Eccentric Connectivity Index of HAC$_5$C$_7$[p,q] and HAC$_5$C$_6$C$_7$[p,q] Nanotubes

Ali Iranmanesh[*], Yaser Alizadeh

Department of Mathematics, Faculty of Mathematical Sciences, Tarbiat Modares University, P.O. Box 14115-137, Tehran, Iran

Abstract

For a simple connected graph G, Eccentric connectivity index denoted by $\xi^c(G)$ is defined as: $\xi^c(G) = \sum_{i \in V(G)} (E(i) \times d(i))$, where $E(i)$ is the eccentricity of vertex i, $d(i)$ is the degree of vertex i and $V(G)$ is the set of vertices of G. Eccentricity of vertex i in a graph G is the path length from verte i to vertex j that is farthest from i. In this paper, an algorithm is presented for computing the Eccentric connectivity index of any simple connected graph. Furthermore the Eccentric connectivity index is computed for HAC$_5$C$_7$[p,q] and HAC$_5$C$_6$C$_7$[p,q] Nanotubes by GAP program.

1. Introduction

An important graph theory application is the numerical characterization of chemical structures with graph invariants that can be polynomials, spectra, atomic or molecular topological indices [1,2].

A topological index is a numerical descriptor of the molecular structure based on certain topological features of the corresponding molecular graph. Topological indices are also used as a measure of structural similarity or diversity and thus they may give a measure of the diversity of chemical databases. The main use of topological indices is that of numerical descriptors of the chemical structure in QSPR and QSAR models [3-8]. Because isomorphic

---

[*] Corresponding author
Email address: iranmanesh@modares.ac.ir

graphs have identical values for any given topological index, these indices are graph invariant, i.e. their values are not dependent on a particular labeling of the molecular graph.

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. Degree of vertex u is denoted by $d(u)$. Eccentric connectivity index [9] is a topological index and denoted by $\xi^c(G)$ is defined as:

$$\xi^c(G) = \sum_{i \in V(G)} (E(i) \times d(i)),$$

where $E(i)$ is the eccentricity of vertex i. Eccentricity of vertex i in a graph G is the path length from vertex i to vertex j that is farthest from i. In this paper, an algorithm is presented for computing the Eccentric connectivity index of any simple connected graph. Furthermore the Eccentric connectivity index is computed for $HAC_5C_7[p,q]$ and $HAC_5C_6C_7[p,q]$ Nanotubes by GAP program. In a series of papers some topological indices are computed for some nanotubes [10-18].

2. An algorithm for computing the eccentric connectivity index of any graph

In this section we give an algorithm for computing the Eccentric connectivity index of any simple connected graph. The steps of the algorithm are as follows:

   I.   At first, we assign to any vertex one number.

   II.   The set of vertices that are adjacent to vertex i is denoted by $N(i)$.

  III.   The number of vertices in $N(i)$ is equal to degree of vertex i, $d(i)$.

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 $D_{i,0} = \{i\}$. With the above notations, we have the following relations:

   [1] $V = \bigcup_{t \geq 0} D_{i,t}$, $i \in V(G)$

   [2] $E(u) = Max\{t \,|\, D_{u,t} \neq \phi\}$

   [3] $d(u) = |N(u)|$

According to the above relations, by determining $D_{i,t}, t \geq 1$ and $N(i)$ for every vertex i, we can obtain the Eccentric connectivity index of the graph.

IV. $D_{i,1} = N(i)$, because the distance between vertex i and its adjacent vertices is equal to 1, For each vertex $j \in D_{i,t}$, $(t \geq 1)$, 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

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

By the above equation, we can determine the sets $D_{i,t}$ for every vertex i.

3. Computing the eccentric connectivity index of $HAC_5C_7[p,q]$ nanotubes by GAP program

$HAC_5C_7[p,q]$ nanotube is constructed of C_5C_7 nets (Fig 1). 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. In this section we compute the Eccentric connectivity index of $HAC_5C_7[p,q]$ nanotubes by GAP program.
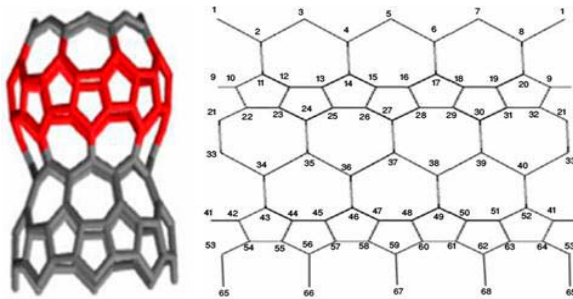

Figure1. $HAC_5C_7[4, 2]$ nanotubes.

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 $3pq$.

K_4: The vertices of the third row in each period whose number is $3pq$.

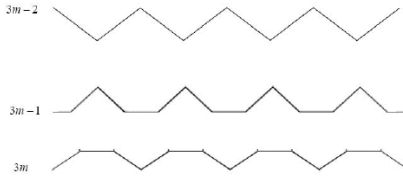K_5: The last vertices of the graph whose number is p.

Figure2. Rows of m-th period.

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 joint of these programs.

```
p:=15; q:=15;# (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;
 D:=[];
for i in [1..n] do
  D[i]:=[];
  u:=[i]; D[i][1]:=N[i];
  u:=Union(u,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]);
  if D[i][t+1]=[] then r:=0;fi;
  t:=t+1;
     od; od;
 C:=[];  d:=[]; Ec:=0;
for i in [1..n] do
   d[i]:=Size(N[i]);
   C[i]:=Size(D[i])-1;
  Ec:=Ec+C[i]*d[i];
 od;
 Ec;
```

p	q	Eccentric connectivity index
3	3	2898
3	4	5184
4	5	10776
5	4	8655
6	5	16200
7	7	37002
7	8	48384
8	6	31344
9	7	47898
10	10	53700
15	15	364410

Table1. Eccentric connectivity index of $HAC_5C_7[p,q]$ Nanotubes

4. Computing the eccentric connectivity index of $HAC_5C_6C_7[p,q]$ by GAP program

A $C_5C_6C_7$ net is a trivalent decoration made by alternating C_5, C_6 and C_7. In this section, similar to previous section we compute the Eccentric connectivity index of $HAC_5C_6C_7[p,q]$ nanotubes by GAP program.
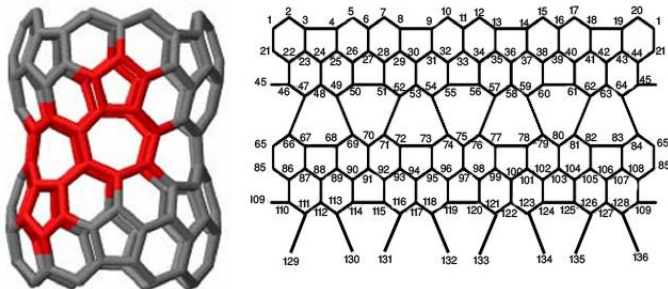

Figure3. $HAC_5C_6C_7[4,2]$ Nanotubes

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 $16pq + 2p$. The Eccentric connectivity index of $HAC_5C_6C_7[p,q]$ Nanotubes is computed for some p and q (Table 2).

	q	Eccentric connectivity index
3	3	6300
3	4	10530
4	5	22200
5	4	20700
6	5	38232
7	7	81312
7	8	101934
8	6	77328
9	7	116640
10	10	237900
15	15	805320

Table2. Eccentric connectivity index $HAC_5C_6C_7[p,q]$ Nanotubes

References

[1]   A. T. Balaban, *Chemical Applications of Graph Theory*, Academic Press, London, 1976.

[2]   J. Devillers, A. T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR,* Gordon & Breach, Reading, 1999.

[3]   R. Garcia-Domenech, A. Villanueva, J. Galvez, R. Gozalbes, Application de la topologie moleculaire a la prediction de la viscosite liquide des composes organiques, *J. Chim. Phys*. **96** (1999) 1172–1185.

[4]   J. V. de Julian-Ortiz, C. de Gregorio Alapont, I. Rios-Santamarina, R. Garrcia-Domenech, J. Galvez, Prediction of properties of chiral compounds by molecular topology, *J. Mol. Graphics Mod.* **16** (1998) 14–18.

[5]   L. Pogliani, Modeling enthalpy and hydration properties of inorganic compounds, *Croat. Chem. Acta*. **3** (1997) 803–817.

[6]   O. Ivanciuc, T. Ivanciuc, A. T. Balaban, Quantitative structure-property relationship study of normal boiling points for halogen-/ oxygen-/ sulfur-containing organic compounds using the CODESSA program, *Tetrahedron* **54** (1998) 9129–9142.

[7]   R. Garcia-Domenech, C. de Gregorio Alapont, J. V. de Ju lian-Ortiz, J. Galvez, L. Popa, Molecular connectivity to find betablockers with low toxicity, *Bioorg. Med. Chem. Lett*. **7** (1997) 567–572.

[8]   L. B. Kier, L. H. Hall, *Molecular Connectivity in Structure-Activity Analysis*, Res. Studies Press, Letchworth, 1986.

[9]   V. Sharma, R. Goswami, A. K Madan, Eccentric connectivity index: A novel highly discriminating topological descriptor for structure-property and structure-activity studies, *J. Chem. Inf. Comput. Sci.* **37** (1997) 273–282.

[10]   V. Kumar, S. Sardana, A. K. Madan, Predicting anti-HIV activity of 2,3-diaryl-1,3-thiazolidin-4-ones: computational approach using reformed eccentric connectivity index, *J. Mol. Mod.* **10** (2004) 399–407;

[11]   A. Iranmanesh, Y. Alizadeh, Computing Wiener and Schultz indices of $HAC_5C_7[p, q]$ nanotube by GAP program, *Am. J. Appl. Sci*. **5** (2008) 1754–1757.

[12]   A. Iranmanesh, Y. Alizadeh, Computing the Szeged and PI indices of $VC_5C_7[p,q]$ nanotubes, *Int. J. Mol. Sci*. **9** (2008) 131–144.

[13]   A. Iranmanesh, Y. Alizadeh, Computing some topological indices by GAP program, *MATCH Commun. Math. Comput. Chem*. **60** (2008) 883–896.

[14]   A.Iranmanesh, O. Khormali, PI index of $HAC_5C_7[p,q]$ nanotube, *J. Comput. Theor. Nanosci.* **5** (2008) 131–139.

[15]   A. Iranmanesh, Y. Pakravesh, Szeged index of $HAC_5C_6C_7[k, p]$ nanotubes, *Ars Comb.* **7** (2007) 3606–3617.

[16]   A. Iranmanesh, Y. Pakravesh, A. Mahmiani, PI and edge-Szeged index of $HC_5C_7[k, p]$ nanotubes, *Util. Math.* **77** (2008) 65–78.

[17]   A. Iranmanesh, Y. Pakravesh, Detour index of $TUC_4C_8(S)$ nanotubes, *Ars Comb.* **84** (2007) 247–254.

[18]   A. Iranmanesh, A. Mahmiani, Y. Pakravesh, Szeged index of HC5C7[r, p] nanotubes, *Ars Comb.* **89** (2008) 309–319.