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Some Topological Indices of Family of C_{12n+4} Fullerenes

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ABSTRACT

A method for computing topological indices based on distances in a simple connected graph is presented. The method is used to obtain closed formulas for topological indices of infinite series of molecular graphs. Also a GAP program is given to compute the distances between vertices in a simple connected graph. Input of the program is the set of adjacent vertices of each vertex that is denoted by *N(i)*. By using the presented GAP program, for each vertex *i*of graph *G*, the set of vertices that their distance to vertex *i* is *t*, can be computed and these sets are denoted by $D_{i,t}$. Some topological indices based on distance such as Wiener index, Molecular topological index (MTI), Schultz index, Modified Schultz index, Szeged index and vertex Padmakar-Ivan (PI_v) index can be expressed in terms of the sets of $D_{i,t}$. So these topological indices can be computedby the GAP program for a simple connected graph. Let I be a topological index and $\{G_n\}$ be a series of molecular graphs. If there exists a polynomial *P (n)* such that $I(G_n) = P(n)$. Then by using the presented method, we can find the polynomial P (n) and also prove that the polynomial is unique. The method is applied to obtain closed formulas (as polynomials) for Molecular topological index (MTI), Schultz indices, Szeged index and vertex Padmakar-Ivan (PI_v) index of an infinite family of C_{12n+4} fullerenes and also the obtained results about Cyclic phenylenes$R_h$is reported.
KEYWORDS: Molecular topological index (MTI), Schultz index, Modified Schultz index, Szeged index, vertex Padmakar-Ivan index (PI_v), C_{12n+4} fullerenes.

1. INTRODUCTION

A topological index of a molecular graph *G* is a numeric quantity invariant under automorphisms of *G*. Hundreds of different topological indices have been investigated so far and used in the Quantitative Structure Properties Relationships (QSPR)studies, with various degrees of success. Most of the more useful invariants belong to one of two broad classes: they are either distance based, or bond-additive. The first class contains the indices that are defined in terms of distances between pairs of vertices; the second class contains the indices defined as the sums of contributions over all edges. Topological indices based on the distances in graph are widely used for establishing relationships between the structure of a molecular graph and their physicochemical properties. Wiener index [1] is the first topological index based on distance and is defined as the sum of distances between all pairs of vertices in a graph.Many methods were proposed for computing based distance topological indices (especially Wiener index) of classes of graphs. For example, cut method [2] was applied for Wiener index, Schultz index and Szeged index ofbenzenoid graphs and partial Hamming graphs [3, 4].The cut method cannot be applied to any classes of graphs.In this paper, we give a method for calculating based distance topological indices of a simple connected graph. The method is discussed onfamily of fullerenes $C_{12n+4}$and cyclic phenylenesand on five topological indices: Molecular topological index, Schultz index, Modified Schultz index, Szeged index and vertexPadmakar-Ivan index. We do not consider the Wiener index of C_{12n+4} because it was earlier treated in [5].

2. Definitions and preliminaries

Let *G* be a simple connected graph, the vertex and edge sets of *G* is 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 of a graph *G* was introduced by Schultz in 1989 [6] and is denoted by MTI. It is defined as:

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

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 molecular topological index has found interesting chemical application [7-10]. Let G be a simple connected graph, *MTI(G)*can be expressed as follow [11]:

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

Where $D_u = \sum_{v \in V(G)} d(u,v)$ is the sum of distances between vertex *u*and all other vertices of the graph *G*.The Schultz index [8] is defined as:

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

The main chemical applications of this index were established in a series of studies [9,12].
Klavžar and Gutman in [13] defined the modified Schultz index as:

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

The Szeged index [14, 15] is another such topological indicesand is closely related to the Wiener index; in particular, the Wiener and the Szegedindex coincide on trees. The Szeged index is a vertex-multiplicative type index that takes into account the wayvertices of a given molecular graph *G* are distributed.
Let *e=uv* be an edge of a graph *G*. The number of vertices of *G*lying closer to vertex *u* than vertex *v* is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices of vertices of *G*lying closer to vertex *v* than vertex *u*.The Szeged index is defined as:

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

Khadikar and Co-authors [16,17] defined a new topological index and named itPadmakar-Ivan index. It is defined as:

$$PI(G) = \sum_{e=uv \in E(G)} m_u(e).m_v(e),$$

Where $m_u(e)$ is the number of edges of *G* lying closer to vertex u than vertex *v*.Applications of the PI index to QSRP/QSAR were studied in [18]. The index was mostlycompared with the Wiener and the Szeged index.
The vertex version of PI index was also considered [19], defined as

$$\mathrm{PI}_v(G) = \sum_{e=uv \in E(G)} n_u(e) + n_v(e).$$

We refer the reader to a number of recent papers concerned with computing some distance based topological indices of several classes of graphs [20-22]

3. Fullerenes C_{12n+4}.

A fullerenes graph is planar, 3-regular and 3-connected graph and consist of the networks of pentagons and hexagons.Fulfilling the EULER's theorem, to form a closed spherical structure, fullerene has to contain exactly 12 pentagons and $\frac{N}{2} - 10$ hexagons where *N*is the number of vertices of the fullerene. The molecular graph of C_{12n+4} fullerene is illustrated in Figure 1 where *n* is the number of layers with 12 vertices. These fullerenes were studied for example in [23-25].

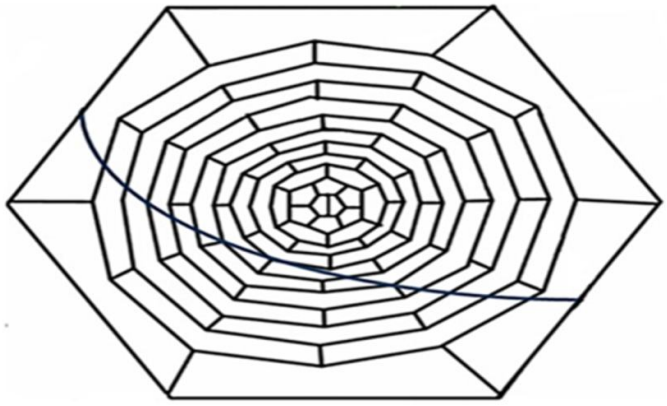

Figure1. C_{12n+4} fullerene, n=11.

4. MAIN RESULTS

In this section, a method and a GAP program [22] for computing thedistances between vertices of a graph are given. We use this method to compute theMTI index, Schultz index, Modified Schultz index, Szeged index and vertex-PI index of C_{12n+4} for some values of n and then we obtain explicit formulas of these indices for fullerenes C_{12n+4}.

Eccentricity of the vertex u in a graph G is the path length from the vertex u to the vertex v that is farthest from u. i.e.,

$$\varepsilon(u) = max\{d(u,v) | v \grave{o} V(G)\}$$

We denote the set of vertices that their distance to vertex $u$is t, by $D_{u,t}$. The distance between vertex u and itsadjacent vertices is 1, hence$D_{u,1} = N(u)$.Let j be a vertex in $D_{u,t}$. For each vertex w in $N(j)$, the distance between u and $wd(u,w)$, is $t-1$ or t or $t+1$. Therefor we have:

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

Using the above relation and induction, the sets $D_{u,t} 1 \le t \le \varepsilon(u)$, can be obtained for each vertex u.

In a series of papers, an algorithm was presented for computing the sets $D_{u,t}$ [28, 30].

For computing the topological indices based on distance, it is sufficient to obtain the sets $D_{u,t}$ for each vertex $u$and $1 \le t \le \varepsilon(u)$.

By obtaining the sets $D_{u,t}$ and the following relations, the topological indices such as the MTI index, Schultz index, Modified Schultz index, Szeged index and vertex PI index could be computed.

1. $\varepsilon(u) = max\left\{t \left| D_{u,t} \neq \phi \right.\right\}$,
2. $\delta_u = \left| D_{u,1} \right|$,
3. $n_u(e) = \sum_{t=1}^{\varepsilon(u)} \left| D_{u,t} \setminus \left(D_{v,t} \cup D_{v,t-1} \right) \right|$,
4. $D_u = \sum_{t=1}^{\varepsilon(u)} t \times \left| D_{u,t} \right|$,
5. $W(G) = \sum_{u \in V(G)} \sum_{t=1}^{\varepsilon(u)} t \times \left| D_{u,t} \right|$,
6. $S(G) = \sum_{u \in V(G)} \sum_{t=1}^{\varepsilon(u)} \sum_{v \in D_{u,t}} (\delta_u + \delta_v) t$,
7. $MS(G) = \sum_{u \in V(G)} \sum_{t=1}^{\varepsilon(u)} \sum_{v \in D_{u,t}} (\delta_u \delta_v) t$.

Let $e = uv$ be an edge of graph G and $j \in D_{u,t}$. Then $d(v, j) = t-1 \text{or } t \text{ or } t+1$. Hence we have:

8. $n_u(e) = \sum_{t=1}^{\varepsilon(u)} \left| D_{u,t} \cap D_{v,t+1} \right|$

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

```
D:=[];u:=[];
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}
```

Topological indices of C_{12n+4} fullerenes

The computed values ofthe MTI index, Schultz index, Modified Schultz index, Szegedindex and PI_v index of C_{12n+4} for some values of *n* are given in Table1.

n	MTI(C_{12n+4})	S(C_{12n+4})	MS(C_{12n+4})	PI_v(C_{12n+4})	Sz(C_{12n+4})
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
14	1481448	740004	1110006	36700	1096038
15	1822500	910476	1365714	42556	1352838
⋮	⋮	⋮	⋮	⋮	⋮
100	565553040	282771156	424156734	2119276	424236678

Table1. Some values of the topological indices of C_{12n+4}.

Lemma 4.1: If *p(n)* and *q(n)* are two polynomials of degrees *r*and *s* respectively $r \le s$ and have more than *s* points in common, then p(n)=q(n).

Proof: It is obvious that the degree of the polynomial *(p-q)(n)*is at most *s* and has more than *s* roots but every nonzero polynomial of degree *s* has *s* real roots at most. Hence *(p-q)(n)* = 0 and the proof is completed.

We start by computing the formula of MTI(C_{12n+4}). Our aim is to find a closed formula for polynomialMTI(C_{12n+4}) as a polynomial*p(n)*. At first, we need to determine a constant upperbound on the degree of *p(n)*. Let *G* be a graph with diameter *d* and *k* vertices. It is easy to see that for each vertex *u*, $D_u \le (k-1)d$. Since $d\left(C_{12n+4}\right) = 2n-1$ for $n \ge 7$ and vertices of $C_{12n+4}$are of degree 3 it follows that for each vertex u, $D_u < (12n+3)(2n-1) = 24n^2 - 12n - 3$,

$$\mathrm{MTI}\left(\mathrm{C}_{12n+4}\right) = 3\sum_{u\in V\left(\mathrm{C}_{12n+4}\right)} (\mathrm{D}_u + 3) < 3(12\mathrm{n}+4)\left(24n^2 - 12\mathrm{n}\right) = 864n^3 - 144n^2 - 144n.$$

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

Polynomial $p(n) = 576n^3 - 1152n^2 - 11004n - 27360,\ n \ge 7$, interpolate the values of $\mathrm{MTI}\left(\mathrm{C}_{12n+4}\right),\ n \ge 7$ in Table 1. We claim that MTI(C_{12n+4})= p(n), $n \ge 7$. It follows because as just said, $\mathrm{MTI}\left(\mathrm{C}_{12n+4}\right)$ is a polynomial with degree at most 3 and has more than 4 points in common with $\mathrm{p}(\mathrm{n})$. Hence by lemma 3.1, $\mathrm{MTI}\left(\mathrm{C}_{12n+4}\right) - \mathrm{p}(\mathrm{n})$ is a polynomial with degree at most 3 but it hasmore than 4 roots therefor it must be zero and then $\mathrm{MTI}\left(\mathrm{C}_{12n+4}\right) = \mathrm{p}(\mathrm{n})$.

We continue with the Schultz index of C_{12n+4} by an analogous method. Since $S(C_{12n+4}) = \sum_{\{u,v\}\subseteq V(C_{12n+4})} 6d(u,v) < 6\binom{12n+4}{2}(2n-1)$ the polynomial of $S(C_{12n+4})$ is at most cubic. Hence it should suffice to compute the interpolation polynomial of four values of $S(C_{12n+4})$, $n \geq 7$. Therefor

$$S(C_{12n+4}) = 288n^3 - 576n^2 + 5448n - 13644, n \geq 7.$$

Since C_{12n+4} is a 3-regular then

$$MS(C_{12n+4}) = \frac{3}{2}S(C_{12n+4}) = 432n^3 - 864n^2 + 8172n - 20466,\ n \geq 7.$$

It is easy to see that for the edge uv, $n_u + n_v \leq |V(C_{12n+4})| = 12n + 4$ and the number of edges of C_{12n+4} is 18n+12 hence $PI_v(C_{12n+4}) < (12n+4)(18n+12)$ and $PI_v(C_{12n+4})$ is a quadratic polynomial. By fitting a quadratic polynomial through the three values of $\mathrm{PI}_v(\mathrm{C}_{12n+4})\, n \geq 7,$ we have:

$$PI_v(C_{12n+4}) = 216n^2 - 408n + 76,\ n \geq 7.$$

Finally, $Sz(C_{12n+4})$ is at most cubic polynomial. Indeed, this follows because for pair vertices u and v, $n_u n_v \leq \frac{1}{4}(12n+4)^2$. On the other hand it interestingly turned out that the polynomial $Sz(C_{12n+4})$ equals interpolation polynomial for $n \geq 12,$ hence we have

$$Sz(C_{12n+4}) = 432n^3 - 864n^2 + 9264n - 49722,\ n \geq 12.$$

Topological indices of Cyclicphenylenes

The cyclic phenylenes were studied in [26, 27]. Cyclic phenylene is denoted by $R_h$where $h$is the number of hexagons and $h \geq 3$. Its structure should be clear from the example of R_6depicted in Fig.2.

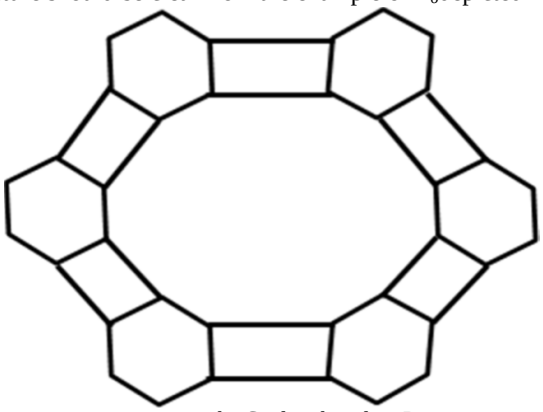

Figure 2. The Cyclic phenyleneR_6

The obtained results for R_h are:

$$MTI(R_h) = 48h^3 + 180h^2 - 124h,$$
$$Sc(R_h) = 48h^3 + 180h^2 - 168h,$$
$$MSc(R_h) = 64h^3 + 224h^2 - 196h,$$
$$PI_v(R_h) = 48h^2,$$
$$Sz(R_h) = 36h^3 + 144h^2 - 144h,$$

Concluding

A method is presented here for obtaining closed formulas for topological indices of families of graphs. The method is illustrated on the family of C_{12n+4} fullerenes and Cyclicphenylenesand on five distance based topological indices: Molecular topological index (MTI),Schultz index, Modified Schultz index, Szeged index

and vertex Padmakar-Ivan (PI_v) index. Also a GAP program is given to compute distances and topological indices based on distances in a simple connected graph.

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