Digest Journal of Nanomaterials and Biostructures Vol. 4, No.1, March 2009, p. 7 - 10

COMPUTING SCHULTZ POLYNOMIAL, SCHULTZ INDEX OF C_{60} FULLERENE BY GAP PROGRAM

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In this paper, we give a GAP program for computing the Schultz polynomial of any graph. Also we compute the Schultz index and Schultz polynomial of C_{60} fullerene by this program.

(Received January 6, 2009; accepted January 21, 2009)

Keywords: Fullerene**,** Schultz polynomial, Schultz index, GAP programming.

1. Introduction

Topological indices are the numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. 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. Such indices based on the distances in graph are widely used for establishing relationships between the structure of molecular graph and their physicochemical properties. Let G be a connected graph. The vertex-set and edge-set of G 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 $u \in V(G)$ is the number of vertices joining to u and denoted by δ_u.

One of the topological index is Schultz index and denoted by MTI. This index was introduced by Schultz in 1989, as the molecular topological index [1], and it is defined by:

$$MTI(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (\delta_u + \delta_v) d(u,v) \tag{1}$$

The Schultz polynomial of G is defined as:

$$H(G,x) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (\delta_u + \delta_v) x^{d(u,v)} \tag{2}$$

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

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$$H'(G,1) = MTI(G) \tag{3}$$

The molecular topological index studied in many papers [2-5]. In a series of paper some topological indices are computed [6-10].

2. Results

According to the equation (3) we can obtain the Schultz index of the graph by the Schultz polynomial.

In this section we give an algorithm for obtaining the Schultz polynomial for any graph.

For this purpose, the following algorithm is presented:

1- We number the vertices of the graph.

2- We determine all of adjacent vertices set of the vertex u, $u \in V(G)$ and this set denoted by N(u).

The set of vertices that their distance to vertex u is equal to $t\ (t \geq 0)$ is denoted by $D_{u,t}$ and consider $D_{u,0}\{u\}$, $\delta_{u,t} = \sum_{v \in D_{u,t}} \delta_v$. We have the following relations:

- $\sum_{v \in V(G)} d(u,v) = \sum_{t \geq 1} t \times \left| D_{u,t} \right|$, $\forall u \in V(G)$
- $\delta_u = \left| N(u) \right|$
- $V(G) = \bigcup_{t \geq 1} D_{u,t}$ $\forall u \in V(G)$
- $H(G,x) = \frac{1}{2} \sum_{u \in V(G)} \sum_{t \geq 1} (\left| D_{u,t} \right| \times \delta_u + \delta_{u,t}) x^t$

According to the above relations, by determining $D_{u,t}$, $t \geq 1$, we can obtain the Schultz polynomial of the graph G.

3- The distance between vertex i and its adjacent vertices is equal to 1, therefore $D_{u,1} = N(u)$. For each $v \in D_{u,t}$, $t \geq 1$, the distance between each vertex of set $N(v) \setminus (D_{u,t} \cup D_{u,t-1})$ and the vertex u is equal to $t+1$, thus we have

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

3. Discussion and conclusions

In this section we compute the Schultz polynomial and Schultz index of C_{60} Fullerene by GAP program. Fullerenes are cage-like molecules formed as a twenty-sided geometric shape. In order to name fullerenes, letter C is followed by the number of carbon atoms existent in the networks of fullerenes. (e.g. C_{60}).Fullerens 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. 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.

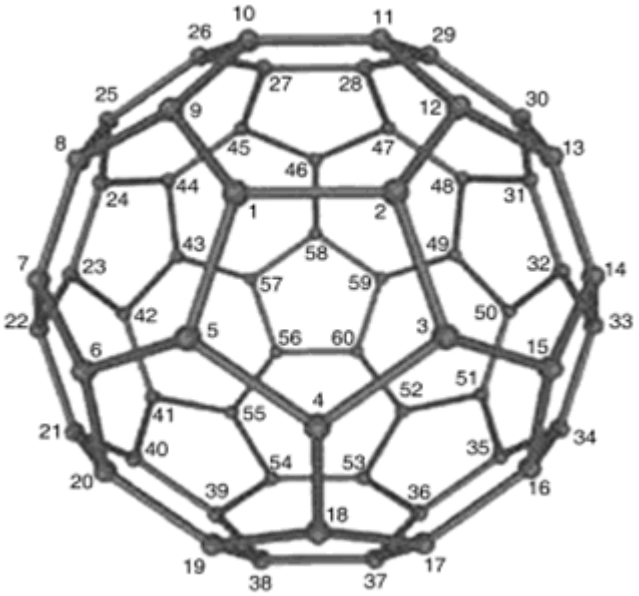

Fig. 1. C_{60} fullerene

The following program computes the Schultz polynomial's coefficients of C_{60} fullerene.

```
n:=60; k:=[];N:=[];
k[1]:=[1..5]; k[2]:=[6..20]; k[3]:=[21..40];
k[4]:=[41..55]; k[5]:=[56..60];
for i in [1..5] 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 4) in [1,2]);
for i in [1..9] do
 x:=D2[i]; N[D3[i+1]][3]:=x; N[x][3]:=D3[i+1];
od;
D4:=Difference(k[3],D3);
D5:=Filtered(k[4],i->(i mod 3)<>1);
for i in [1..9] do
 x:=D4[i]; N[D5[i+1]][3]:=x; N[x][3]:=D5[i+1];
od;
D6:=Difference(k[4],D5);
for i in [1..4] do
x:=D6[i]; N[k[5][i+1]][3]:=x; N[x][3]:=k[5][i+1];
od;
N[1]:=[2,5,9]; N[5]:=[1,4,6]; N[6]:=[5,7,20]; N[20]:=[19,21,6];
N[21]:=[20,22,40]; N[40]:=[39,41,21]; N[41]:=[40,42,55];
N[55]:=[54,56,41]; N[56]:=[55,57,60];N[60]:=[52,56,59];
```

```
md:=1; 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;
md:=MaximumList([md,Size(D[i])]);
od;
p:=[];
for i in [1..md] do p[i]:=0; od;
for t in [1..md] do
 for i in [1..n] do
x:=0;
for j in D[i][t] do
x:=x+Size(N[j]); od;
 p[t]:=p[t]+((Size(D[i][t]))*v[i]+x);
 od;od;
p:=p/2;#(p is the set the Schultz polynomial's coefficients of C60 fullerene)
```

Table1. The Schultz polynomial, Schultz index of C_{60} fullerene

$H(C_{60},x)$	$540x+ 1080x^2+1440x^3 +1800x^4+1800x^5+1800x^6+1440x^7 +540x^8+180x^9$
$MTI(C_{60})$	50040

References

[1] H. P. Schultz. J. Chem. Inf. Comput. Sci. **29**, 227 (1989).
[2] A. A. Dobrynin. Croat. Chem. Acta. **72**, 869 (**1999**).
[3] H. P. Schultz, J. Chem. Inf. Comput. Sci. **40**, 1158 (2000).
[4] S. Klavžar, I. Gutman. Disc. Appl. Math. **80**, 73 (**1997**).
[5] I. Gutman. J. Chem. Inform. Comput. Sci. **34**, 1087 (**1994**).
[6] A. Iranmanesh, Y. Alizadeh. Am. J. Applied Sci. **5**, 1754 (2008).
[7] A. Iranmanesh, Y. Alizadeh. Am. J. Applied Sci. **5,** 1754 (2008)
[8] A. Iranmanesh, B. Soleimani. MATCH Commun. Math Comput. Chem. ***57***, 251 (2007).
[9] A.Iranmanesh, O. Khormali. J. Comput. Theor. Nanosci. **5,** 131 (2008).
[10] A. Iranmanesh, Y. Pakravesh. Ars Combinatoria. **7**, 3606 (2007).