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ECCENTRIC CONNECTIVITY POLYNOMIAL OF C_{12n+2} FULLERENES

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The eccentricity connectivity polynomial of a molecular graph G is defined as EC(G,x) = Σa∈V(G)xecc(a), where ecc(a) is defined as the length of a maximal path connecting a to another vertex of G. In this paper this polynomial is computed for an infinite family of fullerenes.

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1. Introduction

Carbon exists in several allotropic forms in nature. Fullerenes are zero-dimensional nanostructures, discovered experimentally in 1985[1]. Fullerenes are carbon-cage molecules in which a number of carbon atoms are bonded in a nearly spherical configuration. Let p, h, n and m be the number of pentagons, hexagons, carbon atoms and bonds between them, in a given fullerene F. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is $n = (5p+6h)/3$, the number of edges is $m = (5p+6h)/2 = 3/2n$ and the number of faces is $f = p + h$. By the Euler's formula $n - m + f = 2$, one can deduce that $(5p+6h)/3 - (5p+6h)/2 + p + h = 2$, and therefore $p = 12$, $n = 2h + 20$ and $m = 3h + 30$. This implies that such molecules, made entirely of n carbon atoms, have 12 pentagonal and $(n/2 - 10)$ hexagonal faces, while $n \neq 22$ is a natural number equal or greater than 20[2].

Throughout this paper, graph means simple connected graph. The vertex and edge sets of a graph G are denoted by V(G) and E(G), respectively. If $x, y \in V(G)$ then the distance $d(x,y)$ between x and y is defined as the length of a minimum path connecting x and y. The eccentric connectivity index of the molecular graph G, $\xi^c(G)$, was proposed by Sharma, Goswami and Madan[3]. 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 $ecc(u) = Max\{d(x,u) \mid x \in V(G)\}$, see [4-8] for details. The radius and diameter of G are defined as the minimum and maximum eccentricity among vertices of G, respectively.

We now define the eccentric connectivity polynomial of a graph G, ECP(G,x), as $ECP(G,x) = \Sigma_{a\in V(G)}deg_G(a)x^{ecc(a)}$. Then the eccentric connectivity index is the first derivative of ECP(G, x) evaluated at $x = 1$.

Herein, our notation is standard and taken from the standard book of graph theory[9-14].

2. Main results and discussion

The aim of this section is to compute ECP(G,x), for an infinite family of fullerenes. Before going to calculate this polynomial for graph operations, we must compute ECP(G,x), for some well-known class of graphs.

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Example1. Consider fullerene graph C_{20} (figure 1). One can see that the for every $x \in V(G)$, ecc(x)=5. So, $ECP(G,x) = \sum_{a \in V(G)} deg(a)x^{ecc(a)} = 3\sum_{a \in V(G)} x^5 = 60x^5$.

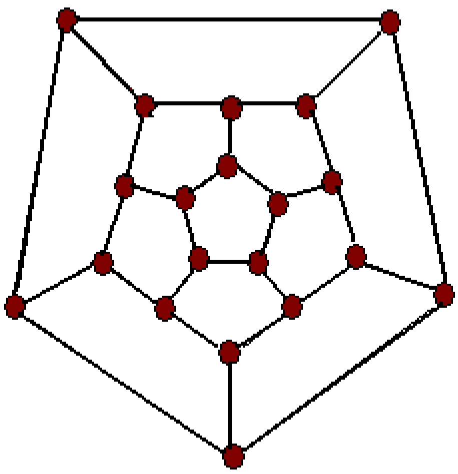

Fig. 1. Graph of fullerene C_{20}

Lemma2. The EC polynomial for a k- regular graph is: $ECP(G,x) = k\sum_{a \in V(G)} x^{ecc(a)}$.

So, the EC polynomial for fullerene graph is $ECP(G,x) = 3\sum_{a \in V(G)} x^{ecc(a)}$.

Example3. Suppose K_n denotes the complete graph on n vertices. Then For every $v \in V(K_n)$, $deg(v)$= n-1 and ecc(v)=1. So, $ECP(G,x) = (n-1)\sum_{a \in V(G)} x = n(n-1)x$.

In Table 1, the EC polynomials of C_{12n+2} fullerenes, Figure 2, are computed, $2 \le n \le 9$. If $n \ge 10$ then we have the following general formula for the EC polynomial of this class of fullerenes.

Theorem4. The EC polynomial of C_{12n+2}, $n \ge 10$, fullerenes are computed as follows:

$$ECP(C_{12n+2},x) = 18x^n + 36x^{n+1}\frac{x^{n-1}-1}{x-1} + 24x^{2n}.$$

Proof. From Figure 2, one can see that there are three types of vertices of fullerene graph C_{12n+2}. These are the vertices of the central and outer polygons, and, other vertices of C_{12n+2}. Obviously, we have:

Vertices	**ecc(x)**	**No.**
The Type 1 Vertices	2n	8
The Type 2 Vertices	n	6
Other Vertices	n+i $(1 \le i \le n)$	12

By using these calculations and Figure3, the theorem is proved. ■

Some exceptional cases are given in the following table:

Table1. Some exceptional cases of C_{12n+2} fullerenes.

Fullerenes	EC Polynomials
C_{26}	$72x^5+6x^6$
C_{38}	$114x^7$
C_{50}	$36x^7+102x^8+12x^9$
C_{62}	$72x^8+72x^9+42x^{10}$
C_{74}	$36x^8+72x^9+54x^{10}+36x^{11}+24x^{12}$
C_{86}	$72x^9+54x^{10}+36x^{11}+36x^{12}+36x^{13}+24x^{14}$
C_{98}	$12x^9+18x^{10}+12x^{11}+12x^{12}+12x^{13}+12x^{14}+12x^{15}+8x^{16}$
C_{110}	$18x^{10}+12x^{11}+12x^{12}+12x^{13}+12x^{14}+12x^{15}+12x^{16}+12x^{17}+ 8x^{18}$

Corollary5. The diameter of C_{12n+2}, $n \geq 5$, fullerenes is 2n.

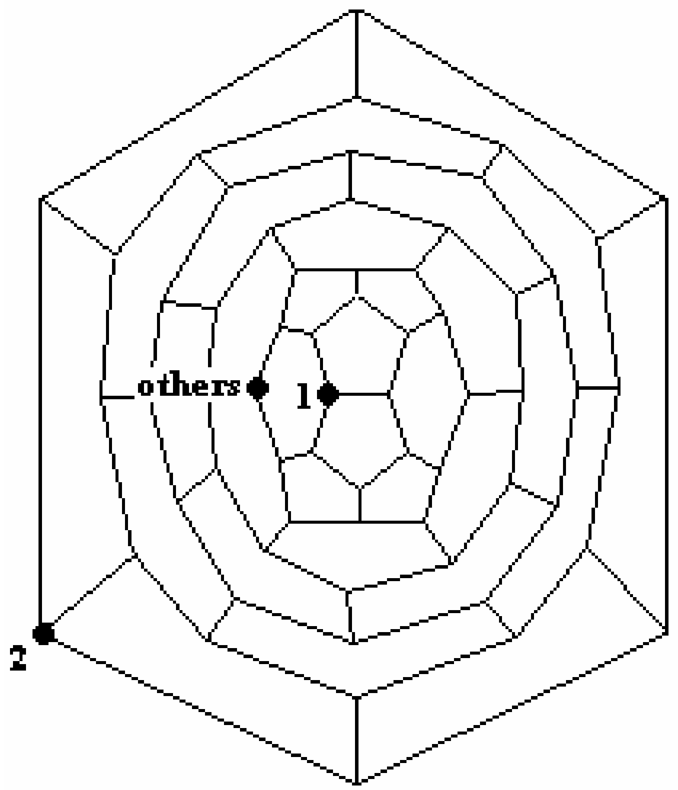

Fig. 2. The Molecular Graph of the Fullerene C_{12n+2}

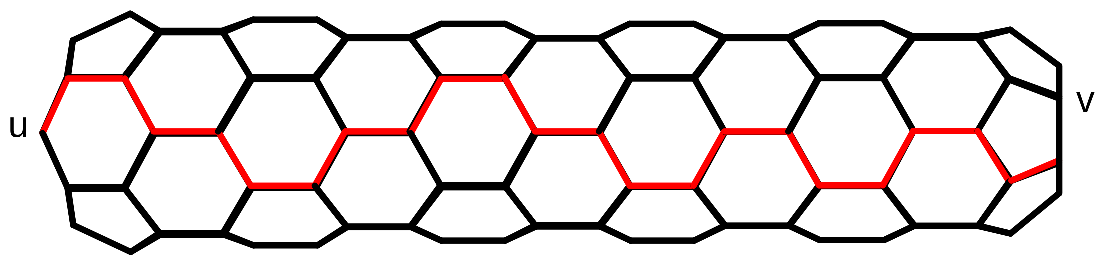

Fig. 3. The Value of ecc(x) for Vertices of Central and Outer Polygons.

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