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Eccentric connectivity polynomials of fullerenes

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The eccentric connectivity polynomial of a molecular graph G is defined as $ECP(G,x) = \Sigma_{x\in V(G)}x^{ecc(x)}$, where ecc(x) is defined as the length of a maximal path connecting x to a vertex of G. In this paper this polynomial is computed for an infinite family of fullerenes.

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1. Introduction

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. Then F made entirely of n carbon atoms, have 3n/2 edges, 12 pentagonal and $(n/2 - 10)$ hexagonal faces, while $n \neq 22$ is a natural number equal or greater than 20 [2].

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is an important tool for studying molecular structures [3-7]. This theory has an important effect in the development of chemical sciences.

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[8]. 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 $ecc(u) = Max\{d(x,u) \mid x \in V(G)\}$ [9-14]. 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.

2. Main results and discussion

The aim of this section is to compute *ECP(G,x)*, for an infinite family of fullerenes. We encourage the reader to consult papers [15-27] for background material as well as basic computational techniques. In Table 1, the EC polynomials of C_{12n+2} fullerenes, Fig. 1, are computed, $2 \leq n \leq 7$.

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

Fullerenes	EC Polynomials
C_{60}	$60x^9$
C_{84}	$84x^{11}$
C_{108}	$84x^{12}+24x^{13}$
C_{132}	$60x^{12}+24x^{13}+24x^{14}+24x^{15}$
C_{156}	$36x^{12}+24x^{13}+24x^{14}+24x^{15}+24x^{16}+24x^{17}$
C_{180}	$12x^{12}+24x^{13}+24x^{14}+24x^{15}+24x^{16}+24x^{17}+24x^{18}+24x^{19}$

When $n \geq 8$, we have the following general formula for the EC polynomial of this class of fullerenes:

Theorem 1. The EC polynomial of $C_{12(2n+1)}$, $n \geq 8$, fullerenes are computed as $ECP(C_{12(2n+1)},x) = 12x^{n+5}+24\,x^{n+6}\,\frac{x^n-1}{x-1}$.

Proof. From Fig. 2, one can see that there are two types of vertices of fullerene graph $C_{12(2n+1)}$. These are the vertices of the central hexagon and other vertices of $C_{12(2n+1)}$. Obviously, we have:

Vertices	ecc(x)	No.
The Type 1 Vertices	$n + i$ $(6\leq i \leq n+5)$	24
The Type 2 Vertices	$n + 5$	12

By using these calculations and Fig. 2, the theorem is proved.

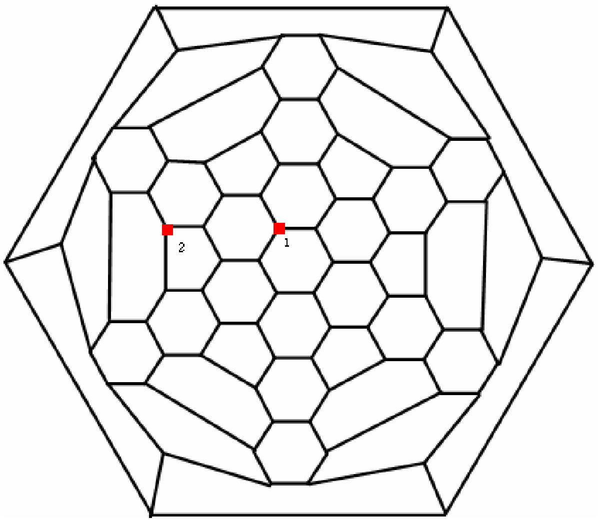

Fig. 1. The Molecular graph of the Fullerene $C_{12(2n+1)}$.

Corollary. The diameter of $C_{12(2n+1)}$ fullerene, $n \geq 2$ is $2n + 5$.

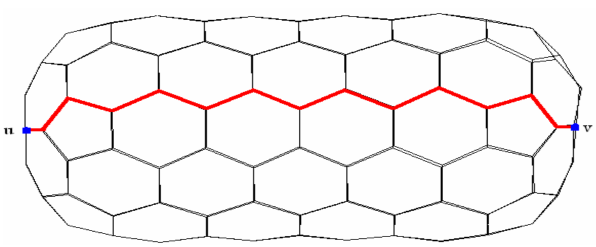

Fig. 2. The value of ecc(x) for vertices of central and outer hexagons.

In Table 2, the EC polynomials of C_{12n+4} fullerenes, Fig. 3, are computed, $2 \leq n \leq 7$. For $n \geq 8$ we have the following general formula for the EC polynomial of this class of fullerenes.

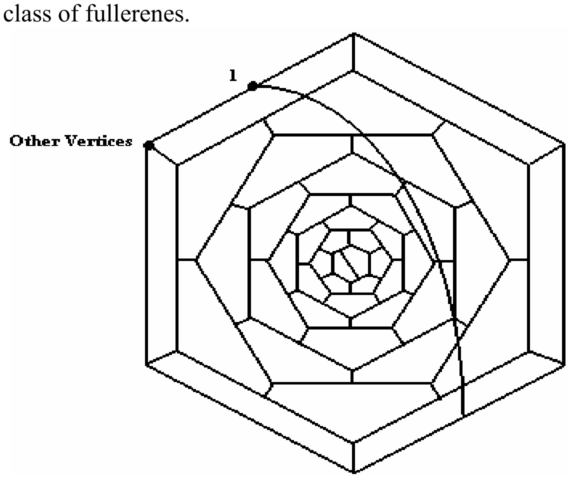

Fig. 3. The molecular graph of the Fullerene C_{12n+4}.

Theorem 2. The EC polynomial of the fullerene C_{12n+4}($n \geq 8$), fullerenes are computed as follows:

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

Proof. From Fig. 3, one can see that there are two types of vertices of fullerene graph C_{12n+4}. These are the vertices of the central pentagons and other vertices of C_{12n+4}. Obviously, we have:

Vertices	ecc(x)	No.
The Type 1 Vertices	2n+1	4
Other Vertices	n+i ($1 \leq i \leq n+1$)	12

By using these calculations and Fig. 4, the theorem is proved.

Corollary. The diameter of C_{12n+4} fullerenes, $n \geq 4$, is $2n+1$.

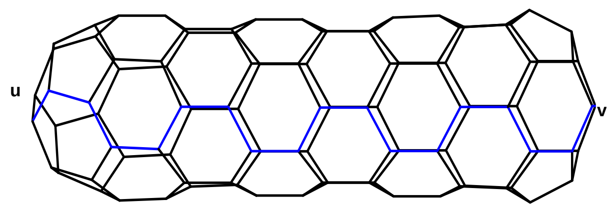

Fig. 4. The value of ecc(x) for vertices of central and outer polygons.

Some exceptional cases are given in the following table:

Fullerenes	EC Polynomials
C_{28}	$12x^5+16x^6$
C_{40}	$36x^7+4x^8$
C_{52}	$12x^7+32x^8+8x^9$
C_{64}	$24x^8+24x^9+12x^{10}+4x^{11}$
C_{76}	$12x^8+24x^9+12x^{1}0+12x^{11}+12x^{12}+4x^{13}$
C_{88}	$24x^9+12x^{10}+12x^{11}+12x^{12}+12x^{13}+12x^{14}+4x^{15}$

Table 2. Some exceptional cases of C_{12n+4} Fullerenes.

3. Concluding remarks

In this paper a method for computing eccentric connectivity index of fullerenes is presented. We apply our method on two infinite families of fullerenes. Our calculation given here is efficient and can be applied in general to other fullerenes.

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