Digest Journal of Nanomaterials and Biostructures, Vol. 4, No. 1, March 2009, p. 67-72

COMPUTING SZEGED AND SCHULTZ INDICES OF $HAC_5C_6C_7[p,q]$ NANOTUBE BY GAP PROGRAM

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In this research, we give a GAP program for computing the Szeged and Schultz indices of any graph. Also we compute the Szeged and Schultz indices of $HAC_5C_6C_7[p,q]$ by this program.

(Received January 14 2009; accepted February 12, 2009)

Keywords: Szeged index, Schultz index, Nanotube, GAP programming.

1. Introduction

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 $A(i,j)$. Let e be an edge of a graph G connecting the vertices u and v. Define two sets $N_1(e|G)$ and $N_2(e|G)$ as follows:

$N_1(e|G)=\{x \in V(G)|d(x,u)<d(x,v)\}$ and
$N_2(e|G)=\{x \in V(G)|d(x,v)<d(x,u)\}$.

The number of elements of $N_1(e|G)$ and $N_2(e|G)$ are denoted by $n_1(e|G)$ and $n_2(e|G)$ respectively.

A topological index was introduced by Gutman and called the Szeged index, abbreviated as Sz [1] and defined as

$$Sz(G)=\sum_{e\in E(G)} n_1(e|G).n_2(e|G).$$

Schultz index (MTI) is a topological index was introduced by Schultz in 1989, as the molecular topological index [2], and it is defined by:

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

In this paper, we give an algorithm that enables us to compute the Szeged and Schultz indices of any graph. Also by this algorithm, we compute the Szeged and Schultz indices of $HAC_5C_6C_7[p,q]$ nanotube .

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2. Result

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

1- We assign to any vertex one number.

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

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

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

b) $(D_{i,t} \setminus D_{j,t}) \subseteq (D_{j,t-1} \cup D_{j,t+1})$, $t \geq 1$.

c) $(D_{i,t} \cap D_{j,t-1}) \subseteq N_2(e|G)$ *and* $D_{i,t} \cap D_{j,t+1} \subseteq N_1(e|G)$ $t \geq 1$.

d) $(D_{i,1} \cup \{i\}) \setminus (D_{j,1} \cup \{j\}) \subseteq N_1(e|G)$ *and* $(D_{j,1} \cup \{j\}) \setminus (D_{i,1} \cup \{i\}) \subseteq N_2(e|G)$.

According to the above relations, by determining $D_{i,t}$, $t \geq 1$, we can obtain $N_1(e|G)$ and $N_2(e|G)$ for each edge e and therefore the Szeged and Schultz indices of the graph G is computed. In the continue we obtain the $D_{i,t}$, $t \geq 1$, for each vertex i.

3- 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).

4- In the start of program we set SZ and Sc equal to zero and T equal to empty set. In the end of program the values SZ and Sc are equal to the Szeged and Schultz indices of the graph G respectively. For each vertex $i, 1 \leq i \leq n$, and each vertex j in $N(i)$, we determine $N_1(e|G)$ and $N_2(e|G)$ for edge $e = ij$, then add the values of $n_1(e|G).n_2(e|G)$ to SZ . Since the edge ji is equal to ij, we add the vertex i to T and continue this step for the vertex i+1 and for each vertex in $N(i+1) \setminus T$.

GAP stands for Groups, Algorithms and Programming [3]. The name was chosen to reflect the aim of the system, which is group theoretical software for solving computational problems in group theory. The last years have seen a rapid spread of interest in the understanding, design and even implementation of group theoretical algorithms. GAP software was constructed by GAP's team in Aachen. We encourage the reader to consult Refs. [4] and [5] for background materials and computational techniques related to applications of GAP in solving some problems in chemistry and biology. The molecular topological index studied in many papers [6-9]. In a series of papers, the Szeged and Schultz indices of some nanotubes computed [10-13], another topological indices are computed [14-18].

3. Disscussion and conclusions

A $C_5C_6C_7$ net is a trivalent decoration made by alternating C_5, C_6 and C_7. It can cover either a cylinder or a torus. In this section we compute the Szeged and Schultz indices of $HAC_5C_6C_7$ nanotube by GAP program.

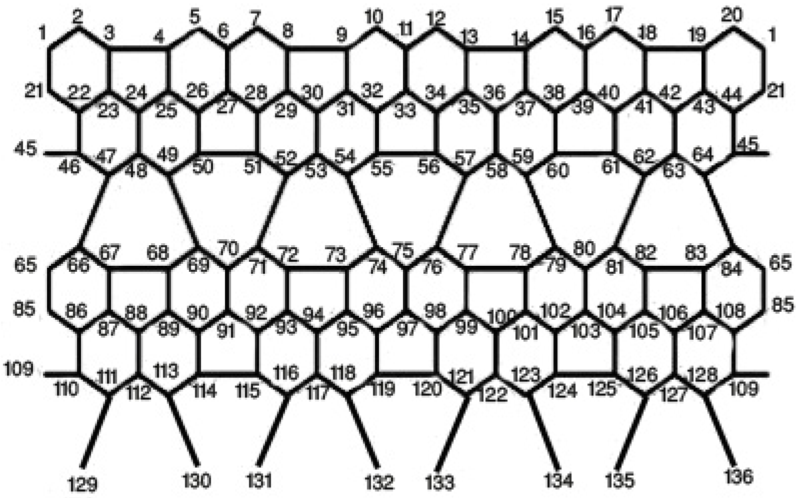

Fig. 1. $HAC_5C_6C_7[4,2]$ *Nanotube*

We denote the number of pentagons in the first row by p. In this nanotube the three first rows of vertices and edges are repeated alternatively; we denote the number of this repetition by q. In each period, there are $16p$ vertices and $2p$ vertices are joined to the end of the graph and hence the number of vertices in this nanotube is equal to $16pq+2p$.

We partition the vertices of this graph to following sets:

K_1: The vertices of first row whose number is $5p$.

K_2: The vertices of the first row in each period except the first one whose number is $5p(q-1)$.

K_3: The vertices of the second rows in each period whose number is $6pq$.

K_4: The vertices of the third row in each period whose number is $5pq$.

K_5: The last vertices of the graph whose number is $2p$.

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.

The following program computes the Szeged and Schultz indices of $HAC_5C_6C_7[p,q]$ nanotube for arbitrary p and q.

```
p:=9; q:=9;#(for example)
n:=16*p*q+2*p;
N:=[]; K1:=[1..5*p]; V1:=[2..5*p-1];
for i in V1 do
 if i mod 5 =1 then N[i]:=[i-1,i+1,(i-1)*(6/5)+1+5*p];
  elif (i mod 5) in [0,2] then N[i]:=[i-1,i+1];
   elif i mod 5=3 then N[i]:=[i-1,i+1,(i-3)*(6/5) +3+5*p];
    elif i mod 5=4 then N[i]:=[i-1,i+1,(i-4)*(6/5)+5+5*p]; fi; od;
N[1]:=[2,5*p,5*p+1]; N[5*p]:=[1,5*p-1];
k:=[5*p+1..16*p*q];
k2:=Filtered(k,i->i mod (16*p) in [1..5*p]);
```

```
    for i in k2 do
 x:=i mod (16*p);
 if x mod 5=1 then N[i]:=[i-1,i+1,(x-1)*(6/5) +1+i-x+5*p];
  elif x mod 5=2 then N[i]:=[i-1,i+1,i-5*p+1];
   elif x mod 5=3 then N[i]:=[i-1,i+1,(x-3)*(6/5)+3+i-x+5*p];
    elif x mod 5=4 then N[i]:=[i-1,i+1,(x-4)*(6/5)+5+i-x+5*p];
     elif x mod 5=0 then N[i]:=[i-1,i+1,i-5*p];fi;
 if x=1 then N[i]:=[i+1,i-1+5*p,i+5*p];fi;
 if x=5*p then N[i]:=[i-1,i-5*p,i-5*p+1];fi; od;
k3:=Filtered(k,i->i mod(16*p) in [5*p+1..11*p]);
for i in k3 do
 x:= (i-5*p) mod (16*p);
 if x mod 6=1 then N[i]:=[i-1,i+1,(x-1)*(5/6)+ i-x-5*p+1];
  elif x mod 6=2 then N[i]:=[i-1,i+1,(x-2)*(5/6)+2+i-x+6*p];
   elif x mod 6=3 then N[i]:=[i-1,i+1,(x-3)*(5/6)+3+i-x-5*p];
    elif x mod 6=4 then N[i]:=[i-1,i+1,(x-4)*(5/6)+4+i-x+6*p];
     elif x mod 6=5 then N[i]:=[i-1,i+1,(x-5)*(5/6)+4+i-x-5*p];
      elif x mod 6=0 then N[i]:=[i-1,i+1,x*(5/6)+1+i-x+6*p];fi;
 if x=1 then N[i]:=[i+1,i+6*p-1,i-5*p];fi;
 if x=6*p then N[i]:=[i-1,i+1,i-6*p+1];fi; od;
k4:=Filtered(k,i-> i mod (16*p) in Union([11*p+1..16*p-1],[0]));
for i in k4 do
 x:=(i-11*p) mod (16*p);
  if x mod 5 =1 then N[i]:=[i-1,i+1,(x-1)*(6/5)+i-x-6*p];
   elif x mod 5 =2 then N[i]:=[i-1,i+1,(x-2)*(6/5)+2+i-x-6*p];
    elif x mod 5 =3 then N[i]:=[i-1,i+1,i-1+5*p];
     elif x mod 5 =4 then N[i]:=[i-1,i+1,(x-4)*(6/5)+4+i-x-6*p];
      elif x mod 5 =0 then N[i]:=[i-1,i+1,i+5*p];fi;
 if x=1 then N[i]:=[i-1,i+1,i-1+5*p];fi;
 if x=5*p then N[i]:=[i-1,i-5*p+1,i+5*p];fi; od;
K5:=[16*p*q+1..n];
for i in K5 do
 x:=i-16*p*q;
 if x mod 2=0 then
     y:=(5/2)*x +16*p*q -5*p;
  else  y:=(5/2 )*(x-1) +3+16*p*q -5*p; fi;
 N[i]:=[y];  N[y][3]:=i; od;
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]);
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]);
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; T:=[]; sz:=0;
for i in [1..n-1] do
```

```
N1:=[];
  for j in Difference(N[i],T) do
    N2:=[];
    N1[j]:=Union(Difference(N[i],Union([j],N[j])),[i]);
    N2[i]:=Union(Difference(N[j],Union([i],N[i])),[j]);
      for t in [2..Size(D[i])-1] do
        for x in Difference(D[i][t],Union(D[j][t],[j])) do
          if not x in D[j][t-1] then
             AddSet(N1[j],x);
           elif x  in D[j][t-1] then
            AddSet(N2[i],x);
         fi; od; od;
   sz:=sz+Size(N1[j])*Size(N2[i]);
  od;   Add(T,i); od;
sz; # (The value of sz  is equal to Szeged index of the graph)
Sc; # (The value of Sc is equal to Schultz index of the graph)
```

Table1. Szeged and Schultz indices of $HAC_5C_6C_7[p,q]$ nanotube

p	q	Szeged	Schultz
3	2	213156	183522
3	3	668817	504438
4	3	1630276	1009944
5	6	23666605	10253380
6	4	12971040	5618280
6	6	41602488	15656184
7	5	39636947	14297514
7	8	154028763	47942944
8	8	232136832	65446528

References

[1] P.P. Khadikar, N.V. Deshpande, P.P. Kale, A.A. Dobrynin, I. Gutman, G. Domotor, J. Chem. Inf. Comput. Sci. **35**, 545 (1995).
[2] H.P. Schultz. J. Chem. Inf. Comput. Sci. **29,** 227 (1989).
[3] M. Schonert, et al., GAP, Groups, Lehrstuhl De fur Mathematik, RWTH: Achen, (1992).
[4] M. Dabirian, A. Iranmanesh. MATCH Commun. Math. Comput. Chem. **54**, 75 (2005),
[5] N. Trinajstic, CRC Press: Boca Roton, FL, (1992)
[6] H.P. Schultz, J. Chem. Inf. Comput. Sci. **40**, 1158 (2000).
[7] S. Klavžar, I. Gutman. Disc. Appl. Math. **80**, 73 (1997).
[8] I. Gutman. J. Chem. Inf. Comput. Sci. **34**, 1087 (1994).
[9] A.A. Dobrynin. Croat. Chem. Acta. **72**, 869 (1999).
[10] A. Iranmanesh, Y. Alizadeh. Am. J. Applied Sci., **5**, 1754 (2008).
[11] A. Iranmanesh, Y. Alizadeh. International Journal of Molecular Sciences, **9,** 131 (2008).
[12] A. Iranmanesh, O. Khormali. Journal of Computational and Theoretical Nanoscience, (in press).

[13] A. Iranmanesh, B. Soleimani, A. Ahmadi. Journal of Computational and Theoretical Nanoscience, **4**, 147 (2007).
[14] A. Iranmanesh, Y. Alizadeh and S. Mirzaei, Digest Journal of Nanomaterials and Biostructures . **4**, 7 **(** 2009).
[15] A. Iranmanesh, B. Soleimani. MATCH Commun. Math Comput. Chem. **57**, 251 (2007).
[16] A. Iranmanesh, O. Khormali. Journal of Computational and Theoretical Nanoscience. **5,** 131 (2008).
[17] A. Iranmanesh, Y. Pakravesh. Ars Combinatoria. **7**, 3606 (2007).
[18] A. Iranmanesh, B. Soleimani, MATCH Commun. Math. Comput. Chem. **57**, 251 (2007).