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# COMPUTING HYPER WIENER AND SCHULTZ INDICES OF TUZC6[P,Q] NANOTUBE BY GAP PROGRAM

ALI IRANMANESH*, YASER ALIZADEH[a]
*Department of Mathematics, Tarbiat Modares University*
*P. O. Box: 14115-137, Tehran, Iran*
[a]*Department of Mathematics, Tarbiat Modares University*
*P. O. Box: 14115-137, Tehran, Iran*

In this paper, we give an algorithm for computing the Wiener and Schultz indices of any graph and by this algorithm; we obtain the hyper Wiener and Schultz indices of TUZC6 [p,q] nanotube.

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## 1. 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. The hyper-Wiener index is one of the recently conceived distance-based graph invariants, used as a structure-descriptor for predicting physico–chemical properties of organic compounds. The hyper-Wiener index was invented by Randic´ (1993) and was eventually extensively studied [2, 3]. Let G be a connected graph. The vertex-set and edge-set of G denoted by V(G) and E(G) respectively. The distance between the vertices u and v, d(u,v), in a graph is the number of edges in a shortest path connecting them. Two graph vertices are adjacent if they are joined by a graph edge. 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 hyper Wiener index of a graph G is denoted by W*W (G)* and defined as:

$$WW(G)=\frac{1}{2}\sum_{i<j} d(i,j)+\frac{1}{2}\sum_{i<j} d(i,j)^2 \qquad (1)$$

where $d(i, j)$ stands for the distance between the vertices $i$ and $j$ in the graph $G$.
Another topological index is Schultz index and denoted by MTI. This index was introduced by Schultz in 1989, as the molecular topological index [4], and it is defined by:

* Corresponding author: iranmanesh@modares.ac.ir

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

In this paper, we give an algorithm for computing the hyper-Wiener and Schultz indices of any graph and by this algorithm we obtain the hyper-Wiener and Schultz indices of TUZC6 [p,q] nanotube.

## 2. An algorithm for computing of the hyper-Wiener and Schultz indices of a graph

In this section, we give an algorithm that enables us to compute the hyper-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 $i$, $i \in V$ (G) and this set denoted by N(i ). 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 $D_{i,0} = \{i\}$. Let $e = ij$ be an edge connecting the vertices $i$ and $j$, then we have the following result:

a) $V = \bigcup_{t\geq 0} D_{i,t}$ , $i \in V$ (G).

b) $$\sum_{j\in V(G)} d(i,j) = \sum_{t\geq 1} t \times |D_{i,t}| \ , \ \sum_{j\in V(G)} d(i,j)^2 = \sum_{t\geq 1} t^2 \times |D_{i,t}|, \forall i \in V(G)$$

c) $$WW(G) = \frac{1}{4} \sum_{i\in V, t\geq 1} (t+t^2) \times |D_{i,t}|$$

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

$$= \sum_{i\in V(G)} v(i) \times \sum_{j\in V(G)} (d(i,j)+A(i,j)) = \sum_{i\in V(G)} v(i) \times \left( \sum_{j\in N(i)} 2 + \sum_{j\in V(G)\setminus N(i)} d(i,j) \right)$$

$$= \sum_{i\in V(G)} \left( 2v(i)^2 + v(i) \times \sum_{j\in D_{i,t}\, t\geq 2} t \times |D_{i,t}| \right)$$

According to the above relations, by determining $D_{i,t}, t \geq 1$, we can obtain the Hyper-Wiener and Schultz indices of the graph G. In the continue we obtain $D_{i,t}$, $t \geq 1$, for each vertex $i$.

(i) 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:

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

According to the above equation we can obtain $D_{i,t}$, $t \geq 2$, for each $i \in V$ (G). The molecular topological index studied in many papers [5-8]. In a series of papers, the Wiener and Schultz indices of some nanotubes computed [9-13].

## 3. Disscussion and conclusions

In this section, according to the above algorithm we write a program by GAP [14] to compute the hyper Wiener and Schultz indices of $TUZC_6[p,q]$ nanotube. $TUZC_6[p,q]$ nanotube is a carbon nanotube formed from a graphite sheet that is rolled up so that it has a zigzag edge.

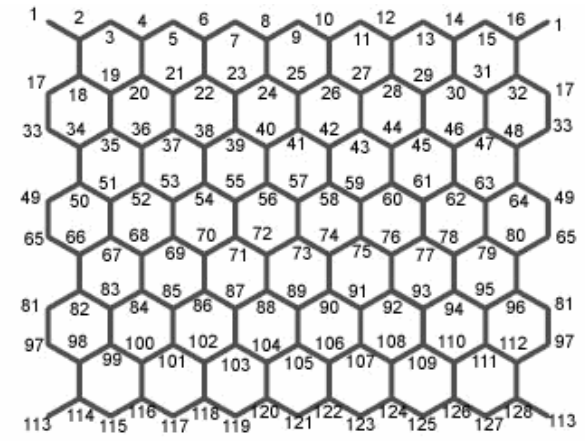

*Fig. 1. Nanotube* $TUZC_6[8,8]$.

We denote the number of hexagon in the first row by $p$ and the number of rows by $q$. In each row, there are $2p$ vertices and hence the number of vertices in this nanotube is equal to $2pq$. The following program computes the hyper Wiener and Schultz indices of $TUZC_6[p,q]$ nanotube for arbitrary p and q.

```
p:=4; q:=5; #(for example)
n:=2*p*q; N:=[];
K1:=[1..2*p]; V1:=[2..2*p-1];
for i in V1 do
  if i mod 2=0 then N[i]:=[i-1,i+1,i+2*p];
   else N[i]:=[i-1,i+1]; fi; od;
N[1]:=[2,2*p]; N[2*p]:=[1,2*p-1,4*p];
K:=[2*p+1..n];
K2:=Filtered(K,i->i mod (4*p) in [1..2*p]);
for i in K2 do
   if i mod 2 =0 then N[i]:=[i-1,i+1,i+2*p];
 else N[i]:=[i-1,i+1,i-2*p]; fi;
    if i mod (4*p)=1 then N[i]:=[i+1,i-2*p,i+2*p-1]; fi;
    if i mod (4*p)=2*p then N[i]:=[i-1,i-2*p+1,i+2*p];
fi; od;
K3:=Filtered(K,i->i mod (4*p) in Union([2*p+1..4*p-1],[0]));
for i in K3 do
     if i mod 2=0 then N[i]:=[i-1,i+1,i-2*p];
  else N[i]:=[i-1,i+1,i+2*p]; fi;
 if i mod (4*p)=2*p+1 then N[i]:=[i+1,i+2*p-1,i+2*p]; fi;
     if i mod (4*p)=0 then N[i]:=[i-1,i-2*p,i-2*p+1]; fi; od;
for i in [n-2*p+1..n] do
    if q mod 2=1 then
        if i mod 2 =0 then N[i]:=[i-1,i+1];
     else N[i]:=[i-1,i+1,i-2*p]; fi;
        if i mod (4*p)=1 then N[i]:=[i+1,i-2*p,i+2*p-1];  fi;
        if i mod (4*p)=2*p then N[i]:=[i-1,i-2*p+1];fi;
    else
      if i mod 2=0 then N[i]:=[i-1,i+1,i-2*p];
     else N[i]:=[i-1,i+1]; fi;
   if i mod (4*p)=2*p+1 then N[i]:=[i+1,i+2*p-1]; fi;
   if i mod (4*p)=0 then N[i]:=[i-1,i-2*p,i-2*p+1]; fi;
 fi; od;
```

```
ww:=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]);
ww:=ww+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]);
ww:=ww+(((t+1)^2)+(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;
ww:=ww/4; #(The  hyper Wiener index of the graph)
Sc; #(The Schultz index of the graph)
```

*Table 1. The hyper Wiener and Schultz indices of $TUZC_6$ [p,q]*

| p | q | Hyper Wiener | Schultz |
|---|---|---|---|
| 3 | 2 | 273 | 822 |
| 3 | 3 | 900 | 2352 |
| 4 | 3 | 2080 | 4816 |
| 5 | 6 | 32475 | 51090 |
| 6 | 4 | 16296 | 28356 |
| 6 | 6 | 53046 | 79452 |
| 7 | 5 | 48930 | 73780 |
| 7 | 8 | 201488 | 246330 |
| 8 | 8 | 289920 | 340912 |

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