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An algorithm for computing the Randic and Zagreb indices of a graph

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

In this paper, we give an algorithm that enables us to compute the Randic and Zagreb indices of any graph. Also by this algorithm, we compute the Randic and Zagreb indices for $VAC_5C_6C_7[p,q]$ nanotubes.

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1. Introduction

A topological index is a single unique number characteristic of the molecular graph and is mathematically known as the graph invariant. Mathematical characterization of graphs, including-molecular graphs, can be accomplished using graph invariants. A graph invariant is a graph theoretical property that has the same value for isomorphic graphs [1,2].

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. Molecular topology has been shown to be an excellent tool for a quick and accurate prediction of physico-chemical and biological properties [3-7].

Let G be a connected graph. The vertex-set and edge-set of *G* denoted by *V(G)* and *E(G)* respectively.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 *deg(i)*. Randic index or connectivity index was introduced by Milan Randic in 1975 [9] and is defined by $R(G)=\sum_{ij}\frac{1}{\sqrt{\deg(i)\deg(j)}}$, where ij runs over all edges in G.

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajestic, [10]. They are defined as:

$$M_1(G)=\sum_{v\in V(G)}\deg(v)^2, \tag{1}$$

$$M_2(G)=\sum_{uv\in E(G)}\deg(u)\deg(v). \tag{2}$$

We refer the reader to consult [11-16] for historical background, computational techniques and mathematical properties of the Randic and Zagreb indices.

2. Main results

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

- At first, 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 is denoted by *N(i)*.

The degree of any vertex *i* equals the number of adjacent vertices to *i*. Therefore, by determining the adjacent vertices of each vertex; its degree can also be obtained.

At the beginning of the program, we set *R(G)*, M_1 and M_2 equal to zero. Then we perform the following operation for each vertex *i*:

- We add $(deg(i))^2$ to M_1, then for each vertex *j* in the set of adjacent vertices to vertex i, we add the value *(deg(i)).(deg(j))* to M_2 and $\frac{1}{\sqrt{\deg(i).\deg(j)}}$ to *R(G)*.

At the end of this operation, *R(G)*, M_1 and M_2 are equal to the Randic, first and the second Zagreb indices respectively. Therefore, by determining the vertices adjacent to the vertex of each graph and the above operation, the Randic and Zagreb indices of that graph can be obtained.

3. Discussion

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 Randic and Zagreb indices of $VAC_5C_6C_7[p,q]$ nanotubes by GAP program [17].

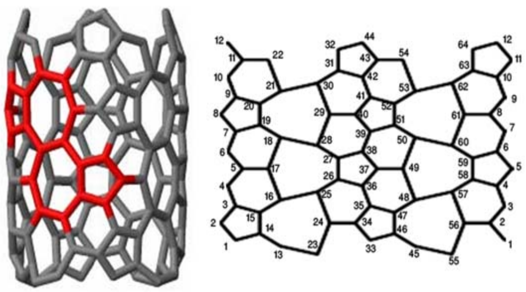

Fig. 1. $VAC_5C_6C_7[2,3]$ nanotube.

According to the first step of the algorithm, we lable the vertices of the graph as figure1 and then determine the set of adjacent vertices of any vertex. The number of vertices of $VAC_5C_6C_7[p,q]$ is 16pq. The first part of the program determine the sets *N(i)* for any vertex i. and then the second part compute the Randic and Zagreb indices of $VAC_5C_6C_7[p,q]$ nanotubes.

```
p:=2; q:=2;# (for example)
n:=16*p*q; N:=[];
K1:=[1..6*p];
for i in K1 do
  x:= i mod 6;
  if x mod 2=0 then N[i]:=[i-1,i+1];
elif x mod 6=1 then N[i]:=[i-1,i+1,(5/6)*(i-1)+2+6*p];
elif x mod 6 in [3,5] then N[i]:=[i-1,i+1,(5/6)*(i-x)+x+6*p];fi;
od;
K:=[6*p+1..n-5*p];
K2:=Filtered(K, i->i mod (16*p) in [1..6*p]);
for i in K2 do
x:= i mod (16*p);
if x mod 6=1 then N[i]:=[i-1,i+1,(5/6)*(x-1)+2+i-x+6*p];
elif x mod 6 in [2,4] then y:=x mod 6;
N[i]:=[i-1,i+1,(5/6)*(x-y)+y+i-x-5*p];
elif x mod 6 in [3,5] then y:=x mod 6;
N[i]:=[i-1,i+1,(5/6)*(x-y)+y+i-x+6*p];
elif x mod 6=0 then N[i]:=[i-1,i+1,(5/6)*x+i-x-5*p];fi;
if x=1  then N[i]:=[i+1,i+6*p+1];fi;
if x=6*p  then N[i]:=[i-1,i-6*p];fi;
od;
K3:=Filtered(K, i->i mod (16*p) in [6*p+1..11*p]);
for i in K3 do
  x:= (i-6*p) mod (16*p);
  if x mod 5 =1 then N[i]:=[i-1,i+1,i+5*p];
elif x mod 5 =2 then N[i]:=[i-1,i+1,(6/5)*(x-2)+1+i-x-6*p];
elif x mod 5 =3 then N[i]:=[i-1,i+1,(6/5)*(x-3)+3+i-x-6*p];
elif x mod 5 =4 then N[i]:=[i-1,i+1,i+5*p-1];
elif x mod 5 =0 then N[i]:=[i-1,i+1,(6/5)*(x-5)+5+i-x-6*p];fi;
if x=1  then N[i]:=[i+1,i+5*p];fi; if x=5*p then N[i]:=[i-1,i-5*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,i-5*p];
elif x mod 5 in [2,4] then y:=x mod 5;
N[i]:=[i-1,i+1,(6/5)*(x-y)+y+i-x+5*p];
elif x mod 5=3 then N[i]:=[i-1,i+1,i-5*p+1];
elif x mod 5=0 then N[i]:=[i-1,i+1,(6/5)*x+i-x+5*p];fi;
if x=1 then N[i]:=[i+1,i-5*p];fi; if x=5*p then N[i]:=[i-1,i+6*p];fi;
od;
K5:=[n-5*p+1..n];
for i in K5 do x:=i+5*p-n;
if x mod 5=1 then N[i]:=[i-1,i+1,i-5*p];
elif x mod 5 in [2,4] then y:=x mod 5;
N[i]:=[i-1,i+1,(6/5)*(x-y)+y];N[(6/5)*(x-y)+y][3]:=i;
elif x mod 5=3 then N[i]:=[i-1,i+1,i-5*p+1];
elif x mod 5=0 then N[i]:=[i-1,i+1,(6/5)*x]; N[(6/5)*x][3]:=i;fi;
if x=1 then N[i]:=[i+1,i-5*p];fi; if x=5*p then N[i]:=[i-1,6*p];fi;
od;
N[1]:=[2,6*p+2];N[6*p]:=[6*p-1,n]; D:=[]; v:=[];
```

```
deg:=[];
R:=0;
M1:=0;
M2:=0;
for i  in [1..n] do
  deg[i]:=Size(N[i]);
od;
for i  in [1..n] do
   M1:=M1+(deg[i])^2;
for j in N[i] do
 M2:=M2+deg[i]*deg[j];
#R:=R+ ER(1/((deg[i]*deg[j])));
 od;
od;
```

```
#R:=R/2; #(this value is equal to Randic index of the graph)
```

```
M1; #( the value of M1 is equal to the first Zagreb index)
```

```
M2:=M2/2; #(the value of M2 is equal to the second Zagreb index)
```

Table 1. The Randic and Zagreb indices of $VAC_5C_6C_7[p,q]$ nanotubes.

p	q	The Randic index	The first Zagreb index	The second Zagreb index
3	3	71.79796	1206	1761
3	4	95.73061	1608	2348
4	5	159.6633	1638	2409
5	4	159.7306	2760	4076
5	6	239.5959	4140	6114
6	5	239.6633	4170	6175
7	7	391.5286	6846	10157

4. Conclusions

An algorithm has been presented for computing the Randic and Zagreb indices of any connected simple graph. According to the algorithm and using the GAP program, we can write a program to compute these indices quickly. This method has been used here for the first time. We test the algorithm to calculate the Randic and Zagreb indices of $VAC_5C_6C_7[p,q]$ nanotubes.

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*Corresponding author: iranmanesh@modares.ac.ir