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A Study of Fullerenes by MEC Polynomials

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The modified eccentric connectivity polynomial of a molecular graph, G, is defined as $\Lambda(G,x) = \sum_{a \in V(G)} n_G(a) x^{\varepsilon_G(a)}$ where $\varepsilon_G(a)$ is the eccentricity of vertex a and $n_G(a)$ is the sum of the degrees of its neighborhoods. In this paper, the polynomial for three infinite classes of fullerenes is computed.

Keywords: Fullerene, modified eccentric connectivity polynomial, eccentric connectivity polynomial.

1. INTRODUCTION

A topological index is a graphic invariant used in a structure property correlations. Topological indices defined by the distance function d(-,-) are called distance-based topological indices. Here for arbitrary vertices x and y, the distance d(x,y) is defined as the length of a minimal path connecting x and y. The Wiener index[1] is the first distance-based topological index. It is defined as the sum of all distances between the vertices of a graph G.

Fullerenes are zero-dimensional nanostructures which were discovered experimentally in 1985.[2] They are carbon-cage molecules in which a number of carbon atoms are bonded in a nearly spherical configuration. For a given fullerene, F, let p, h, n and m be the number of pentagons, hexagons, carbon atoms and bonds between them. Because each atom lies in exactly three faces and each edge lies in two 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. From Euler's formula, n – m + f = 2, we can deduce that (5p+6h)/3 – (5p+6h)/2 + p + h = 2 and that p = 12, n = 2h + 20 and m = 3h + 30. This outcome implies that molecules of this type, which are made entirely of n carbon atoms, have 12 pentagonal faces and (n/2 – 10) hexagonal faces; it also implies that $n \neq 22$ is a natural number equal to or greater than 20.[3]

Throughout this paper, the word graph means a simple connected graph. The vertex and edge sets of graph G are denoted by V(G) and E(G), respectively. The eccentric connectivity index of molecular graph G, $\xi(G)$, was proposed by Sharma, Goswami and Madan.[4] It is defined as $\xi(G) = \Sigma_{u \in V(G)} \deg_G(u).\varepsilon_G(u)$, where $\deg_G(x)$ denotes the degree of vertex x in G and $\varepsilon_G(u)= \mathrm{Max}\{d(x,u) \mid x \in V(G)\}$.[5-8] The radius and diameter of G are defined as the minimum and maximum eccentricity among vertices of G, respectively.

We now define the modified eccentric connectivity (MEC) polynomial of graph G as $\Lambda(G,x) = \sum_{a \in V(G)} n_G(a) x^{\varepsilon_G(a)}$ where $n_G(a)$ is the sum of the degrees of the neighbors of vertex a. As a result, MEC index is the first derivative of this polynomial for $x = 1$. For example, if K_n denotes the complete graph on n vertices, then, for every $v \in V(K_n)$, $deg(v)$ = n – 1 and $\varepsilon_G(v) = 1$. Hence, $\Lambda(G,x) = (n-1)^2 \sum_{a \in V(G)} x = n(n-1)^2 x$.

Throughout this paper, we use standard notation taken mainly from a standard book of graph theory. Basic computational techniques and background materials can be found in the references.[9-13]

2. MAIN RESULTS AND DISCUSSION

The goal of this paper is to compute the MEC polynomial of some classes of fullerenes. To do this, we begin with a result which is crucial in the paper.

Lemma 1. The MEC polynomial of a k-regular graph is $\Lambda(G, x) = k^2 \sum_{a \in V(G)} x^{\varepsilon_G(a)}$.

With Lemma 1, the MEC polynomial of a fullerene can be easily represented as

$$\Lambda(G, x) = 9 \sum_{a \in V(G)} x^{\varepsilon_G(a)}.$$

Table 1 shows the computations of some exceptional cases of the MEC polynomial of C_{12n+2} fullerenes (Fig. 1). For $n \geq 10$, we get Theorem 2.

Theorem 2. The MEC polynomial of C_{12n+2} fullerenes for $n \geq 10$ is computed as follows:

$$\Lambda(C_{12n+2}, x) = 54x^n + 36x^{n+1}\frac{x^{n-1}-1}{x-1} + 72x^{2n}.$$

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Proof. Figure 1 confirms the possibility of the vertex set being partitioned into three subsets: A, B and C. As shown in Figure 1, subset A contains all the vertices of the central octagon, subset B contains all the vertices of the outer hexagon of C_{12n+2}, and subset $C = V(C_{12n+2}) - A \cup B$. Therefore,

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

we have the following calculations.

With these calculations and Figure 2, the theorem 2 is proved.

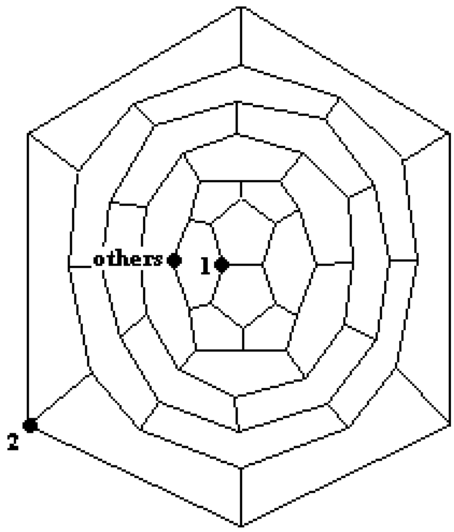

Fig. 1. The molecular graph of the fullerene C_{12n+2}.

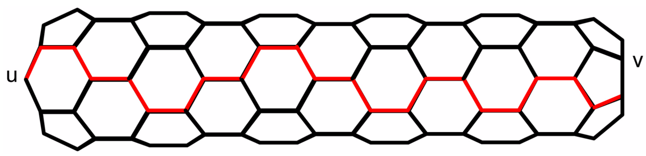

Fig. 2. A maximum path for computing $\varepsilon_G(u)$ and $\varepsilon_G(v)$ in C_{12n+2}.

Some exceptional cases are given in Table 1.

Corollary 3. Consider the fullerene graph C_{12n+2}. Then $\Lambda(C_{12n+2}) = 54n^2 + 144n$.

Consider the C_{12n+4} fullerene depicted in Figure 3. Table 2 shows the computations of some exceptional cases of the MEC polynomials. When $n \ge 8$, we have the following general formula:

Theorem 4. The MEC polynomial of a C_{12n+4} fullerene is computed as follows:

$$\Lambda(C_{12n+4},x) = 108x^{n+1}\frac{x^{n-1}-1}{x-1} + 36x^{2n+1}.$$

Proof. Figure 4 shows that there are two types of vertices: the vertices of the central pentagons and the vertices of

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

C_{12n+4}. Obviously, we have:

With these calculations and Figure 3, the theorem is proved.

Some exceptional cases are given in Table 2.

Corollary 5. The MEC index of a C_{12n+4} fullerene is computed as follows:

$$\Lambda(C_{12n+4}) = 162n^2 + 180n + 36.$$

Table 3 shows the computations of some exceptional cases of the MEC polynomial of C_{18n+10} fullerenes (Fig. 5). For $n \ge 14$, we get the following general formula:

Theorem 6. The MEC polynomial of a C_{18n+10} fullerene for $n \ge 14$ is computed as follows:

$$\Lambda(C_{18n+10},x) =$$

$$162x^{n+2} \times \frac{x^{n-2}-1}{x-1} + 135(x^{2n} + x^{2n+1}) + 81x^{2n+2} + 63x^{2n+3}$$

Table 1. Some exceptional cases of C_{12n+2} fullerene

Fullerenes	EC Polynomials
C_{26}	$216x^5+18x^6$
C_{38}	$342x^7$
C_{50}	$108x^7+306x^8+36x^9$
C_{62}	$216x^8+216x^9+126x^{10}$
C_{74}	$108x^8+216x^9+162x^{10}+108x^{11}+72x^{12}$
C_{86}	$216x^9+162x^{10}+108x^{11}+108x^{12}+108x^{13}+72x^{14}$
C_{98}	$36x^9+54x^{10}+36x^{11}+36x^{12}+36x^{13}+36x^{14}+36x^{15}+24x^{16}$
C_{110}	$54x^{10}+36x^{11}+36x^{12}+36x^{13}+36x^{14}+36x^{15}+36x^{16}+36x^{17}+ 24x^{18}$

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

Fullerenes	Modified eccentric connectivity polynomials
C_{28}	$36x^5 + 48x^6$
C_{40}	$108x^7 + 12x^8$
C_{52}	$36x^7 + 96x^8 + 24x^9$
C_{64}	$72x^8 + 72x^9 + 36x^{10} + 12x^{11}$
C_{76}	$36x^8 + 72x^9 + 362x^{1}0 + 36x^{11} + 36x^{12} + 12x^{13}$
C_{88}	$72x^9 + 36x^{10} + 36x^{11} + 36x^{12} + 36x^{13} + 36x^{14} + 12x^{15}$

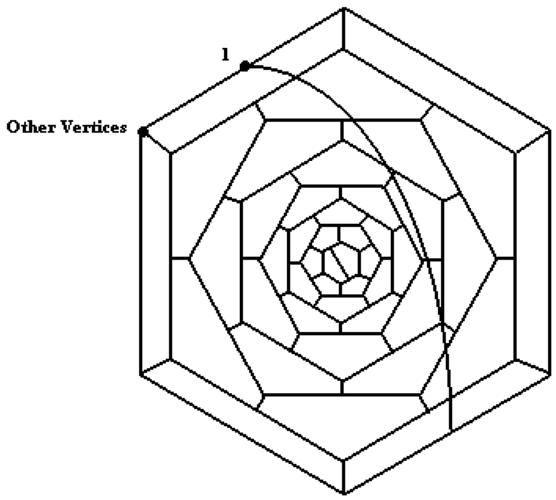

Fig. 3. The molecular graph of the fullerene C_{12n+4}.

Proof. Figure 6 shows that there are four types of vertices of fullerene graph C_{18n+10}. Obviously, we have:

Vertices	ecc(x)	No.
The Type 1 Vertices	2n+3	7
The Type 2 Vertices	2n+2	9
The Type 3 Vertices	2n,2n+1	15
Other Vertices	n+i (2 i n-1)	18

With these calculations and Figure 5, the theorem is proved.

Some exceptional cases are given in Table 3:

Corollary 7. The MEC index of C_{18n+10} is computed as $\Lambda(C_{18n+10}) = 243n^2 - 117n + 189$.

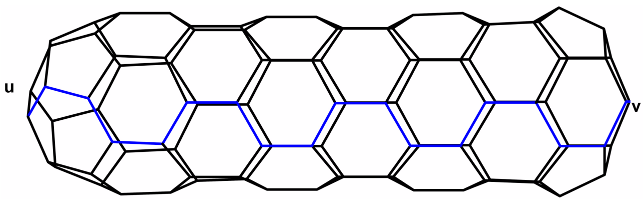

Fig. 4. A Maximal path for calculation of $\varepsilon_G(u)$ and $\varepsilon_G(v)$ in C_{12n+4}.

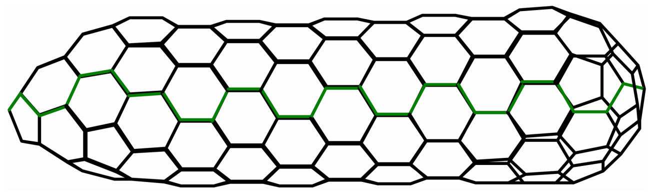

Fig. 5. Maximal path for calculation of $\varepsilon_G(u)$ and $\varepsilon_G(v)$ in C_{18n+10}.

Table 3. Some exceptional cases of C_{18n+10} fullerene

Fullerenes	Modified eccentric connectivity polynomials
C_{82}	$201x^{10}+45x^{11}$
C_{100}	$54x^{10}+150x^{11}+66x^{12}+30x^{13}$
C_{118}	$108x^{11}+117x^{12}+63x^{13}+39x^{14}+27x^{15}$
C_{136}	$54x^{11}+108x^{12}+81x^{13}+63x^{14}+45x^{15}+36x^{16}+21x^{17}$
C_{154}	$108x^{12}+81x^{13}+63x^{14}+54x^{15}+63x^{16}+45x^{17}+27x^{18}+21x^{19}$
C_{172}	$54x^{12}+81x^{13}+63x^{14}+54x^{15}+63x^{16}+54x^{17}+45x^{18}+45x^{19}+ 27x^{20}+21x^{21}$
C_{190}	$81x^{13}+63x^{14}+54x^{15}+72x^{16}+54x^{17}+54x^{18}+54x^{19}+45x^{20}+45x^{21}+27x^{22}+21x^{23}$
C_{208}	$27x^{13}+63x^{14}+54x^{15}+72x^{16}+54x^{17}+54x^{18}+54x^{19}+ 54x^{20}+ 54x^{21}+ 45x^{22}+ 45x^{23} +27x^{24}+21x^{25}$
C_{226}	$63x^{14}+54x^{15}+72x^{16}+54x^{17}+54x^{18}+54x^{19}+54x^{20}+54x^{21}+54x^{22}+54x^{23}+45x^{24}+45x^{25}+27x^{26}+21x^{27}$
C_{244}	$36x^{15}+72x^{16}+54x^{17}+54x^{18}+54x^{19}+54x^{20}+54x^{21}+54x^{22}+54x^{23}+54x^{24}+54x^{25}+45x^{26}+45x^{27}+27x^{28}+21x^{29}$

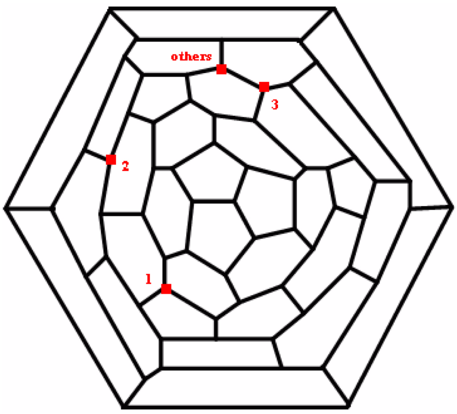

Fig. 6. The molecular graph of the fullerene C_{18n+10}.

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