Balaban and Randic Indices of IPR C$_{80}$ Fullerene Isomers, Zigzag Nanotubes and Graphene

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Abstract:

In this paper an algorithm for computing the Balaban and Randic indices of any simple connected graph was introduced. Also these indices were computed for IPR C$_{80}$ fullerene isomers, Zigzag nanotubes and graphene by GAP program.

Keywords: Balaban index, Randic index, IRP C$_{80}$ Fullerene isomers, Zigzag nanotubes, Graphene, GAP program.

1. INTRODUCTION

Topological descriptors are derived from hydrogen-suppressed molecular graphs, in which the atoms are represented by vertices and the bonds by edges. The connections between the atoms can be described by various types of topological matrices (e.g., distance or adjacency matrices), which can be mathematically manipulated so as to derive a single number, usually known as graph invariant, graph-theoretical index or topological index[1,2].

Topological indices 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 [3-7].

Let G be a connected graph. The vertex-set and edge-set of *G* are 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 δ_i. The Balaban index of a molecular graph G was introduced by A.T. Balaban [8,9]. It is denoted by J(G) and defined

as $J(G) = \dfrac{m}{\mu+1} \displaystyle\sum_{ij \in E(G)} \dfrac{1}{\sqrt{d(i)d(j)}}$ where *m* is the

number of edges of G and $\mu(G)$ is the cyclomatic number of G. Noting that the cyclomatic number is the minimum number of edges that must be removed from G in order to transform it to an acyclic graph; it can be calculated using $\mu(G) = m - n + 1$ where *n* is the number of vertices and *d(i)* is the sum of distances between vertex i and all other vertices of G, and the summation goes over all edges from the edge set *E(G)*.

The Balaban index appears to be a very useful molecular descriptor with attractive properties

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[10,11]. 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 [12-14]. Randic or connectivity index was introduced by Milan Randic in 1975 [15] defined as $R(G) = \sum_{ij} \dfrac{1}{\sqrt{\delta_i \delta_j}}$, where j runs over all edges in G. In a series of papers, Balaban and Randic indices of some nanotubes are computed [16-18]. In this paper we give an algorithm for computing the Balaban and Randic indices of any graph. Also, by using GAP program [19], we compute these indices for IPR C_{80} fullerene isomers, zigzag nanotubes and graphene. IPR fullerenes are described in [20-22].

2. An algorithm for computing the Balaban and Randic indices

In this section an algorithm for computing the Balaban and Randic indices of any graph was introduced.

I. At first, one number was assigned to each vertex.

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

The set of vertices that their distance to vertex u is equal to t $(t \geq 0)$ is denoted by $D_t(u)$ and consider $D_0(u) = \{u\}$. So, the following relations are obtained:

- $V(G) = \bigcup_{t \geq 0} D_t(u), \ \forall u \in V(G)$

- $d(u) = \sum_{v \in V(G)} d(u,v) = \sum_{t \geq 1} t \times |D_t(u)| , \forall u \in V(G)$

- $\delta_u = |N(u)|$

According to the above relations, we can obtain the Balaban index by determining the $D_t(u)$ for every vertex u.

III. 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 be-

tween each vertex of $N(j) \setminus (D_{i,t} \bigcup D_{i,t-1})$ and the vertex i is equal to $t+1$. Thus we have:

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

According to the above equation we can obtain $D_{i,t}, \ t \geq 2,$ for each $i \in V(G)$. By determining the sets $D_{i,t}$ we can compute the Balaban and Randic indices of G.

3. Computing the Balaban and Randic indices for IPR C_{80} fullerene isomers

Fullerenes consist of the networks of pentagons and hexagons. To be a closed shape, a fullerene should exactly have 12 pentagon faces, but the number of hexagons faces can be extremely variable. Fullerenes were discovered in 1985 by Robert Curl, Harold Kroto and Richard Smalley at the University of Sussex and Rice University, and are named after Richard Buckminster Fuller. The fullerene gallery at the address http://www.cochem2.tutkie.tut.ac.jp/Fuller/fsl/fsl.html presents many of them including non-IPR ones. Seven possible IPR isomers C_{80} are shown in Figure 1.
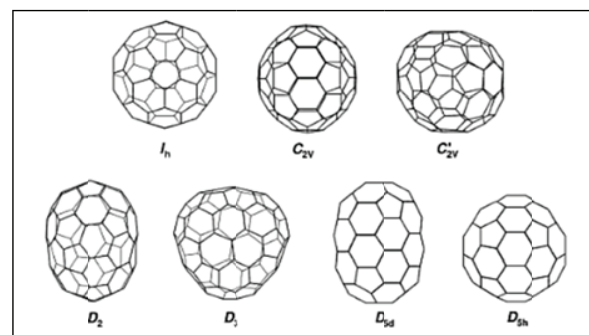
Figure 1: Seven possible isomers of C_{80} with their symmetry according to an Atlas of fullerene [23].

For computing these indices for IPR C_{80} fullerene isomers, one number is firstly assigned to any vertex of the graph and then according to the above algorithm, we can write a GAP program to determine $N(i)$ and $D_{i,t}$. Take the IPR isomer D5h of C_{80}

fullerene and assign to any vertex of the graph one number as in Figure 2.

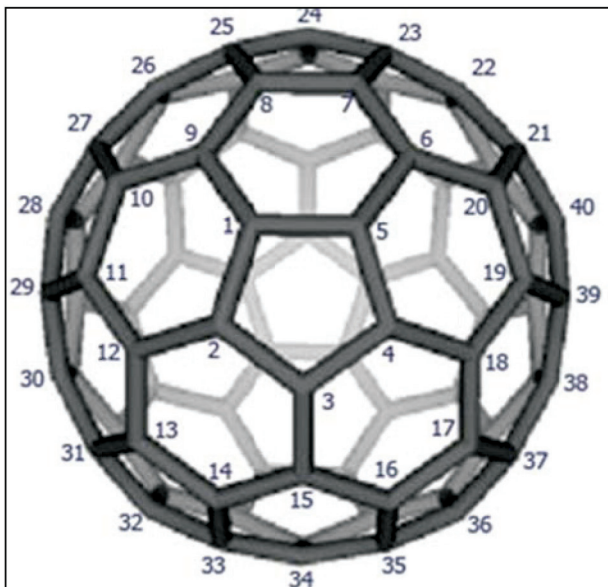**Figure 2:** *The IPR isomer D$_{5h}$ of C80 Fullerene which is numbered.*

Using the following GAP program, the Balaban and Randic indices for the above IPR isomer of C$_{80}$ fullerene are computed as follows:

```
n:=80; k:=[]; N:=[];
k[1]:=[1..5]; k[2]:=[6..20]; k[3]:=[21..40];
k[4]:=[41..60]; k[5]:=[61..75]; k[6]:=[76..80];
for i in [1..6] do
 y:=Size(k[i]);
 for j in [1..y] do
  x:=k[i][j];
  N[x]:=[x-1,x+1];
 od;
od;
D1:=[9,12,15,18];
for i in [1..4] do
 x:=D1[i]; N[i][3]:=x; N[x][3]:=i;
od;
D2:=Difference(k[2],Filtered(k[2],i->(i      mod
3)=0));
D3:=Filtered(k[3],i->(i mod 2)=1);
for i in [1..9] do
```

```
 x:=D3[i+1]; N[D2[i]][3]:=x; N[x][3]:=D2[i];
od;
D4:=Difference(k[3],D3);
D5:= Filtered(k[4],i->i mod 2=1);
for i in [1..9] do
 x:=D5[i+1]; N[D4[i]][3]:=x; N[x][3]:=D4[i];
od;
D6:=Difference(k[4],D5);
D7:= Filtered(k[5],i->(i mod 3)<>2);
for i in [1..9] do
 x:=D7[i+1]; N[D6[i]][3]:=x; N[x][3]:=D6[i];
od;
D8:=Difference(k[5],D7);
for i in [1..4] do
 x:=k[6][i+1]; N[D8[i]][3]:=x; N[x][3]:=D8[i];
od;
N[1]:=[2,5,9];      N[5]:=[1,4,6];      N[6]:=[5,7,
20];N[20]:=[6,19,21];N[21]:=[20,22,40];
N[40]:=[21,39,41];   N[41]:=[40,42,60];N[60]:=[
61,59,41];N[61]:=[60,62,75]; N[74]:=[73,75,76];
N[75]:=[58,61,74];          N[76]:=[74,77,80];
N[80]:=[71,76,79];
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]);
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;
m:=(1/2)*Sum(v)-n+1;
d:=[];deg:=[];
for i in [1..n] do
d[i]:=0;
deg[i]:=Size(N[i]);
for t in [1..Size(D[i])] do
d[i]:=d[i]+t*Size(D[i][t]);
od;od;
B:=0;R:=0;
for i in [1..n] do
```

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for j in N[i] do
B:=B+ER(1/((d[i]*d[j])));
R:=R+ ER(1/((deg[i]*deg[j])));
od;
od;
B:=m*B/2;#(this value is equal to Balaban index of the graph)
*R:=R/2; #(this value is equal to Randic index of the graph)*

Similar programs were applied for computing the Balaban and Randic indices of other IPR isomers C_{80} fullerene and results are shown in Table 1. For all C_{80} isomers, the Randic index is constant, and it's equal to 13.333.

Table 1: *The Balaban index of IPR C80 Fullerene isomers.*

IPR isomers of C_{80} fullerene	Balaban index
D_{5d}	0.81074
D_2	0.80994
C_{2v}	0.80701
D_3	0.80915
$C`_{2v}$	0.80499
D_{5h}	0.80281
lh	0.79822

4. Computing the Balaban and Randic indices for Zigzag nanotubes and graphene

In this section, the Balaban and Randic indices of zigzag nanotubes and grapheme were computed similar to those given for IPR C_{80} fullerene.
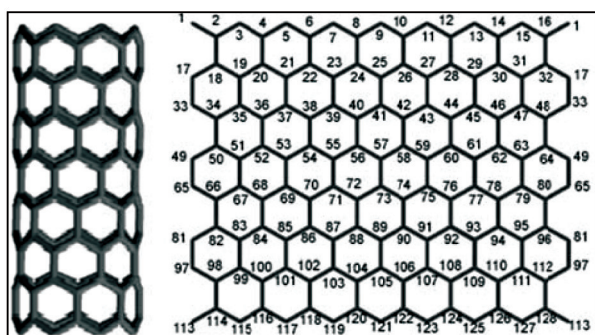
Figure 3: *Zigzag[8,8] nanotube.*

To do this we denote the number of hexagons in the first row by and the number of rows by . In each row, there are vertices and hence the number of vertices in this nanotubes is equal to . 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;
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]);
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;
m:=(1/2)*Sum(v)-n+1;
d:=[];deg:=[];
for i in [1..n] do
d[i]:=0;
deg[i]:=Size(N[i]);
for t in [1..Size(D[i])] do
d[i]:=d[i]+t*Size(D[i][t]);
od;od;
B:=0;R:=0;
```

```
for i in [1..n] do
 for j in N[i] do
 B:=B+ER(1/((d[i]*d[j])));
R:=R+ ER(1/((deg[i]*deg[j])));
od;od;
B:=m*B/2;#(this value is equal to Balaban index
of the graph)
R:=R/2; #(this value is equal to Randic index of the
graph)
```

By a similar way, the Balaban and Randic indices for graphene can be obtained. The number of hexagons in the first row is denoted by and the number of rows by .
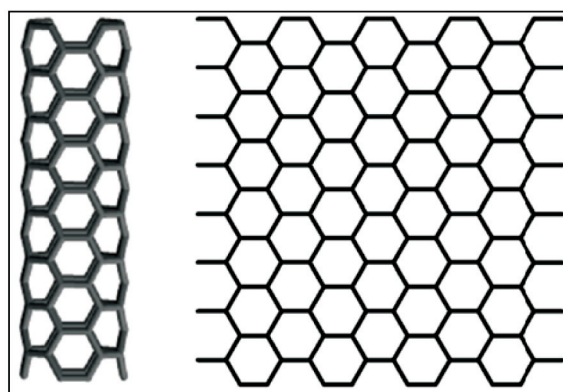

Figure 4: *Graphene[4,8] nanotube.*

Table 2: *Balaban and Randic indices of zigzag[p,q] nanotubes and graphene[p,q].*

P	q	Balaban index of zigzag[p,q]	Randic index of zigzag[p,q]	Balaban index of grapheme[p,q]	Randic index of grapheme[p,q]
2	2	1.95970	3.93265	1.71379	7.93265
2	3	1.67044	5.93265	1.42196	11.93265299
4	5	1.096412	19.86531	0.82065	39.86530
3	5	1.16766	14.89898	0.92423	29.89897
6	4	1.03259	23.79796	0.70617	47.79795
5	3	1.27712	14.83163	0.88425	29.83163
7	7	0.73099	48.76429	0.51655	97.76428

The Randic index of zigzag[p,q] nanotubes and graphene are equal to

$$R(zigzag) = p\left(\frac{2\sqrt{6} + 3q - 5}{3} \right) \text{ and }$$

$$R(graphene) = p\left(2q - \frac{5}{3} + \frac{4}{\sqrt{6}} \right),$$

respectively. For example, we obtained the Balaban and Randic indices of zigzag[p,q] and graphene nanotubes for some p and q by GAP program. In Table 2, these numbers are presented.

5. CONCLUSION

An algorithm has been presented for computing the Balaban and Randic indices of any connected simple graph. According to this algorithm and using the GAP program, a program can be written to compute these indices quickly. This method has been used here for the first time. We tested the algorithm to calculate the Balaban and Randic indices of IPR C80 fullerene isomers, zigzag nanotubes and graphene.

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