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# Wiener index of $SC_5C_7$[p,q] nanotubes

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Let *G* be a simple connected graph with vertex set *V (G)* and edge set *E(G)*. The distance between two vertices *u* and *v* is the number of edges in the shortest path between *u* and *v* that is denoted by *d(u, v)*. The Wiener index is the first topological index based on distance and is defined as the sum of distances between all pairs of vertices in a graph. In the other word: $W(G)=\frac{1}{2}\sum_{\{i,j\}\subseteq V(G)} d(i,j)$. In this paper, a method for computing the Wiener index of a simple graph is presented and we apply this method for computing the Wiener index of family of $SC_5C_7$ [p, q] nanotubes.

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## 1. Introduction

Let G be a connected graph. The vertex-set and edge-set of G denoted by and respectively. The distance between vertices u and v of G is denoted by d(u, v) and diameter of G is denoted by diam(G). The Wiener index of G is denoted by W (G) and is defined by

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

Topological indices are numerical parameters derived from the molecular structure and are used in the study of biological activities and physico-chemical properties of molecular graphs. In the latter the topological distance between two vertices is the number of edges in the shortest path between these. The distance based topological indices are widely studied in mathematical chemistry. Wiener index is the first distance based topological index introduced by chemist Harold Wiener [1] in 1947. It is used to determine physical properties of types of alkanes known as paraffin. It found numerous applications in the modelling of biological, physico-chemical properties.

For a review, historical details and further bibliography on the chemical applications of the Wiener index see [2-4]. In a series of papers other topological indices for some nanotubes are computed [5-16].

## 2. Main result

For computing the Wiener index, it's sufficient to obtain the distances between vertices. In this section, we give a method to compute the distances between vertices and Wiener index of any simple connected molecular graph. $D_{u,t}$ denotes the set of vertices that their distance to vertex *u* is equal to *t*. We denote the adjacent vertices to vertex *u* by *N (u)*. It is easy to see that for each vertex u, the sets $D_{u,t}$ ($t \geq 0$) partition the vertex set of the graph.

$$V=\bigcup_{t\geq 0} D_{u,t} \quad u\in V$$

$$W(G)=\frac{1}{2}\sum_{u\in V}\sum_{t=1}^{diam(G)} t\times\left|D_{u,t}\right|$$

By determining the sets $D_{u,t}$ for all vertices of graph *G*, we can obtain the Wiener index and diameter of *G*. Also some other information about *G* such as eccentricity of vertices can be determined. In the following, a method for computing the sets $D_{u,t}$ is explained. Put $D_{u,0} = u$ and $D_{u,1} = N(u)$ for each vertex *u*. Suppose the set $D_{u,t}$ was computed, the set $D_{u,t+1}$ can be computed by the relation

$$D_{u,t+1}=\bigcup_{v\in D_{u,t}}(N(v)\setminus(D_{u,t}\bigcup D_{u,t-1}) \quad t\geq 1.$$

## 3. Computing the Wiener index of $SC_5C_7$[p,q] nanotube by GAP program

A $C_5C_7$ net is a trivalent decoration made by alternating $C_5$ and $C_7$. It can cover either a cylinder or a torus. The structure of $SC_5C_7$[p,q] should be clear from Fig. 1. In this section we compute the Wiener index of $SC_5C_7$[p,q] nanotube by GAP program.

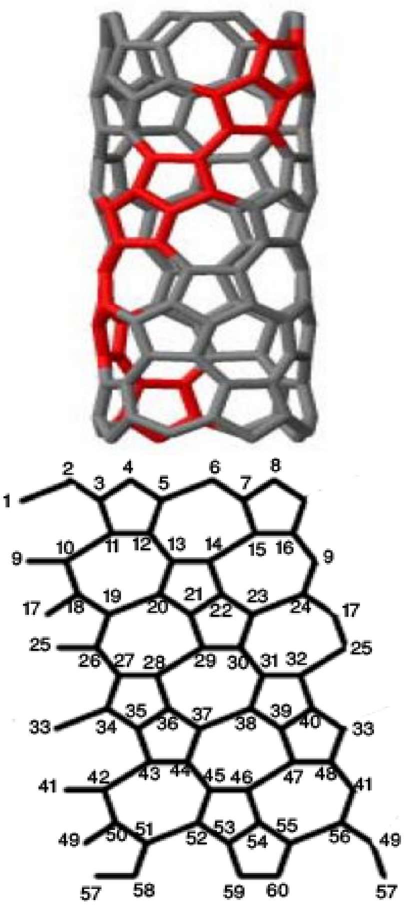


*Fig. 1. $SC_5C_7[4,2]$ nanotube.*

We denote the number of pentagons in the first row by p, in this nanotube the four first rows of vertices and edges are repeated alternatively, we denote the number of this repetition by $q$ .In each row there are $4p$ vertices, except last row which there are $2p$ vertices, and hence the number of vertices in this nanotube is equal to $16pq-2p$ .

We partition the vertices of the graph to following sets:

$K_1$ : The vertices of the first row.

$K_2$ : The vertices of the first row in each period, except the first one.

$K_3$ : The vertices of the second rows in each period.

$K_4$ : The vertices of the third row in each period.

$K_5$ : The vertices of the fourth row in each period.

$K_6$ : The last vertices of the graph.

We write a program to obtain the adjacent vertices set to each vertex in the sets $K_i$ , i=1…6. We can find the adjacent vertices set to each vertex by joining of these programs.

The following program computes the Wiener index of $SC_5C_7$[p,q] nanotube for arbitrary p and q. In Table 1, results are shown for some *p* and *q*.

```
p:=4; q:=2; #(for example)
n:=16*p*q-2*p; N:=[]; K1:=[1..4*p];
for i in K1 do
if i mod 4=1 then N[i]:=[i-1,i+1,i+4*p-1];
elif i mod 2=0 then N[i]:=[i-1,i+1];
elif i mod 4=3 then N[i]:=[i-1,i+1,i+4*p];fi;
od;
N[1]:=[2,4*p,8*p]; N[4*p]:=[4*p-1,1];
K:=[4*p+1..n-2*p];K2:=Filtered(K,i->i mod
(16*p) in[1..4*p]);
for i in K2 dox:=i mod (16*p);
if x mod 4 =1 then N[i]:=[i-1,i+1,i+4*p-1];
elif x mod 4=2 then N[i]:=[i-1,i+1,i-4*p+1];
elif x mod 4=3 then N[i]:=[i-1,i+1,i+4*p];
elif x mod 4=0 then N[i]:=[i-1,i+1,i-4*p];fi;
if x=1 then N[i]:=[i+1,i+4*p-1,i+8*p-1]; fi;
if x=4*p then N[i]:=[i-1,i-4*p,i-4*p+1]; fi;
od;
K3:=Filtered(K,i->i mod (16*p)
in[4*p+1..8*p]);
for i in K3 dox:=(i-4*p) mod (16*p);
if x mod 4=1 then N[i]:=[i-1,i+1,i+4*p-1];
elif x mod 4=2 then N[i]:=[i-1,i+1,i+4*p];
elif x mod 4=3 then N[i]:=[i-1,i+1,i-4*p];
elif x mod 4=0 then N[i]:=[i-1,i+1,i-4*p+1];fi;
if x=1 then N[i]:=[i+1,i+4*p-1,i+8*p-1]; fi;
if x=4*p then N[i]:=[i-1,i-4*p+1,i-8*p+1]; fi;
od;
K4:=Filtered(K,i->i mod (16*p)
in[8*p+1..12*p]);
for i in K4 dox:=(i-8*p) mod (16*p);
if x mod 4=1 then N[i]:=[i-1,i+1,i+4*p];
elif x mod 4=2 then N[i]:=[i-1,i+1,i-4*p];
elif x mod 4=3 then N[i]:=[i-1,i+1,i+4*p-1];
elif x mod 4=0 then N[i]:=[i-1,i+1,i-4*p+1];fi;
if x=1 then N[i]:=[i+1,i+4*p-1,i+4*p]; fi;
if x=4*p then N[i]:=[i-1,i-4*p+1,i-8*p+1]; fi;
od;
K5:=Filtered(K,i->i mod (16*p) in
Union([12*p+1..16*p-1],[0]));
for i in K5 dox:=(i-12*p) mod (16*p);
if x mod 4=1 then N[i]:=[i-1,i+1,i-4*p];
elif x mod 4=2 then N[i]:=[i-1,i+1,i-4*p+1];
elif x mod 4=3 then N[i]:=[i-1,i+1,i+4*p-1];
elif x mod 4=0 then N[i]:=[i-1,i+1,i+4*p];fi;
if x=1 then N[i]:=[i+1,i+4*p-1,i-4*p]; fi;
if x=4*p then N[i]:=[i-1,i-4*p+1,i+4*p]; fi;
od;
K6:=[n-2*p+1..n];
for i in K6 dox:=i mod (4*p);
if i mod 2=0 then N[i]:=[i-1,i+x-1-4*p];
else N[i]:=[i+1,i+x-1-4*p]; fi;
```

```
N[i+x-1-4*p][3]:=i;
od;
N[n-2*p+1]:=[n-6*p+1,n-2*p+2]; N[n-6*p+1][3]:=n-2*p+1;
w:=0;
D:=[];
for i in [1..n] do
  D[i]:=[]; u:=[i];  D[i][1]:=N[i];
  u:=Union(u,D[i][1]); w:=w+Size(D[i][1]);
s:=1;  t:=1;
while s<>0 do
   D[i][t+1]:=[];
for j in D[i][t] do
for m in Difference(N[j],u) do
AddSet(D[i][t+1],m);
od; od;
u:=Union(u,D[i][t+1]);
w:=w+(t+1)*Size(D[i][t+1]);
  if D[i][t+1]=[]  then  s:=0;
fi;
t:=t+1;
od;
od;
w:=w/2; # (This value is equal to the Wiener index of the graph )
```

*Table 1. Wiener index of $SC_5C_7$[p,q].*

| P | q | Wiener index $SC_5C_7$[p,q] |
|---|---|---|
| 2 | q | $(4096/3)q^3 - 512q^2 + (2444/3)q - 410,\ q > 1$ |
| 3 | q | $3072q^3 - 1152q^2 + 4200q - 3105,\ q > 2$ |
| 4 | q | $(16384/3)q^3 - 2048q^2 + (39824/3)q - 12792,\ q > 3$ |
| 5 | q | $(25600/3)q^3 - 3200q^2 + (97280/3)q - 38435,\ q > 4$ |
| 6 | q | $12288q^3 - 4608q^2 + 67296q - 94524,\ q > 5$ |
| 7 | q | $(50176/3)q^3 - 6272q^2 + (374150/3)q - 202405,\ q > 6$ |
| 8 | q | $(65536/3)q^3 - 8192q^2 + (638144/3)q - 391520,\ q > 7$ |
| 9 | q | $27648q^3 - 10368q^2 + 340758q - 701280,\ q > 8$ |
| 10 | q | $(102400/3)q^3 - 12800q^2 + (1558520/3)q - 1181840,\ q > 9$ |
| 11 | q | $(123904/3)q^3 - 15488q^2 + (2281664/3)q - 1895069,\ q > 10$ |
| 12 | q | $49152q^3 - 18432q^2 + 1077168q - 2917404,\ q > 11$ |
| 13 | q | $(173056/3)q^3 - 21632q^2 + (4451252/3)q - 4339855,\ q > 12$ |
| 14 | q | $(200704/3)q^3 - 25088q^2 + (5987492/3)q - 6269480,\ q > 13$ |
| 15 | q | $76800q^3 - 28800q^2 + 2629980q - 8830725,\ q > 14$ |

## 4. Conclusions

A method has been presented for computing the Wiener index of any simple connected graph. According to the method and using the GAP program, we can prepare a program to compute the Wiener index of a simple connected graph quickly. We apply the method to calculate the Wiener index of $SC_5C_7$[p,q] nanotubes.

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