

Computing Schultz and modified Schultz indices of C_{80} fullerene by GAP program

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In this paper, we give a GAP program for computing the Schultz and the modified Schultz indices of C_{80} fullerene.

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1. Introduction

Topological indices are real numbers related to a structural graph of a molecule. It does not depend on the labeling or pictorial representation of a graph. Such indices based on the distances in graph are widely used for establishing relationships between the structure of a molecular graph and their physicochemical properties. Usage of topological indices in biology and chemistry began in 1947 when chemist Harold Wiener [1] introduced Wiener index to demonstrate correlation between physicochemical properties of organic compounds and the index of their molecular graphs.

Let G be a simple connected graph, the vertex and edge sets of G denoted by $V(G)$ and $E(G)$, respectively. The distance between two vertices u and v of G is denoted by $d(u, v)$ and it is defined as the number of edges in a shortest path connecting u and v .

The “molecular topological index” (Schultz index) was introduced by Harry Schultz [2]. The Schultz index is defined as:

$$S(G) = \sum_{\{u,v\} \subseteq V(G)} (\delta_u + \delta_v) d(u, v)$$

where δ_u is degree of vertex u .

Klavzar and Gutman in [3] defined the modified Schultz index as:

$$MS(G) = \sum_{\{u,v\} \subseteq V(G)} (\delta_u \delta_v) d(u, v)$$

In a series of paper another topological indices are computed [4-22].

In this paper we give an algorithm for obtaining the Schultz and the modified Schultz indices of any graphs. Then by this algorithm, we compute these indices for C_{80} fullerene by GAP program.

2. Results

In this section we give an algorithm for obtaining the Schultz and the modified Schultz indices for any graph. For this purpose, the following algorithm is presented:

At first, we label the vertices of the graph, then we determine all of adjacent vertices set of the vertex u , $u \in V(G)$ and this set is denoted by $N(u)$.

The set of vertices that their distance to vertex u is equal to t ($t \in \mathbb{N}$) is denoted by $D_t(u)$.

$$D_t(u) = \{v \mid d(u, v) = t\}$$

$$D_0(u) = \{u\}$$

$$D_1(u) = N(u)$$

The distance between each vertex of set $N(v) \setminus (D_t(u) \cup D_{t-1}(u))$ and the vertex u is equal to $t+1$, thus we have:

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

We have the following relations:

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

$$S(G) = \sum_{\{u,v\} \subseteq V(G)} (\delta_u + \delta_v) d(u, v)$$

$$MS(G) = \sum_{\{u,v\} \subseteq V(G)} (\delta_u \delta_v) d(u, v)$$

3. Results and discussion

Fullerenes are cage-like molecules formed as a twenty-sided geometric shape.

Fullerenes consist of the networks of pentagons and hexagons. To be a closed shape, a fullerene should exactly have 12 pentagon sides, but the number of hexagon sides can be extremely variable. The degree of any vertex u of fullerene graph is equal to 3. In order to name fullerenes, letter C is followed by the number of carbon.

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.

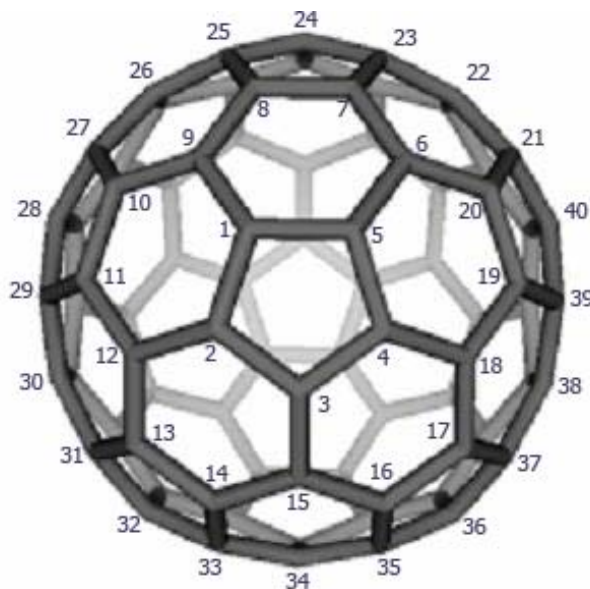


Fig. 1. C_{80} fullerene.

There are seven IPR-satisfying isomers for C_{80} . For these seven isomers, the Schultz and the modified Schultz indices are computed by the following GAP program [23] in Table1.

By the following program we can compute the Schultz and the modified Schultz indices of C_{80} fullerene:

```
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:=[]; 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;
  S:=0; MS:=0; Deg:=[];
  for i in [1..n] do
    Deg[i]:=Size(N[i]);
  od;
  for i in [1..n] do
    for t in [1..Size(D[i])] do
      for j in D[i][t] do
```

```

S:=S+(Deg[i]+Deg[j])*t;
MS:=MS+(Deg[i]*Deg[j]*t);
od;
od;
od;
S:=S/2;
MS:=MS/2;

```

Table 1. Schultz and modified Schultz indices of isomer's C_{80} fullerene.

Isomers of C_{80} fullerene	Schultz index	modified Schultz index
No.1-D5d	105600	158400
No.2-D2	104040	156060
No.3-C2v	104112	156168
No.4-D3	104472	156708
No.5-C2v	104208	156312
No.6-D5h	104724	157086
No.7-lh	105000	157500

4. Conclusions

An algorithm has been presented for computing the Schultz and the modified Schultz indices of any graphs. 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 these indices for C_{80} fullerene.

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