ECCENTRIC CONNECTIVITY POLYNOMIAL OF C_{12n+4} FULLERENES

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Fullerenes C_n can be drawn for $n = 20$ and for all even $n \geq 24$. They have n carbon atoms, $3n/2$ bonds, 12 pentagonal and $n/2$-10 hexagonal faces. The eccentricity connectivity polynomial of a molecular graph G is defined as $EC(G,x) = \Sigma_{a\in V(G)}deg_G(a)x^{ecc(a)}$, 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 is one of the most fascinating of all materials. It is the basis of all life and of all organic chemistry. One of its forms, diamond, is the hardest of all known materials and has the highest thermal conductivity. Fullerenes are a family of carbon allotropes, molecules composed entirely of carbon, in the form of a hollow sphere, ellipsoid, tube, or plane. Spherical fullerenes are also called buckyballs, and cylindrical ones are called carbon nanotubes or buckytubes. Graphene is an example of a planar fullerene sheet. Fullerenes are similar in structure to graphite, which is composed of stacked sheets of linked hexagonal rings, but may also contain pentagonal (or sometimes heptagonal) rings that would prevent a sheet from being planar.

Fullerenes are zero-dimensional nanostructures, discovered experimentally in 1985.[1] Fullerenes C_n can be drawn for $n = 20$ and for all even $n \geq 24$. They have n carbon atoms, $3n/2$ bonds, 12 pentagonal and $n/2$-10 hexagonal faces. The most important member of the family of fullerenes is C_{60}.[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].

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2. Main results and discussion

The aim of this section is to compute ECP(G,x), for an infinite family of fullerenes. To do this, we first draw these compounds by HeperChem[15] and then compute their adjacency and distance matrices by TopoCluj[16]. Next, we apply some GAP[17] programs to compute the ecc(u) for given vertex u of these nanomaterials. Final step of this process is analyzing data obtained by our GAP programs. These programs are accessible from the authors upon request.
In Table 1, the EC polynomials of C_{12n+4} fullerenes, Figure 3, are computed, $2 \le n \le 7$. For $n \ge 8$ we have the following general formula for the EC polynomial of this class of fullerenes.
Theorem4. The EC polynomial of the fullerene $C_{12n+}4(n \ge 8)$, fullerenes are computed as follows:

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

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 ($1 \le i \le n+1$)	12

By using these calculations and Figure2, the theorem is proved. ■
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}	$24x^9+12x^{10}+12x^{11}+12x^{12}+12x^{13}+12x^{14}+4x^{15}$

Table1. Some exceptional cases of C_{12n+4} fullerenes.

Corollary5. The diameter of C_{12n+4}, $n \ge 4$, fullerenes is 2n+1.

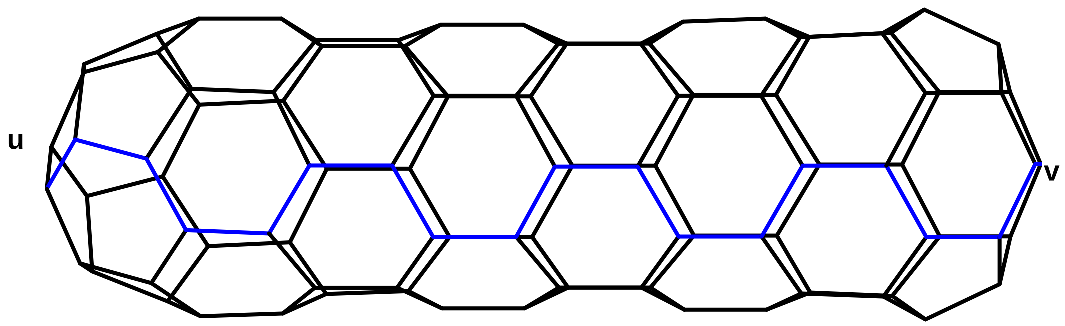

Fig. 2. The Value of ecc(x) for Vertices of Central and Outer Polygons.

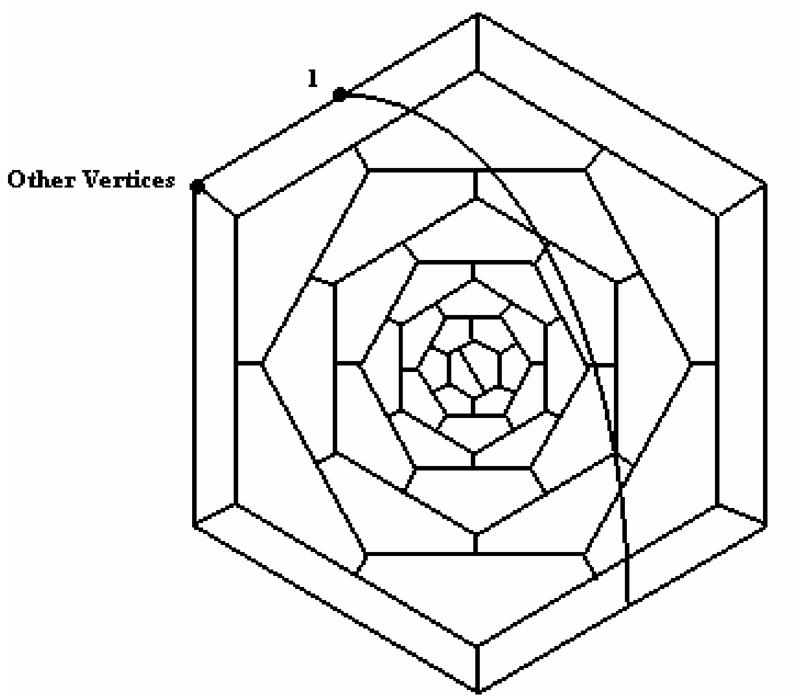

Fig. 3. The Molecular Graph of the Fullerene C_{12n+4}

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