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Computing Eccentric Distance Sum for an Infinite Family of Fullerenes

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Abstract

In this paper, a method for computing eccentric distance sum index of fullerenes is presented.

1. Introduction

Carbon is an important element and has almost infinite number of allotropes. The two most common allotropes of carbon are diamond and graphite. Discovery of C_{60} has opened up the new branch of carbon allotropes, known as fullerene. Fullerenes are carbon-cage molecules comprised of carbon atoms that are arranged on a sphere with pentagonal and hexagonal faces. Using the graph theory, fullerenes can be modeled as cubic 3-connected graphs which are embedded into a sphere with face lengths being 5 or 6.

Using the Euler's formula, we can conclude that each fullerene contains exactly twelve pentagons, but it does not imply any restriction on the number of hexagons. In fact, it is not difficult to see that mathematical models of fullerenes with precisely α hexagons exist for all

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values of α with the sole exception of α = 1, see [1-3] for more information on chemical, physical, and mathematical properties of fullerenes.

Based on the molecular graph of a chemical compound, a topological index, also known as a connectivity index, is calculated. These indices characterize topology of the graphs and therefore are usually graph invariant.

Throughout this paper, graph means simple connected graph. The vertex and the edge sets of a graph G are denoted by V(G) and E(G), respectively. If x, y ∈ V(G), then the distance d(x,y) between x and y is defined as the length of a minimum path connecting x and y. The diameter of G, denoted by d(G), is maximum distance between pairs of vertices . The eccentric connectivity index of the molecular graph G, $\xi^c(G)$, was proposed by Sharma, Goswami and Madan [4]. It is defined as $\xi^c(G) = \Sigma_{u\in V(G)}\deg_G(u)\ ecc(u)$, where $\deg_G(x)$ denotes the degree of the vertex x in G and ecc(u) = max{d(x,u) | x ∈ V(G)}. The radius and diameter of G are defined as the minimum and the maximum eccentricity among all vertices of G, The index $\xi^c(G)$ was used for the development of mathematical models for the prediction of biological activities of diverse nature, see [5-10]. The Wiener index W(G) of a connected graph G is the sum of all the distances between pairs of vertices of G, i.e., $(G) = \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d(u,v)$.

The eccentric distance sum of *G* (EDS) is defined as :

$\xi^{ds}(G) = \Sigma_{u\in V(G)}\ ecc(u)D(u)$, where $D(u) = \Sigma_{x\in V(G)}\ d(u,x)$ is the sum of all distances from the vertex *u*. Eccentric distance sum was introduced by Gupta, Singh and Madan [5]. It has a vast potential in structure activity/property relationships. In [11] the authors considered the *n*-vertex trees and unicyclic graphs with minimal eccentric distance sums, and in [12] the authors proved that path P_n is the unique extremal trees with *n* vertices having maximum eccentric distance sum, and provided various lower and upper bounds for the eccentric distance sum. Also, some results obtained on the eccentric connectivity index in [13-15].

It turned to have high discriminating power and excellent predictability both with regard to biological and physical properties and to provide valuable leads for the development of safe and potent therapeutic agents of diverse nature.

2. Main results and discussion

The aim of this section is to compute ξ^{ds} (G) for an infinite family of fullerenes.

In Figure 1, we showed that the molecular graph of the fullerene $C_{12(2n+1)}$.

In [16], we computed the eccentric connectivity polynomial of $C_{12(2n+1)}$ fullerene. For compute the EDS index of this type of fullerene, at first we computed this index for some n which is shown in Table 1.

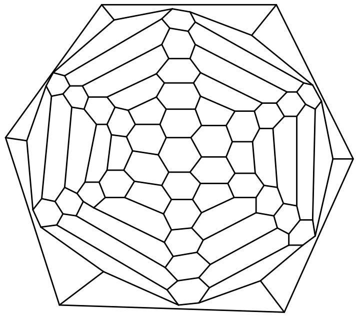

Figure 1. The Molecular Graph of the Fullerene $C_{12(2n+1)}$.

Fullerenes	**ξ^{ds} Index**
C_{60}	151740
C_{84}	436128
C_{108}	909168
C_{132}	1619376
C_{156}	2715648

Table1. Some exceptional cases of $C_{12(2n+1)}$ fullerenes.

By the Maple software [17] and interpolation of our data, we conjecture that

$$\xi^{ds}(G)=600n^4+5520n^3+18984n^2+11712n-21168 \quad , n \geq 7$$

By Figure 1, it is easily to see that the diameter of molecular graph of $C_{12(2n+1)}$ is $2n+5, n \geq 2$ see [16].

By the following propositions, we will prove our conjecture.

Proposition 2.1 If f(x) and g(x) are two polynomials of degrees m and n, respectively $(m \leq n)$ and have more than n points in common, then $f(x) = g(x)$.

Proof: It is obvious that the degree of the polynomial $(f-g)(x)$ is at most n and has more than n roots but every nonzero polynomial of degree n has n real roots at most. So $(f-g)(x)=0$ and the proof is completed.

Proposition 2.2 Let G be a simple connected graph with k vertices, then

$$W(G) \leq \binom{k}{2} \times d(G)$$

and equality is hold if and only if G is a complete graph.

Proof: Straight forward by definition of the Wiener index.

Theorem 2.3 Let G be a connected graph with diameter d(G) , then

$\xi^{ds}(G) \leq 2W(G) \cdot d(G)$

Proof: See Theorem 4.1 in [12].

Corollary 2.4 Let G be a simple connected graph with k vertices, then
$\xi^{ds}(G) \leq 2\binom{k}{2} \cdot (d(G))^2$

Corollary 2.5 Let G be the molecular graph of $C_{12(2n+1)}$ fullerene, then $\xi^{ds}(G) \leq 2\binom{12(2n+1)}{2} \cdot (2n+5)^2 = 2304n^4+13728n^3+25968n^2+16440n+3300$.

Theorem 2.6 The ξ^{ds} of the fullerene $C_{12(2n+1)}$ for $n \geq 7$, is obtain as follows:

$$\xi^{ds}(G) = 600n^4+5520n^3+18984n^2+11712n-21168.$$

Proof: Let $f(n)$ be the eccentric distance index of $C_{12(2n+1)}$ fullerene for $n \geq 7$. By Corollary 2. 5, $f(n)$ is a polynomial of at most degree 4. Two polynomials $f(n)$ and $g(n)=600n^4+5520n^3+18984n^2+11712n-21168$, have more than 4 point in common, so by Proposition 2.1, we have $f(n)=g(n)$.

In continue, we obtain the EDS index for another type of fullerene. In [16], we computed the eccentric connectivity polynomial of C_{12n+4} fullerene. In Figure 2 we show that the molecular graph of C_{12n+4} fullerene:

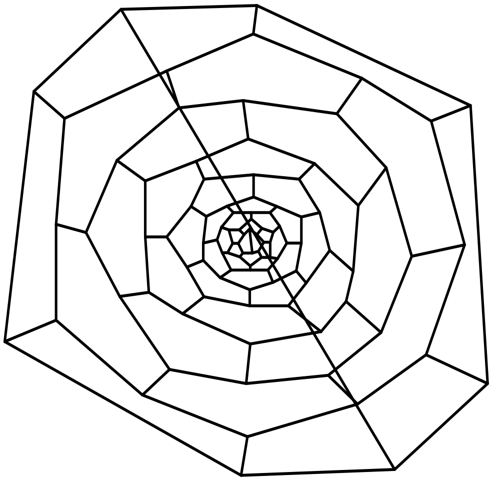

Figure 2. The Molecular Graph of the Fullerene C $_{12n+4}$

In Table 2, the EDS index of C_{12n+4} fullerenes are computed, for some values of n.

Fullerenes	ξ^{ds} **Index**
C_{28}	13372
C_{40}	42696
C_{52}	93784
C_{64}	181976
C_{78}	322020

Table2. EDS index of C_{12n+4} fullerene for some n.

Theorem 2.7 By the above assumptions, the ξ^{ds} index of the fullerene graph C_{12n+4} for $n \geq 10$, is obtain as follows:

$$\xi^{ds}(G)=150n4+216n3+2666n2-4776n+5180.$$

Proof: The proof of this theorem is similar to the proof of the Theorem 2.6.

In follows, we prepare a GAP program to compute the EDS index of any fullerene. This program is prepared by GAP, see [18] for more information.

```
f:=function(M)
local t,S,k,tt,H,i,j,
t:=Size(M);  S:=[]; k:=0;  tt:=0; H:=[];
for i in [1..t] do
            Add(S,Maximum(M[i]));
 od;
for i in [1..t] do
             for j in M[i] do
                     k:=k+j;
           od;
         Add(H,k);k:=0;
od;
for i in [1..t] do
           tt:=tt+H[i]*S[i];
od;
Print("EDS Index:=", tt);
print("*************************************","\n");
print("\n");
```

3. Conclusions

An algorithm has been presented for computing the EDS index of any connected simple graph. According to this algorithm and using the GAP program, we wrote a program to compute this index. We tested the algorithm to calculate the EDS index of C_{12n+4} and $C_{12(2n+1)}$ fullerenes.

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