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SOME TOPOLOGICAL INDICES OF C_{12n+4} FULLERENES

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ABSTRACT. A method for computing some topological descriptors based on distance in a graph, such as the molecular topological index (MTI), Schultz, Modified Schultz, Szeged and vertex PI_v indices in simple connected graphs and in the family of C_{12n+4} fullerenes is presented.

Keywords: *Molecular topological index (MTI), Schultz index, Modified Schultz index, Szeged index, vertex Padmakar-Ivan index (PI_v), C_{12n+4} fullerenes.*

INTRODUCTION

A topological index is real number mathematically derived from the structural graph of a molecule. Hundreds of different topological indices have been investigated so far and used in the Quantitative Structure Property Relationship (QSPR) studies, with various degrees of success. These invariants belong to one of two broad classes: distance-based indices or bond-additive ones. The first class includes indices defined on topological distances between pairs of vertices while the indices of the second class are defined as the sums of contributions over all edges. Topological indices based on the distances in graph are widely used to establish relationships between the structure of a molecular graph and their physicochemical properties. 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(G).

The molecular topological index MTI of G was introduced by Schultz in 1989 [1]. It is defined as:

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$$MTI(G) = \sum_{i\in V(G)} \sum_{j\in V(G)} (a_{ij} + d_{ij})\delta_i \tag{1}$$

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 molecular topological index has found interesting chemical application [2-10]. Mathematical properties of MTI are also described in several articles [11-13]. Let G be a simple connected graph, then MTI can also be expressed as [14]:

$$MTI(G) = \sum_{u\in V(G)} D_u\delta_u + \sum_{u\in V(G)} \delta_u^{\,2} \tag{2}$$

where $D_u = \sum_{v\in V(G)} d(u,v)$ is the sum of distances between vertex i and all other vertices of G. The Schultz index was introduced by Harry Schultz [3]. The non-trivial part of MTI is called the Schultz index and is defined as:

$$S(G) = \sum_{\{u,v\}\subseteq V(G)} (\delta_u + \delta_v) d(u,v) \tag{3}$$

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

The main chemical applications and mathematical properties of this index were established in a series of studies [6,11,15]. Also a comparative study of molecular descriptors showed that the Schultz index and Wiener index are mutually related [14,16].

Klavzar and Gutman in [17] defined the modified Schultz index as:

$$MS(G) = \sum_{\{u,v\}\subseteq V(G)} (\delta_u\delta_v) d(u,v) \tag{4}$$

The Szeged index [18,19] is another such topological index and is closely related to the Wiener index; in particular, the Wiener and the Szeged index coincide in trees. The Wiener index also attracted considerable attention [20, 21].

The Szeged index is a vertex-multiplicative index. Let e=uv be an edge in G. The number of vertices in G lying closer to vertex u than to vertex v is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices in G lying closer to vertex v than vertex u. The Szeged index is defined as:

$$Sz(G) = \sum_{e=uv \in E(G)} n_u(e) \times n_v(e) \tag{5}$$

Khadikar et al. [22, 23] have defined a new topological index and named it Padmakar-Ivan PI index:

$$PI(G) = \sum_{e=uv \in E(G)} m_u(e) \times m_v(e) \tag{6}$$

where $m_u(e)$ is the number of edges of G lying closer to vertex *u* than vertex v. Applications of PI index to QSRP/QSAR were studied in [24]. The index was mostly compared to the Wiener and Szeged indices.

The vertex version of PI index was also considered [25]

$$PI_v(G) = \sum_{e=uv \in E(G)} n_u(e) + n_v(e) \tag{7}$$

In this paper we give a method for computing the MTI, Schultz, Modified Schultz, Szeged and PI_v indices for the family of fullerenes C_{12n+4}. In a series of papers, these indices have been computed for various molecular graphs [26-31].

Computing the MTI, Schultz, Modified Schultz, Szeged and PIv indices in fullerenes C12n+4

Carbon exists in the nature in three allotropic forms: diamond, graphite and fullerenes. Fullerene C_{60} has been discovered by Kroto *et al* in 1985 [32]. Fullerenes are large carbon cage molecules. A fullerene is associated to a planar, 3-regular and 3-connected graph and is tessellated by pentagons and hexagons. The molecular graph of C_{12n+4} fullerenes is illustrated in Figure 1, where *n* is the number of layers of 12 vertices.

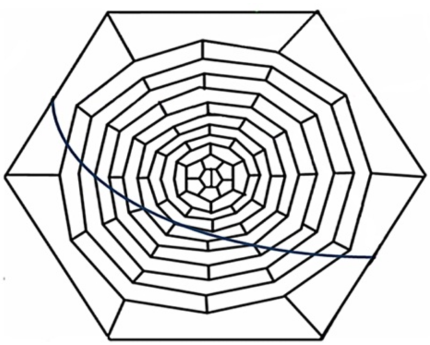

Figure 1. Fullerene C_{12n+4}; n=11

In this section, we give a GAP program for computing the MTI, Schultz, Modified Schultz, Szeged and vertex PI indices in simple connected graphs but also in C_{12n+4} fullerenes.

We denote the set of vertices of which distance to the vertex u is t, by $D_{u,t}$ and $D_{u,o} = \{u\}$. Eccentricity of the vertex u in G is the path length from the vertex u to the vertex v that is farthest from u:

$$\varepsilon(u) = Max\{d(u,v) | v \in V(G)\} \tag{8}$$

For computing the topological indices based on distance, it is sufficient to obtain the sets $D_{u,t}$ for each vertex u and $1 \leq t \leq \varepsilon(u)$. In a series of papers, an algorithm for computing the sets $D_{u,t}$ and some topological indices in molecular graphs was presented [28, 30]. Let $e = uv$ be an edge of G. By obtaining the sets $D_{u,t}$ and following the definition relations, the topological indices such as the MTI, Schultz, Modified Schultz, Szeged and PI_v, could be computed:

$$\varepsilon(u) = Max\{t | D_{u,t} \neq \emptyset\},$$
$$\delta_u = |D_{u,1}|,$$
$$n_u(e) = \sum_{t=1}^{\varepsilon(u)} |D_{u,t} \setminus (D_{v,t} \cup D_{v,t-1})|,$$
$$D_u = \sum_{t=1}^{\varepsilon(u)} t \times |D_{u,t}|,$$
$$S(G) = \sum_{u \in V(G)} \sum_{t=1}^{\varepsilon(u)} \sum_{v \in D_{u,t}} (\delta_u + \delta_v) \times t,$$
$$MS(G) = \sum_{u \in V(G)} \sum_{t=1}^{\varepsilon(u)} \sum_{v \in D_{u,t}} (\delta_u \delta_v) \times t.$$

The following GAP program computes the sets $D_{u,t}$ for any simple connected graph. The input of the program is the adjacent vertices set of each vertex.

```
D:=[];
for i in [1..n] do
D[i]:=[];D[i][1]:=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;
D; # D[i][t] is the set D_{i,t}
```

We computed the MTI, Schultz, Modified Schultz, Szeged and PI_v indices of C_{12n+4} for various values of n and some results are shown in Table 1.

Table 1. Some Topological Indices of C_{12n+4}

n	MTI	Schultz index	Modified Schultz index	PI index	Szeged index
3	14628	7188	10782	924	5072
4	36408	18024	27036	1984	16404
5	71196	35364	53046	3492	38168
6	121680	60552	90828	5440	72958
7	190788	95052	142578	7804	122686
8	281856	140532	210798	190966	190966
9	398268	198684	298026	13900	278834
10	543480	271236	406854	17596	388582
11	720948	359916	539874	21724	522642
12	934128	466452	699678	26284	683526
13	1186476	592572	888858	31276	873798

It is easy to see that the diameter of the molecular graph of C_{12n+4} is $2n-1$ for $n \geq 7$. By interpolation of our data, we conjecture the following formula for MTI (C_{12n+4}).

$$MTI(C_{12n+4})=576n^3-1152n^2+11004n-27360,\ n \geq 7 \qquad (9)$$

In the following, a mathematical method is presented to demonstrate the above conjecture.

Since C_{12n+4} is a 3-regular graph we have the following relation:

$$\begin{aligned} MTI(C_{12n+4}) &= 3 \sum_{u \in V(G)}' D_u + 9(12n+4) \\ &< 3\binom{12n+4}{2}(2n-1) + 108n + 36 \\ &= 432n^3 + 36n^2 + 18n + 36. \end{aligned} \qquad (10)$$

Hence $MTI(C_{12n+4})$ is a polynomial with degree at most 3.

Proposition 1: If p(x) and q(x) are two polynomials of degrees m and n, respectively $(m \leq n)$ and have more than n points in common, then $p(x) = q(x)$.

Proof: $q(x) - p(x)$ is a polynomial with degree at most n and more than n roots. Since a nonzero polynomial of degree n has at most n real roots, hence $q(x) - p(x)$ must be 0 and the proof is completed.

Theorem 1. For $n \geq 7$ we have:

$$MTI(C_{12n+4}) = 576n^3 - 1152n^2 + 11004n - 27360.$$

Proof: Let $P(n) = MTI(C_{12n+4})$ and $q(n) = 576n^3 - 1152n^2 + 11004n - 27360, n \geq 7$. $p(n)$ and $q(n)$ are two polynomial with degrees at most 3 and by Table1, have more than 3 points in common, hence by Proposition 1, we have:

$$MTI(C_{12n+4}) = P(n) = q(n) = 576n^3 - 1152n^2 + 11004n - 27360, n \geq 7.$$

By a similar method, the other topological indices of C_{12n+4} fullerenes can be computed. In the next theorem, the explicit formulas for the Schultz, Modified Schultz, Szeged and PI_v indices of C_{12n+4} fullerenes is presented.

Theorem 2.

$$S(C_{12n+4}) = 288n^3 - 576n^2 + 5448n - 13644, \qquad n \geq 7,$$
$$MS(C_{12n+4}) = 432n^3 - 864n^2 + 8172n - 20466, \qquad n \geq 7,$$
$$PI_v(C_{12n+4}) = 216n^2 - 408n + 76, \qquad n \geq 7,$$
$$Sz(C_{12n+4}) = 432n^3 - 864n^2 + 9264n - 49722, \qquad n \geq 12.$$

CONCLUSIONS

It takes a long time to compute the topological indices based on distances in a graph. In this paper, a method is presented for computing some topological indices such as the MTI, Schultz, Modified Schultz, Szeged and PI_v indices. By the presented method, we can compute the above topological indices for the family of fullerenes C_{12n+4} by the GAP program and present explicit formulas for them.

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