American Journal of Applied Sciences 5 (12): 1754-1757, 2008
ISSN 1546-9239

Computing Wiener and Schultz Indices of HAC_5C_7 [p, q] Nanotube by GAP Program

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Abstract: In this research, we give a GAP program for computing the Wiener and the Schultz indices of any graph. In addition, we compute the Wiener and the Schultz of HAC_5C_7 [p, q] nanotube by this program.

Key words: Wiener index, Schultz index, nanotubes, GAP programming

INTRODUCTION

Topological indices of nanotubes are numerical descriptors that are derived from graph of chemical compounds. Such indices based on the distances in graph are widely used for establishing relationships between the structure of nanotubes and their physicochemical properties. Usage of topological indices in biology and chemistry began in 1947 when chemist Harold Wiener[1] introduced Wiener index to demonstrate correlations between physicochemical properties of organic compounds and the index of their molecular graphs. Wiener originally defined his index (W) on trees and studied its use for correlations of physico- chemical properties of alkanes, alcohols, amines and their analogous compounds[2].

Let G be a connected graph. The vertex-set and edge-set of G denoted by V(G) and E(G), respectively. 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 a graph G is denoted by W (G) and defined as the sum of distances between all pairs of vertices in G:

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

where, d(i, j) is the distance between vertices i and j. Another topological index is Schultz index, the Schultz index (MTI) was introduced by Schultz in 1989, as the molecular topological index[3] and it is defined by:

$$MTI = \sum_{\{i,j\} \subseteq V(G)} v(i)(d(i,j) + A(i,j)). \tag{2}$$

The molecular topological index studied in many papers[4-7].

In a series of papers, the Wiener index of some nanotubes is computed[8-14], another topological indices are computed[15-19]. In this research, we give an algorithm for computing the Wiener and Schultz indices of any graph and by this algorithm; we obtain the Wiener and Schultz indices of $HAC_5C_7[p,q]$ nanotube.

AN ALGORITHM FOR THE COMPUTATION OF THE WIENER AND SCHULTZ INDICES OF A GRAPH

Here, we give an algorithm that enables us to compute the Wiener and Schultz indices of any graph. For this purpose, the following algorithm is presented:

- We assign to any vertex one number
- We determine all of adjacent vertices set of the vertex $i, i \in V$ and this set denoted by N(i)
- In the start of program, we set w = 0, Sc = 0 and at the end of program, the values of $\frac{1}{2}w$ and Sc will be the Wiener and Schultz indices of graph G respectively
- The set of vertices that their distance to vertex i is equal to $t\,(t \geq 0)$ is denoted by $D_{i,t}$ and consider $D_{i,0} = \{i\}$. We have following relations:

$$V = \bigcup_{t \geq 0} D_{i,t} \quad i \in V \tag{3}$$

$$\sum_{j \in V(G)} d(i,j) = \sum_{t \geq 1} t \times \left|D_{i,t}\right| \quad ,\forall i \in V(G) \tag{4}$$

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$$W(G) = \frac{1}{2}\sum_{i\in V, t\geq 1} t\times\left|D_{i,t}\right| \quad (5)$$

$$\begin{aligned} MTI(G) &= \sum_{i\in V(G)} v(i)\times \sum_{j\in V(G)} (d(i,j)+A(i,j)) \\ &= \sum_{i\in V(G)} v(i)\times\left(\sum_{j\in N(i)} 2 + \sum_{j\in V(G)\setminus N(i)} d(i,j)\right) \quad (6) \\ &= \sum_{i\in V(G)}\left(2\,v(i)^2 + v(i)\times\sum_{j\in D_{i,t}\ t\geq 2} t\times\left|D_{i,t}\right|\right) \end{aligned}$$

According to Eq. (5) and (6), by determining these sets, we can obtain the wiener and Schultz indices of the graph.

The distance between vertex i and its adjacent vertices is equal to 1, therefore $D_{i,1} = N(i)$. For each $j\in D_{i,t}$ $t\geq 1$, the distance between each vertex of set $N(j)\setminus(D_{i,t}\cup D_{i,t-1})$ and the vertex i is equal to t+1, thus we have

$$D_{i,t+1} = \bigcup_{j\in D_{i,t}, t\geq 1} (N(j)\setminus(D_{i,t}\cup D_{i,t-1})) \quad (7)$$

According to Eq. (7), we can obtain $D_{i,t}$, $t\geq 2$ for each $i\in V$. In this step, we compute the wiener and Schultz indices of the graph by above relations.

COMPUTING THE WIENER AND SCHULTZ INDICES OF HAC_5C_7 [P, Q] NANOTUBE

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. Here we compute the Wiener and Schultz indices of HAC_5C_7 [p, q] nanotube by GAP program (Fig. 1, Table 1).

We denote the number of heptagons in one row by p. In this nanotube, the three first rows of vertices and edges are repeated alternatively and we denote the number of this repetition by q. In each period there are 8p vertices and p vertices which are joined to the end of the graph and hence the number of vertices in this nanotube is equal to 8pq+p.

We partition the vertices of this graph to following sets:

K_1: The vertices of first row whose number is 2p.
K_2: The vertices of the first row in each period except the first one whose number is 2p(q-1).
K_3: The vertices of the second rows in each period whose number is 3pq.

Table1: Wiener and Schultz indices of HAC_5C_7[p, q] nanotube

p	q	W(G)	MTI(G)
3	1	1167	246
4	2	12236	68376
4	3	35052	199672
5	3	57915	330040
6	4	187068	1078044
7	4	265391	1530130
7	7	1220219	7143010
3	6	134787	786006
4	6	243276	1418392
4	7	379756	2222456
5	7	601855	3522320
6	8	1290348	7573884
7	8	1781535	10458098
7	9	2495731	14683410
8	8	2362824	13872176
9	9	4235085	24921882

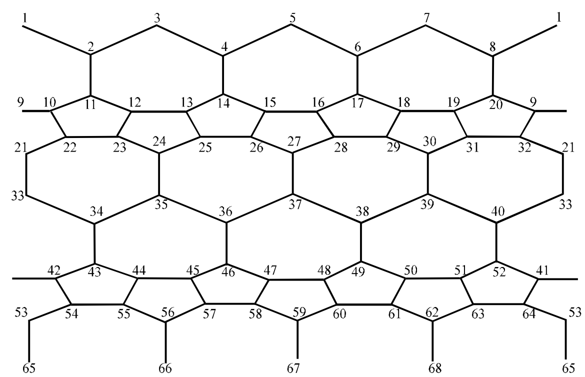

Fig. 1: HAC_5C_7[4, 2]

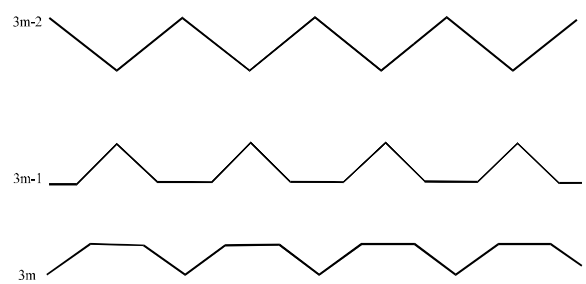

Fig. 2: m-th period

K_4: The vertices of the third row in each period whose number is 3pq.
K_5: The last vertices of the graph whose number is p.

Figure 2 shows the rows of m-th period, 1≤m≤q.

We write a program to obtain the adjacent vertices set to each vertex in the sets K_i, i = 1…5. We can obtain the adjacent vertices set to each vertex by the join of these programs. In this program, the value of x is the assign number of vertex i in that period.

The following program computes the Wiener and Schultz indices of HAC_5C_7 [p, q] nanotube for arbitrary p and q.

```
p: = 3; q: = 2; # (For example)
n: = 8*p*q +p;
N: = [];
K1: = [1..2*p];
V1: = [2..2*p-1];
N[1]: = [2,2*p];
N[2*p]: = [2*p-1,5*p,1];
for i in V1 do
if i mod 2 = 0 then N[i]: = [i-1,i+1,3/2 *i+2*p];
else N[i]: = [i-1,i+1];fi;
od;
k: = [2*p+1..8*p*q];
k2: = Filtered(k,i->i mod (8*p)in [1..2*p]);;
for i in k2 do
x: = i mod (8*p);
if x mod 2 = 1 then N[i]: = [i-1,i+1,(x-1)*(3/2) +1+i-x-3*p];
else N[i]: = [i-1,i+1,x*(3/2) +2*p+i-x];fi;
if x = 1 then N[i]: = [i+1,i-1+2*p,i-3*p];fi;
if x = 2*p then N[i]: = [i-1,i+3*p,i-2*p+1];fi;
od;
k3: = Filtered(k,i->i mod (8*p) in[2*p+1..5*p]);;
for i in k3 do
x: = i mod (8*p);
if (x-(2*p)) mod 3 = 1 then N[i]: = [i-1,i+1,i+3*p-1];
elif (x-(2*p)) mod 3 = 2 then N[i]: = [i-1,i+1,i+3*p];
elif (x-(2*p)) mod 3 = 0 then N[i]: = [i-1,i+1,(2/3) *(x-2*p)+i-x];fi;
if x = 2*p+1 then N[i]: = [i-1+3*p,i-1+6*p,i+1];fi;
if x = 5*p then N[i]: = [i-3*p,i-3*p+1,i-1];fi;
od;
k4: = Filtered(k,i->i mod (8*p) in Union([5*p+1..8*p-1],[0]) );;
for i in k4 do
x: = i mod (8*p);
if (x-(5*p)) mod 3 = 1 then N[i]: = [i-1,i+1,(x-(5*p)-1)*(2/3) +1+(i-x)+8*p];
elif (x-(5*p)) mod 3 = 2 then N[i]: = [i-1,i+1,i-3*p];
elif (x-(5*p)) mod 3 = 0 then N[i]: = [i-1,i+1,i-3*p+1];fi;
if x = 5*p+1 then N[i]: = [i+3*p-1,i+1,i+3*p];fi;
if x = 0 then N[i]: = [i-1,i-3*p+1,i-6*p+1];fi;
od;
K5: = [8*p*q+1 ..8*p*q+p];
for i in K5 do
x: = i-8*p*q;
y: = 8*p*(q-1)+5*p+3*x-2;
N[i]: = [y];
N[y][3]: = i;
od;

w: = 0;
Sc: = 0;
v: = [];
D: = [];
for i in [1..n] do
D[i]: = [];
u: = [i];
D[i][1]: = N[i];
v[i]: = Size(N[i]);
u: = Union(u,D[i][1]);
w: = w+Size(D[i][1]);
Sc: = Sc+v[i]*2*Size(D[i][1]);
r: = 1;
t: = 1;
while r<>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]);
Sc: = Sc+v[i]*(t+1)*Size(D[i][t+1]);
if D[i][t+1] = [] then r: = 0;fi;
t: = t+1;
od;
od;
w: = w/2;
Sc;
```


ACKNOWLEDGEMENT

This research is partially supported by Iran National Science Foundation (INSF) (Grant No. 83120).

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