times 2k + 2(2p-2k) \\ &= 4p^2 + 4(2 + 4 + \cdots + 2k) + 2((2p-2) + (2p-4) + \cdots + (2p-2k)) \\ &= 4p^2 + 8\sum_{i=1}^{k} i + 4\sum_{i=1}^{k}(p-i) \\ &= 4p^2 + 4kp + 2(k^2 + k). \end{aligned}$$

With a similar argument, using Lemma 2, we have

$$\begin{aligned} d_y(k) &= d_y(0) + (d_y(1) - d_y(0)) + (d_y(2) - d_y(1)) + \cdots + (d_y(k) - d_y(k-1)) \\ &= 4p^2 + 4(0 + 2 + \cdots + 2(k-1)) + 2((2p-0) + (2p-2) + \cdots + (2p-2k+2)) \\ &= 4p^2 + 8\sum_{i=1}^{k-1} i + 4\sum_{i=1}^{k-1}(p-i) \\ &= 4p^2 + 4kp + 2(k^2 - k). \end{aligned}$$

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

$$\begin{aligned} d_x(k) &= d_x(p) + (d_x(p+1) - d_x(p)) + (d_x(p+2) - d_x(p+1)) + \cdots + \\ &\qquad (d_x(p+k) - d_x(p+k-1)) \\ &= (10p^2 + 2p) + 4(2p)(k-p) \\ &= 2p^2 + 8kp + 2p. \end{aligned}$$

Similarly we have

$$\begin{aligned} d_y(k) &= d_y(p) + (d_y(p+1) - d_y(p)) + (d_y(p+2) - d_y(p+1)) + \cdots + \\ &\qquad (d_y(p+k) - d_y(p+k-1)) \\ &= (10p^2 - 2p) + 4(2p)(k-p) \\ &= 2p^2 + 8kp - 2p. \end{aligned}$$

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

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

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

$$\begin{aligned} S(l) &= \sum_{k=0}^{l}(4p^2 + 4kp + 2(k^2+k) + 4p^2 + 4kp + 2(k^2-k)) \\ &= \frac{4}{3}l^3 + (4p+2)l^2 + \left(8p^2 + 4p + \frac{2}{3}\right)l + 8p^2. \end{aligned}$$

Therefore, by definition of the Wiener index we have

$$\begin{aligned} W(G) &= \frac{1}{2}\sum_{\{i,j\}\subseteq V(G)} d(i,j) \\ &= 2p\left(\sum_{k=0}^{q-1}\Big(S(k) + S(q-k-1) - S(0)\Big)\right) \\ &= 2p\left(2\sum_{k=0}^{q-1} S(k) - qS(0)\right) \\ &= \frac{pq}{3}\Big(2q^3 + 8pq(3p+q) - 2q - 8p\Big). \end{aligned}$$

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

$$\begin{aligned} S(l) &= \sum_{k=0}^{p}(4p^2 + 4kp + 2(k^2+k) + 4p^2 + 4kp + 2(k^2-k)) + \\ &\qquad \sum_{k=p+1}^{l}((2p^2 + 8kp + 2p) + (2p^2 + 8kp - 2p)) \\ &= 8Pl^2 + (4p^2+8)l + \frac{4}{3}p^3 + 6p^2 + \frac{2}{3}p. \end{aligned}$$

Hence, by definition of Wiener index we have

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

$$
\begin{aligned}
&= 2p\Big(\sum_{k=0}^{q-1}(S(k)+S(q-k-1)-S(0))\Big)\\
&= 2p\Big(2\sum_{k=0}^{q-1}S(k)-qS(0)\Big)\\
&= \frac{p^2}{3}\Big(-2p^3+8qp^2+(12q^2+2)p+16q^3-12q\Big).
\end{aligned}
$$

This completes the proof. □

Now we can use of Wiener index and the quantity $d_x(k)$, which obtained in Lemma 3 and Theorem 1, and compute Schultz index of $T(p,q)$ in short and long cases.

Theorem 2. The Schultz index $MTI(G)$ of $G := TUC_4C_8(S)$ nanotubes is given by

$$
\begin{cases}
pq\Big(16pq(3p+q)+4q(q^2-1)-8p(2p+1)-8q(p+\frac{q}{3})+\frac{116}{3}\Big)-20p & \text{if } q\le p\\
pq\Big(8pq(3p+4q-2)+8p(2p^2-p-2)+36\Big)-p\Big(4p^2(p^2+1)+\frac{8}{3}p(p^2-1)-20\Big) & \text{if } q>p.
\end{cases}
$$

Proof: Put $a_{kt}\in\{x_{kt},y_{kt}\}$, where $0\le t<2p$ and $0\le k<q$. For all vertices $a_{kt}\ne x_{0t},x_{q-1,t}$ of $T(p,q)$, $v(a_{kt})=3$ and $v(a_{x_{0t}})=v(x_{q-1,t})=2$. So

$$
\begin{aligned}
MTI(G) &= \sum_{i,j}v(i)(d(i,j)+A(i,j))\\
&= 3\sum_{i\notin\{x_{0t},x_{q-1,t}\}}(d(i,j)+A(i,j))+2\sum_{i\in\{x_{0t},x_{q-1,t}\}}(d(i,j)+A(i,j))\\
&= \Big(3\sum_{i,j}d(i,j)-\sum_{i\in\{x_{0t},x_{q-1,t}\}}d(i,j)\Big)+\Big(3\sum_{i,j}A_{ij}-\sum_{i\in\{x_{0t},x_{q-1,t}\}}A_{ij}\Big).
\end{aligned}
$$

Note that $\sum_{i,j}A(i,j)=2|V(G)|$ and $|V(G)|=p(6q-2)$. So if $q\le p$ we have

$$
\begin{aligned}
MTI(G) &= 6W(G)-4p\sum_{k=0}^{q-1}d_x(k))+(6p(6q-2)-8p\\
&= 6\Big(\frac{pq}{3}\Big(2q^3+8pq(3p+q)-2q-8p\Big)\Big)\\
&\quad -4p\Big(2pq(2p+q-1)+\frac{2}{3}q(q^2-1)\Big)+(36pq-20p)\\
&= pq\Big(16pq(3p+q)+4q(q^2-1)-8p(2p+1)-8q(p+\frac{q}{3})+\frac{116}{3}\Big)-20p.
\end{aligned}
$$

Now if $q>p$, then

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

$$= 6\left(\frac{p^2}{3}\left(-2p^3 + 8qp^2 + (12q^2+2)p + 16q^3 - 12q\right)\right)$$
$$-4p\left(2pq(2q+p-1) + \frac{2}{3}p(p^2-1)\right) + (36pq - 20p)$$
$$= pq\left(8pq(3p+4q-2) + 8p(2p^2-p-2) + 36\right) - p\left(4p^2(p^2+1) + \frac{8}{3}p(p^2-1) - 20\right).$$

Therefore the is proof is complete . □

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

p	q	$W(G)$	$MTI(G)$	p	q	$W(G)$	$MTI(G)$
2	2	336	1768	8	7	270592	1539392
3	3	2664	14328	9	6	262872	1484532
4	3	5824	31200	9	9	666792	3834576
4	4	11392	62576	10	5	236000	1318400
5	4	20800	114220	10	8	673280	3856120
5	5	35000	195200	12	10	1841760	10642800
6	3	18144	96912	12	12	2814336	16352208
7	4	52864	290276	15	10	3393000	19621500
7	7	189336	1076488	15	12	5123520	29793060
8	5	126080	704000	15	15	8595000	50255400

Table 1. Wiener and Schultz indices in short tubes, TUC4C8(S), $q \leq p$

p	q	$W(G)$	$MTI(G)$	p	q	$W(G)$	$MTI(G)$
2	3	928	5040	7	9	346528	1990352
2	5	3584	20032	7	10	449624	2591932
3	5	9456	52704	8	9	489216	2811776
3	7	22872	129672	9	10	856440	4942980
4	8	64384	367280	9	12	1333584	7739100
4	10	116480	670160	10	13	2123200	12353280
5	10	197000	1134100	10	15	3028000	17678800
5	15	584000	3403000	12	15	4803264	28062432
6	7	126336	717744	12	20	9838464	57809232
6	10	306480	1765560	15	20	17178000	101000100

Table 2. Wiener and Schultz indies in long tubes, TUC4C8(S), $q > p$

Appendix

In this 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.

```
<< 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},{x+1,y-1}},
             {{x+1,y-1},{x,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],
            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[pos[x,y],{y,3q/2-7/2,-3,-3},{x,5/2,3p,3}],1],
            Flatten[Table[neg[x,y],{y,3q/2-3/2,0,-3},{x,5/2,3p,3}],1],
            Flatten[Table[neg[x,y],{y,3q/2-3,0,-3},{x,1,3p,3}],1],
            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,3/2,3p,3}]  (*last piece of row*)
                 ],(*** ** ** ** ** ** ** ** ** ** ** *******)
       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],
            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}] ,
            {{{1,-1/2},{3p,-1/2}}},
            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,y],{y,3q/2-3,0,-3},{x,1,3p,3}],1],
            Table[neg[x,0],{x,5/2,3p,3}],(**)
            Table[pos[x,-1/2],{x,1,3p,3}],(**)
```

```
            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[edgs_] := Module[{vert,G,n,t,e,vv},
    vert=Union[Flatten[edgs,1]];
    n=Length[vert];     t=Length[edgs];
    e ={};     vv=Table[{vert[[t]],VertexLabel -> t},{t,1,n}];
    For[i=1,i <= t,
        z=edgs[[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]
```

Acknowledgement: This work was partially supported by Center of Excellence of Mathematics of Isfahan University of Thecnology (CEAMA).

References

[1] S. Iijima, Nature **354** (1991) 56-58.

[2] S. Iijima and T. Ichlhashi, Nature **363** (1993) 603-605.

[3] H. Wiener, J. Am. Chem. Soc. **69** (1947) 17-20.

[4] S. Wolfram. A system for doing mathematics by computers. Addison-Welesly (1991)

[5] R. Todeschini and V. Consonni, Handbook of Molecular Descriptors, Wiley, Weinheim, 2000.

[6] D. E. Needham, I. C. Wei and P. G. Seybold, J. Am. Chem. Soc. **110** (1988) 4186-4194.

[7] G. Rücker and C. Rücker, J. Chem. Inf. Comput. Sci. **33** (1993) 683-695.

[8] A. A. Dobrynin, and I. Gutman, Publ. Inst. Math. (Beograd) **56** (1994) 18-22.

[9] A. A. Dobrynin, R. Entringer and I. Gutman, Acta Appl. Math. **66** (2001) 211-241.

[10] A. A. Dobrynin, I. Gutman, S. Klavzar and P. Zigert, Acta Appl. Math. **72** (2002) 247-294.

[11] P. E. Johna, M. V. Diudea, Croat. Chem. Acta, **77** (2004) 127-132.

[12] R. Todeschini and V. Consonni, Handbook of Molecular Descriptors, Wiley, Weinheim, 2004.

[13] M. V. Diudea and A. Graovac, MATCH Commun. Math. Comput. Chem. **44** (2001) 93-102.

[14] M. V. Diudea, I. Silaghi-Dumitrescu and B. Parv, MATCH Commun. Math. Comput. Chem. **44** (2001) 117-133.

[15] M. V. Diudea and P. E. John, MATCH Commun. Math. Comput. Chem. **44** (2001) 103-116.

[16] M. V. Diudea, Bull. Chem. Soc. Japan. **75** (2002) 487-492.

[17] M. V. Diudea, MATCH Commun. Math. Comput. Chem. **45** (2002) 109-122.

[18] P. E. John and M. V. Diudea, Croat. Chem. Acta, **77** (2004) 127-132.

[19] M. V. Diudea, M. Stefu, B. Parv and P. E. John, Croat. Chem. Acta, **77** (2004) 111-115.

[20] M. Stefu and M. V. Diudea, MATCH Commun. Math. Comput. Chem. **50** (2004) 133-144.

[21] H. P. Schultz, J. Chem. Inf. Comput.Sci. **29** (1989) 227-228.

[22] H. P. Schultz, J. Chem. Inf. Comput. Sci. **40** (2000) 1158-1159.

[23] S. Klavzär and I. Gutman, Disc. Appl. Math. **80** (1997) 73-81.

[24] I. Gutman, J. Chem. Inf. Comput. Sci. **34** (1994) 1087-1089.

[25] A. A. Dobrynin, Croat. Chem. Acta, **72**(4)(1999) 869-874.

[26] I. Gutman, Graph Theory Notes New York **27** (1994) 9-15.

[27] A. A. Dobrynin and I. Gutman, Publ. Inst. Math. (Beograd) **56** (1994) 18-22.

[28] A. A. Dobrynin, I. Gutman and G. Dömötör, Appl. Math. Lett. **8** (1995) 57-62.

[29] A. A. Dobrynin, I. Gutman, Graph Theory Notes New York **28** (1995) 21-23.

[30] P. V. Khadikar, N. V. Deshpande, P. P. Kale, A. A. Dobrynin, I. Gutman and G. Dömötör, J. Chem. inf. Comput. Sci **35** (1995) 547-550.

[31] P. V. Khadikar and S. Klavžar, J. Chem. Inf. Comput. Sci. **35** (1995) 1011-1014.