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SCHULTZ, MODIFIED SCHULTZ AND SZEGED INDICES OF A FAMILIY OF FULLERENES

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ABSTRACT. Let G be a simple connected graph. Schultz and modified Schultz indices are defined as:

$S(G)=\sum_{\{u,v\}\subseteq V(G)}(\delta_u+\delta_v)d(u,v)$; $MS(G)=\sum_{\{u,v\}\subseteq V(G)}(\delta_u\delta_v)d(u,v)$, where δ_u is the degree of vertex *u* and $d(u,v)$ is the distance between *u* and *v*. Let e be an edge of a graph G connecting the vertices u and v. Define two sets $N_1(e|G)$ and $N_2(e|G)$ as follows:

$N_1(e|G)=\{x\in V(G)|d(x,u)<d(x,v)\}$ and

$N_2(e|G)=\{x\in V(G)|d(x,v)<d(x,u)\}$ .The number of elements of $N_1(e|G)$ and $N_2(e|G)$ are denoted by $n_1(e|G)$ and $n_2(e|G)$ respectively. Szeged index of G is defined as:

$$Sz(G)=\sum_{e\in E(G)}n_1(e|G).n_2(e|G).$$

In this paper we give a GAP program for computing the Schultz, the Modified Schultz and the Szeged indices of a simple connected graph. Also we compute and formulate these indices for a family of fullerenes by the software GAP and MAPLE.

Keywords: *Schultz index, Modified Schultz index, Szeged index, $C_{12\ (n-1)}$ fullerenes.*

INTRODUCTION

A topological index is a numerical quantity that is mathematically derived in a direct and unambiguous manner from the structural graph of a molecule. Let G be a simple connected graph, the vertex and edge sets of G being 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*. Diameter of G is denoted by *d.* Distance is an important concept in graph theory and it has applications in computer science, chemistry, and a variety of other fields. Topological indices based on the distances in graph, like Wiener index [1], are widely used for

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establishing relationships between the structure of a molecular graph and its physicochemical properties.

In connection with certain investigations in mathematical chemistry, Schultz [2] considered a graph invariant that he called “molecular topological index” and denoted by MTI. It is defined as:

$$MTI(G) = \sum_{i=1}^{n}\sum_{j=1}^{n}(A_{ij} + D_{ij})\delta_i$$

where δ_i is the degree of vertex *i* in *G* and A_{ij} and D_{ij} are elements of the adjacency matrix and distance matrix of G respectively.

The essential part of MTI is the *Schultz index S*(G) [3]:

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

where δ_u is degree of vertex *u* and *d(u,v)* denote the distance between vertices *u* and *v*.

Klavzar and Gutman in [4] defined a modified Schultz index as:

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

Let e be an edge of a graph G connecting the vertices u and v. Define two sets $N_1(e|G)$ and $N_2(e|G)$ as follows:

$$N_1(e|G) = \{x \in V(G) | d(x,u) < d(x,v)\} \text{ and}$$

$$N_2(e|G) = \{x \in V(G) | d(x,v) < d(x,u)\}.$$

The number of elements of $N_1(e|G)$ and $N_2(e|G)$ are denoted by $n_1(e|G)$ and $n_2(e|G)$ respectively.

The Szeged index *Sz* was introduced by Gutman [5] and is defined as:

$$Sz(G) = \sum_{e\in E(G)} n_1(e|G).n_2(e|G).$$

Schultz, Modified Schultz and Szeged indices of the following nanotubes and fullerenes are computed: C_{60} fullerene [6], $HAC_5\,C_7$ [p, q] [7], TUC_4C_8[p,q] [8,9], VC_5C_7[p,q] nanotube [10], $HAC_5C_6C_7$[p,q] [11], dendrimer nanostars [12], HC_5C_7[r, p] [13], zigzag nanotube [14].

In this paper, we give a GAP program for computing the Schultz, Modified Schultz and Szeged indices of $C_{12(n-1)}$ fullerenes.

RESULTS AND DISCUSSION

The Schultz, modified Schultz and Szeged indices are topological indices based on distances in a graph.To obtain these indices, it needs to compute the degree of the vertices and the distance between the vertices. The

set of vertices having their distance to the vertex *u* equal to t is denoted by $D_{u,t}$ and the set of vertices adjacent to vertex *u* is denoted by *N(u).*

Let *e=uv* be an edge connecting the vertices *u* and *v*, then we have the following result:

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

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

$$=\sum_{t}\sum_{u\in V(G)}\sum_{v\in D_{u,t}} (\delta_u+\delta_v)t$$

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

$$=\sum_{t}\sum_{u\in V(G)}\sum_{v\in D_{u,t}} (\delta_u\delta_v)t$$

$$(D_t(u)\setminus D_t(v))\subseteq (D_{t-1}(v)\cup D_{t+1}(v)),\ t\geq 1.$$

$$(D_t(u)\cap D_{t-1}(v))\subseteq N_2(e|G) \quad and \quad D_t(u)\cap D_{t+1}(v)\subseteq N_1(e|G), t\geq 1$$

$$(D_1(u)\cup\{u\})\setminus(D_1(v)\cup\{v\})\subseteq N_1(e|G) \ \ and \ \ (D_1(v)\cup\{v\})\setminus(D_1(u)\cup\{u\})\subseteq N_2(e|G).$$

By using the following relations, we can determine the sets $D_{u,t}$.

$$D_{u,1}=N(u),$$

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

According to the above relations, by determining the sets $D_{u,t}$, we can compute the Schultz, the modified Schultz and the Szeged indices of a graph.

The fullerene is a hollow, pure carbon molecule in which the atoms lie at the vertices of a polyhedron with 12 pentagonal faces and any number (other than one) of hexagonal faces. The fullerenes discovered in 1985 by researchers at Rice University, are a family of carbon allotropes named after Buckminster Fuller. Spherical fullerenes are sometimes called buckyballs. A family of Fullerene is $C_{12(n-1)}$ (*n* denote the number of layers) Figure 1.

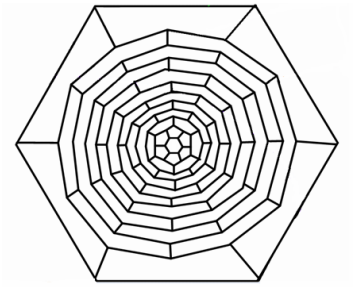

Figure 1. $C_{12(n-1)}$ fullerene (n=11).

By using the following GAP program, we can compute the Shultz, the Modified Schulttz and the Szeged indices of a graph. Input of the program is the set of adjacent vertices.

```
D:=[];  deg:=[];  e:=[];
for i in [1..n] do  D[i]:=[]; D[i][1]:=N[i]; deg[i]:=Size(N[i]);
u:=Union(u,D[i][1]);   r:=1; t:=1; u:=[i];
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;
A:=[]; T:=[];S:=0;  MS:=0;  sz:=0;
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;
for i in [1..n-1] doN1:=[];
for j in Difference(N[i],T) do   N2:=[];
N1[j]:=Union(Difference(N[i],Union([j],N[j])),[i]);
N2[i]:=Union(Difference(N[j],Union([i],N[i])),[j]);
for t in [2..Size(D[i])-1] do
for x in Difference(D[i][t],Union(D[j][t],[j])) do
if not x in D[j][t-1] then    AddSet(N1[j],x);
elif x  in D[j][t-1] then    AddSet(N2[i],x);
fi;
od;
od;
sz:=sz+Size(N1[j])*Size(N2[i]);
od;
Add(T,i);
od;
 S:=S/2; #(The value of S is equal to the Schultz index of the graph)
 MS:=MS/2; #(The value of MS is equal to the Modified Schultz index of the graph)
sz; #(The value of sz is equal to szeged index of the graph
```

In Table 1, the Shultz, the Modified Schulttz and the Szeged indices of $C_{12(n-1)}$ fullerene for some n are computed by the above GAP software.

Table 1. The Shultz, the Modified Schulttz and the Szeged indices of $C_{12(n-1)}$ fullerene.

n	Number of vertices	Schultz index	Modified Schultz index	Szeged index
5	48	28728	43092	29508
6	60	51084	76626	59616
7	72	82224	123336	104052
8	84	123768	185652	166236
9	96	177408	266112	247248
10	108	244872	367308	349332
11	120	327888	491832	474912
12	132	428184	642276	626460
13	144	547488	821232	806532
20	228	2059992	3089988	3083100
24	276	3608568	5412852	5410428
30	348	7158312	10737468	10741740
36	420	12512088	18768132	18779100
41	480	18620928	27931392	27947940
57	672	50845824	76268736	76303140
69	816	90884448	136326672	136374468
76	900	121862808	182794212	182849820
82	972	153447624	230171436	230233740
95	1128	239665392	359498088	359574900
100	1188	279928152	419892228	419974620

In the following, the formulas of these indices are obtained by the software Maple.

The Schultz index of $C_{12(n-1)}$ fullerene is :

$$S(C_{12(n-1)}) = 288\mathrm{n}^3 - 864\mathrm{n}^2 + 5832\mathrm{n} - 15048 \qquad n \geq 8$$

The Modified Schultz of $C_{12(n-1)}$ fullerene is:

$$MS(C_{12(n-1)}) = 432n^3 - 1296n^2 + 8748n - 22572 \qquad n \geq 8,$$

The Szeged indices of $C_{12(n-1)}$ fullerene is:

$$Sz(C_{12(n-1)}) = 432n^3 - 1296n^2 + 9864n - 51780 \qquad n \geq 12.$$

CONCLUSIONS

In this paper, a GAP program for computing the Schultz and Modified Schultz indices of a simple connected graph is presented. Input of the program is the set of adjacent vertices of the graph. The formulas for these indices in $C_{12(n-1)}$ fullerenes are derived by Maple software and examples are computed by the software GAP.

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