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Schultz and Modified Schultz Polynomials of C_{100} Fullerene

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Abstract

In this research, we give a GAP program for computing the Schultz and modified Schultz polynomials of any connected graph. We computing the Schultz and modified Schultz polynomials of isomeres of C_{100} fullerene by this program.

1. Introduction

Topological index is a numerical value associated with chemical consitution purporting fir correlation of chemical strcture with various physical properties, chemical reactivity or biological activity.

The numerical basis for topological indices is provided(depending on how a molecular graph is converted into a numerical value) by either the adjacency matrix or the topological distance matrix. In the latter the topological distance between two vertices is the number of edges in the shortest path between these.

Let G be a connected graph. The vertex-set and edge-set of G denoted by V(G) and E(G) respectively. The degree of a vertex $u \in V(G)$ is the number of vertices joining to u and denoted by δ(u). Distance is an important concept in graph theory and it has applications to computer science, chemistry, and a variety of other fields. The "molecular topological index"

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(Schultz index) was introduced by Harry Schultz in 1989 [1]. The molecular topological index studied in many papers [3-5].

The Schultz index is defined as:

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

Klavzar and Gutman defined the Modified Schultz [2]

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

In [6], Haruo Hosoya used polynomials to generate distance distributions for graphs.

The Schultz polynomial of *G* is:

$$H_1(G,x)=\sum_{\{u,v\}\subseteq V(G)}(\delta_u+\delta_v)x^{d(u,v)}$$

Also the modified Schultz polynomial of G is defined as:

$$H_2(G,x)=\sum_{\{u,v\}\subseteq V(G)}(\delta_u\delta_v)x^{d(u,v)}$$

Observe that the degree of the Schultz polynomial and the modified Schultz polynomial is equal to the diameter of *G*. Also, notice that

$$H_1'(G,x)=S(G)$$

$$H_2'(G,x)=MS(G)$$

In a series of papers the Schultz and the modified Schultz indices for some fullerene are computed[7-10].

In this paper, we give a method for computing the Schultz and the modified Schultz polynomials for any graph and by this method, we obtain these polynomials for C_{100} fullerene by GAP program.

2. Result

In this section we give a method for obtaining Schultz and modified Schultz polynomials 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 ($t \geq 0$) 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:

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

We have the following relations:

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

- $H_1(G,x) = \sum_{\{u,v\} \subseteq V(G)} (\delta_u + \delta_v) x^{d(u,v)} = \frac{1}{2} \sum_{i=1}^{n} \sum_{i \neq j=1}^{n} (\delta_i + \delta_j) x^{d(i,j)} = \frac{1}{2} \sum_{i=1}^{n} \sum_{j \in D_t(i)} (\delta_i + \delta_j) x^t$

- $H_2(G,x) = \sum_{\{u,v\} \subseteq V(G)} (\delta_u \delta_v) x^{d(u,v)} = \frac{1}{2} \sum_{i=1}^{n} \sum_{i \neq j=1}^{n} (\delta_i \delta_j) x^{d(i,j)} = \frac{1}{2} \sum_{i=1}^{n} \sum_{j \in D_t(i)} (\delta_i \delta_j) x^t$

2-1. Fullerene:

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 pentagon sides and no two pentagon networks have any common vertex, but the number of hexagon sides can be extremely variable. The molecular graph of fullerene is 3-regular. There are 120 edges in the molecular graph of C_{100} fullerene.

There are 450 IPR-satisfying isomers for C_{100}. For some isomers, the Schultz and the modified Schultz polynomials are computed by the following GAP program [11] in table1.

```
v:=[]; D:=[]; md:=1;
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;
md:=MaximumList([md,Size(D[i]-1)]);
od;
C:=[];   MC:=[];
for k in [1..md] do
  C[k]:=0;
  MC[k]:=0;
od;
 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])-1] do
        for j in D[i][t] do
       C[t]:=C[t]+(Deg[i]+Deg[j]);
      MC[t]:=MC[t]+(Deg[i]*Deg[j]);
      od;
    od;
 od;
C:=C/2; # (C is the Schultz polynomial's coefficients of C100Fullerene)
MC:=MC/2;# (MC is the modified Schultz polynomial's coefficients of C100 Fullerene)
```

Isomers of C_{100} Fullerene	Schultz polynomials	modified Schultz Polynomials
N0.2-D2	$900x+1800x^2+2520x^3+3240x^4+3600x^5+3960x^6+3888x^7+3540x^8+3036x^9+2064x^{10}+996x^{11}+144x^{12}+12x^{13}$	$1350x+2700x^2+3780x^3+4860x^4+5400x^5+5940x^6+5832x^7+5310x^8+4554x^9+3096x^{10}+1494x^{11}+216x^{12}+18x^{13}$
N0.4-C2	$900x+1800x^2+2520x^3+3240x^4+3600x^5+3948x^6+3864x^7+3546x^8+3024x^9+2154x^{10}+894x^{11}+210x^{12}$	$1350x+2700x^2+3780x^3+4860x^4+5400x^5+5922x^6+5796x^7+5319x^8+4536x^9+3231x^{10}+1341x^{11}+315x^{12}$
N0.14-Cs	$900x+1800x^2+2520x^3+3240x^4+3600x^5+3960x^6+3852x^7+3600x^8+3024x^9+1980x^{10}+1116x^{11}+108x^{12}$	$1350x+2700x^2+3780x^3+4860x^4+5400x^5+5940x^6+5778x^7+5400x^8+4536x^9+2970x^{10}+1674x^{11}+162x^{12}$
N0.36-C2v	$900x+1800x^2+2520x^3+3240x^4+3600x^5+3936x^6+3858x^7+3546x^8+3018x^9+2154x^{10}+1056x^{11}+72x^{12}$	$1350x+2700x^2+3780x^3+4860x^4+5400x^5+5904x^6+5787x^7+5319x^8+4527x^9+3231x^{10}+1584x^{11}+108x^{12}$

N0.184-C1	$900x+1800x^2+2520x^3+3240x^4+3600x^5+3924x^6+3828x^7+3540x^8+3000x^9+2106x^{10}+1152x^{11}+90x^{12}$	$1350x+2700x^2+3780x^3+4860x^4+5400x^5+5886x^6+5742x^7+5310x^8+4500x^9+3159x^{10}+128x^{11}+135x^{12}$
N0.221-C3	$900x+1800x^2+2520x^3+3240x^4+3600x^5+3906x^6+3816x^7+3528x^8+2988x^9+2124x^{10}+1152x^{11}+126x^{12}$	$1350x+2700x^2+3780x^3+4860x^4+5400x^5+5859x^6+5724x^7+5292x^8+4482x^9+3186x^{10}+1728x^{11}+189x^{12}$
N0.321-T	$900x+1800x^2+2520x^3+3240x^4+3600x^5+3960x^6+3852x^7+3600x^8+3024x^9+1980x^{10}+1116x^{11}+108x^{12}$	$1350x+2700x^2+3780x^3+4860x^4+5400x^5+5940x^6+5778x^7+5400x^8+4536x^9+2970x^{10}+1674x^{11}+162x^{12}$
N0.390-D2	$900x+1800x^2+2520x^3+3240x^4+3600x^5+3888x^6+3816x^7+3528x^8+3000x^9+2208x^{10}+1116x^{11}+84x^{12}$	$1350x+2700x^2+3780x^3+4860x^4+5400x^5+5832x^6+5724x^7+5292x^8+4500x^9+3312x^{10}+1674x^{11}+126x^{12}$
N0.395-D2d	$900x+1800x^2+2520x^3+3240x^4+3600x^5+3888x^6+3804x^7+3504x^8+2988x^9+2136x^{10}+1200x^{11}+120x^{12}$	$1350x+2700x^2+3780x^3+4860x^4+5400x^5+5832x^6+5706x^7+5256x^8+4482x^9+3204x^{10}+1800x^{11}+180x^{12}$
N0.450-D5	$900x+1800x^2+2520x^3+3240x^4+3600x^5+3840x^6+3780x^7+3450x^8+2970x^9+2100x^{10}+1230x^{11}+270x^{12}$	$1350x+2700x^2+3780x^3+4860x^4+5400x^5+5760x^6+5670x^7+5175x^8+4454x^9+3150x^{10}+1845x^{11}+405x^{12}$

Table1. Schultz and modified Schultz polynomials of some C_{100} fullerene's isomers

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