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Computing the Higher Randić Index of $HAC_5C_7[p,q]$ and $TUZC_6[p,q]$ Nanotubes by GAP Program

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Abstract

In this paper we give an algorithm for computing the higher Randić index R_t of any graph. Also we compute the higher Randić index R_7 of $HAC_5C_7[p,q]$ and $TUZC_6[p,q]$ nanotubes by GAP program.

1. Introduction

One of the main distinctive characteristics of modern chemistry is the use of theoretical tools for the molecular modeling of physicochemical processes, chemical reaction, medicinal and toxicological events, etc., in which chemicals are involved. The success of the molecular modeling is judged by the insights that it offers on the nature of the processes studied, which permit better comprehension and their rational modification. These properties, measured experimentally, are almost invariably expressed in quantitative terms, for instance boiling point, refraction index, transition state energy, percentage of inhibition of some enzymatic activity, lethal dose, and so forth. The paradigm for the modeling of such properties is the relationship that exists between them and the molecular structure of chemical. This fact highlights the first challenge for molecular modeling: the properties are expressed as number while the molecular structure is not. The way to solve this problem is by using molecular descriptors, which are numbers representing information about different molecular features, to describe quantitatively the properties under study. These models are known as quantitative

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structure-property (QSPR) and quantitative structure-activity relationships (QSAR), depending on the physicochemical or biological nature of the properties studied, respectively.
A topological index is a single unique number characteristic of the molecular graph and is mathematically known as the graph invariant. The topological index of a molecule is a non-empirical numerical quantity that quantifies the structure and the branching pattern of the molecule. Therefore, the topological analysis of a molecule involves translating its molecular structure into a characteristic unique number (or index) that may be considered a descriptor of the molecule under examination.
Topological indices of nanotubes are numerical descriptors that are derived from graphs of chemical compounds. Such indices based on the distances in a 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 the chemist Harold Wiener [1] introduced the so-called Wiener index to demonstrate correlations between physicochemical properties of organic compounds and the index of their molecular graphs. In a series of papers, the other topological indices of some nanotubes are computed [2-6], [7-10].

Let G = (V,E) be a simple, connected and finite graph with vertex set V = {1, 2, . . . , n}and edge set E. Let d_i be the degree of the vertex i for $i = 1,2,...n$.The neighborhood of a vertex $i \in V$, denoted by N_i, is the set of vertices adjacent to i.

Another topological index was introduced by Milan Randić in 1975 [11, 12] and called the Randić index or connectivity index, $R_1(G)$, and is defined by

$$R_1(G) = \sum_{ij} \frac{1}{\sqrt{d_i d_j}},$$

where ij runs over all edges in G.

Topological indices, namely Wiener index, Randić's connectivity index based on distances are used to describe the molecular structure of a series of alkylcupferrons used as mineral collectors in the beneficiation of a Canadian uranium ore. There is a linear relation between any of these topological indices and the separation efficiency of the alkylcupferrons considered. The data fit into two separate curves, differentiating the alkylcupferrons into two subclasses, one with rigid rod-like methyl substituents and the other with flexible alkyl substituents. As in the case of Wiener index, connectivity index has also been correlated with

physical properties such as density and heat of vaporization. In addition, connectivity index is also related to some biological properties [12]. The first order connectivity index is also correlated with the limiting organic concentration for third phase formation in solvent extraction [14]. The connectivity indices are extensively used as molecular descriptors in predicting the retention indices in chromatographic analysis of various isomeric aliphatic, aromatic and polycyclic hydrocarbons [15-17].

The higher Randić index or higher connectivity index [18] is also of interest in molecular graph theory. For $t \geq 1$, the higher Randić index is defined by

$$R_t(G) = \sum_{i_1 i \ldots i_{t+1}} \frac{1}{\sqrt{d_{i_1} d_{i_2} \ldots d_{i_{t+1}}}},$$

where $i_1 i_2 \ldots i_{t+1}$ runs over all paths (that is, $i_{j-1} \neq i_{j+1}$ for $2 \leq j \leq t$ and possibly $i_s = i_m$ for $1 \leq s < m-2$) of length t in G.

2. An algorithm for the computation of the higher Randić index $R_t(G)$, for an arbitrary graph G.

We give an algorithm that enables us to compute the higher Randić index of any graph. For this purpose, the following algorithm is presented:

1. We assign one number to any vertex.
2. We determine all of adjacent vertices set of the vertex $i, i \in V$(G) and this set is denoted by N(i).
3. At the start of program we set R_t equal to zero. At the end of program the value of $\frac{1}{2} R_t$ is equal to the higher Randić index of the graph G.
4. For each vertex i we determine all paths of lengths t starting from this vertex like $ii_1 i_2 \ldots i_t$, then add the value of $\frac{1}{\sqrt{d_i d_{i_1} \ldots d_{i_t}}}$ to R_t.

For each vertex i_1 in N_i, the edge ii_1 is a path of length 1 and for each vertex i_2 in $N_{i_1} \setminus \{i\}$, $ii_1 i_2$ is a path of length 2. By following this procedure, for each vertex i_{t-1} in $N_{i_{t-2}} \setminus \{i, i_1, i_2 \ldots i_{t-3}, i_{t-2}\}$ the path $ii_1 \ldots i_{t-1}$ is a path of length t-1. Also for each vertex i_t in

$N_{i_{t-1}} \setminus \{i_1, i_2 ... i_{t-2}, i_{t-1}\}$ the path $ii_1 ... i_{t-1} i_t$ is a path of length t. So we can determine all path of length t, $t \geq 1$.

3. Computing the higher Randić index R_7 of $HAC_5C_7[p,q]$ 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. In this section we compute the higher Randić index of $HAC_5C_7[p,q]$ nanotube by GAP program.

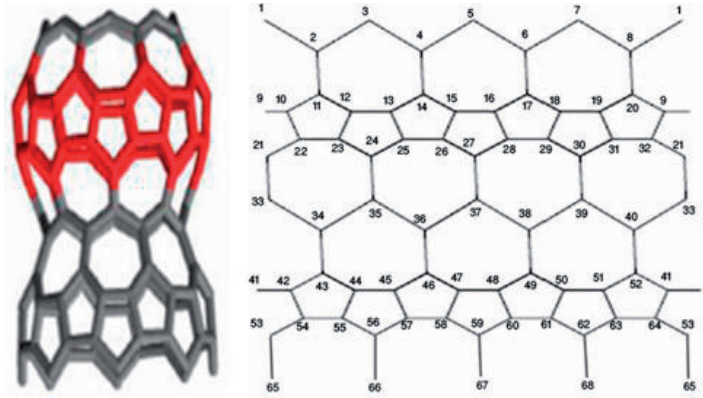

Figure1: HAC_5C_7 [4, 2] nanotube.

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.

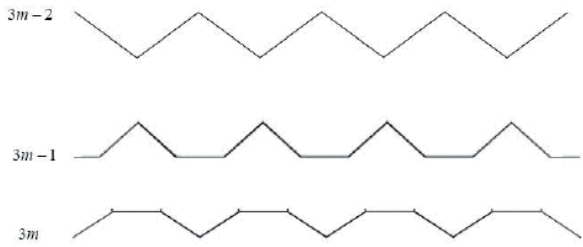

Figure2: Rows of m-th period.

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 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 higher Randić index R_7 of $HAC_5C_7[p,q]$ nanotube for arbitrary p and q.

```
p:=4; 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;
d:=[];
for i in [1..n] do
 d[i]:=Size(N[i]);
od;
r7:=0;
```

```
for i in [1..n] do
  for j in N[i] do
   for x in Difference(N[j],[i]) do
    for y in Difference(N[x],[i,j]) do
     for s in Difference(N[y],[i,j,x]) do
      for t in Difference(N[s],[i,j,x,y]) do
       for k in Difference(N[t],[i,j,x,y,s]) do
        for m in Difference(N[k],[j,x,y,s,t]) do
        r7:=r7+ER(1/(d[i]*d[j]*d[x]*d[y]*d[s]*d[t]*d[k]*d[m]));
        od;
       od;
      od;
     od;
    od;
  od;
od;
    r7:=r7/2; #(This value is equal to the higher Randić index R7 of the graph)
```

4. Computing the Higher Randić index R_7 of $TUZC_6[p,q]$ nanotube by GAP program

In this section we compute the higher Randić index R_7 of $TUZC_6[p,q]$ nanotube similar to the previous section.

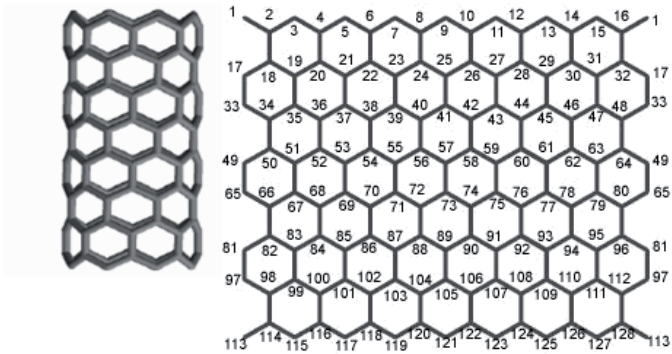

Figure3: Nanotube $TUZC_6[8,8]$

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 is the same as the last program.

```
p:=3; q:=8;#(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;
d:=[];
for i in [1..n] do
 d[i]:=Size(N[i]);
od;
r7:=0;
for i in [1..n] do
   for j in N[i] do
     for x in Difference(N[j],[i]) do
       for y in Difference(N[x],[i,j]) do
        for s in Difference(N[y],[i,j,x]) do
         for t in Difference(N[s],[i,j,x,y]) do
          for k in Difference(N[t],[i,j,x,y,s]) do
           for m in Difference(N[k],[j,x,y,s,t]) do
           r7:=r7+ER(1/(d[i]*d[j]*d[x]*d[y]*d[s]*d[t]*d[k]*d[m]));
           od;
          od;
         od;
        od;
      od;
    od;
  od;
od;
r7:=r7/2; #(This value is equal to the higher Randić index R7 of the graph)
```

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