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Eccentric connectivity index of fullerene graphs

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ABSTRACT. The eccentric connectivity index of the molecular graph is defined as $\xi^c(G)=\Sigma_{u\in V(G)}\deg_G(u)\varepsilon(u)$, where $\deg_G(x)$ denotes the degree of the vertex x in G and $\varepsilon(u)=\max\{d(x,u)\ |x\in V(G)\}$. In this paper this polynomial is computed for an infinite class of fullerenes.

Keywords: eccentric connectivity index, eccentricity connectivity polynomial, fullerene.

1. INTRODUCTION

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. Two vertices are adjacent if and only if they are connected by an edge; two edges are adjacent if and only if they have an end vertex in common. For given graph G, it is called a molecular graph if the maximum degree of every vertex reaches to four. Molecular graphs are significantly important in showing the mathematic applications in chemistry. Molecules properties description is of a great value in the science of chemistry and pharmacology. A topological index is a numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. In an exact phrase, if Λ denotes the class of all finite graphs then a topological index is a function Top from Λ into real numbers with

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this property that Top(G) = Top(H), if G and H are isomorphic. Obviously, the number of vertices and the number of edges are topological index. The *Wiener index* [1] is the first reported distance based topological index defined as half sum of the distances between all the pairs of vertices in a molecular graph [2]. *Topological indices* are abundantly being used in the *QSPR* and *QSAR* researches. So far, many various types of topological indices have been described.

If For two vertices $x, y \in V(G)$ the distance $d(x, y)$ is defined as the length of a shortest path between them. The eccentric connectivity index of the molecular graph G, $\xi^c(G)$, was proposed by Sharma, Goswami and Madan as [3]

$$\xi^c(G) = \Sigma_{u \in V(G)} \deg_G(u)\varepsilon(u),$$

where $\deg_G(x)$ denotes the degree of the vertex x in G and $\varepsilon(u)=\max\{d(x,u)|x \in V(G)\}$, see [4-8] for details. The eccentric connectivity polynomial of a graph G defined by Doslić et.al as [9]

$$\xi^c(G, x) = \Sigma_{a \in V(G)} \deg_G(a) x^{\varepsilon(a)}.$$

Then the eccentric connectivity index is the first derivative of $\xi^c(G, x)$ evaluated at $x = 1$.

In the past years, nanostructures involving carbon have been the focus of an intense research activity which is driven to a large extent by the quest for new materials with specific applications. Fullerene is one of the main objects of nanostructures. Kroto and his team discovered the most stable fullerene C_{60} and by this discovery the fullerene era was started. A fullerene is a cubic 3- connected planar graphs whose faces are cycles C_s and C_r, satisfying in Euler's formula. So, by using Euler's theorem we can construct fullerenes with faces pentagons and hexagons, fullerenes with faces triangles and hexagons, fullerene with faces quadrangles and hexagons and even fullerenes with pentagonal and heptagonal faces. Denoted by (4,6) fullerenes means a fullerenes whose faces are quadrangles and hexagons. Let q, h, n and m be the number of pentagons, hexagons, carbon atoms and bonds between them, in a given (4,6) fullerene F. Since F is cubic, $m = 3n/2$ and by Euler's theorem $n - 3n/2 + f = 2$. This means

$$f = 2 + n/2 = q + h. \tag{1}$$

On the other hand, $n - m + f = (4q + 6h)/3 - (4q + 6h)/2 + q + h = 2$, leads us to conclude that $q = 6$. Hence, by using equation (1) we have $h = n/2 - 4$, while $n \neq 10$ is a natural number equal or greater than 8, see [10, 11]. In this paper by a fullerene we mean a (4,6) fullerene.

A bijection $\sigma: V \longrightarrow V$ by this properties that if $e = uv$ is an edge, then $\sigma(e)=\sigma(u)\sigma(v)$ is an edge of E is called an automorphism of graph G. The set of all automorphisms of G under the composition of mappings forms a group which is denoted by $Aut(G)$.

A hypercube H_n (Figure 1) can be constructed as follows: the vertex set of H_n are all n-tuples $b_1b_2...b_n$ with $b_i \in \{0,1\}$ and two vertices $x=x_1x_2...x_n$ and $y=y_1y_2...y_n$ are adjacent if and only if $d_G(x,y)=1$.

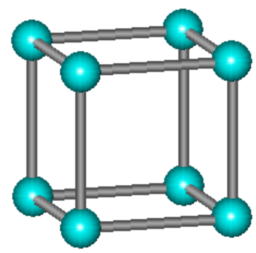

Figure 1. Hypercube H_3.

Herein, our notation is standard and taken from the standard book of graph theory [12].

2. RESULTS AND DISCUSSION

The aim of this section is to compute the eccentric connectivity polynomial of an infinite family of fullerenes with $8n^2$ vertices denoted by F_{8n^2}. Since every fullerene is cubic then every fullerene in this class has $12n^2$ edges. To do this, we first draw these compounds by HeperChem [13] and then compute their adjacency and distance matrices by TopoCluj [14]. Next, we apply a GAP [15] program to compute the $\varepsilon(u)$ for given vertex u. This program is accessible from the authors upon request.

Lemma 1. If G be a k regular graph, then $\xi^C(G) = k\sum_{u\in V(G)}\varepsilon(u)$.

Lemma 2 [8]. Suppose G is a graph, A_1, A_2, ..., A_t are the orbits of Aut(G) under its natural action on $V(G)$ and $x_i \in A_i$, $1 \le i \le t$. Then $\xi^C(G) = \sum_{j=1}^{t}|A_j|\deg(x_j)\varepsilon(x_j)$. In particular, if G is vertex transitive then $\xi^C(G) = k.|V(G)|.r(G)$ for some k.

Proof. It is easy to see that if vertices u and v are in the same orbit, then there is an automorphism φ such that $\varphi(u) = v$. choose a vertex x such that $ecc(u) = d(u,x)$. Since φ is onto, for every vertex y there exists the vertex w such that $y = \varphi(w)$. Thus $d(v, y) = d(\varphi(u), \varphi(w)) = d(u,w)$ and so

$$\varepsilon(v) = \max\{d(v, y)\}_{y\in V(G)} = \max\{d(u,w)\}_{w\in V(G)} = \varepsilon(u).$$

On the other hand, it is a trivial fact that the vertices of a given orbit have equal degrees. Therefore, $\xi^C(G) = \sum_{j=1}^{t} |A_j| \deg(x_j)\varepsilon(x_j)$. If G is vertex transitive then it is k – regular graph, for some k and by Lemma 1, $\xi^C(G) = k.|V(G)| r(G)$. This completes our proof.

In Table 1, the eccentric connectivity polynomials of F_{8n^2} fullerenes (Figure 2) are computed, $4 \le n \le 13$. For $n \ge 14$ we have the following general formula for the eccentric connectivity polynomial of this class of fullerenes.

Theorem 3. The eccentric connectivity polynomial of the fullerene F_{8n^2} ($n \ge 14$), fullerenes are computed as follows:

$$\xi^c(F_{8n^2}, x) = 54x^{n+2} \times \frac{x^{n-2} - 1}{x - 1} + 45(x^{2n} + x^{2n+1}) + 27x^{2n+2} + 21x^{2n+3}.$$

Proof. By means of group action of automorphism group of F_{8n^2} on the set of its vertices, one can see that there are four types of vertices of fullerene graph F_{8n^2}. These are the vertices of the type 1, type 2, type 3 and type 4 of the fullerene F_{8n^2}. Obviously, we have the following table and this completes the proof.

Vertices	ε**(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	$n+i$ ($2 \le i \le n-1$)	18

Corollary 4. The eccentric connectivity polynomial of the fullerene F_{8n^2} ($n \ge 14$), fullerenes is:

$$\xi^c(F_{8n^2}) = 81n^2 + 141n + 108.$$

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Fullerene	*EC* Polynomial
F_{82}	$67x^{10}+15x^{11}$
F_{100}	$18x^{10}+50x^{11}+22x^{12}+10x^{13}$
F_{118}	$36x^{11}+39x^{12}+21x^{13}+13x^{14}+9x^{15}$
F_{136}	$18x^{11}+36x^{12}+27x^{13}+21x^{14}+15x^{15}+12x^{16}+7x^{17}$
F_{154}	$36x^{12}+27x^{13}+21x^{14}+18x^{15}+21x^{16}+15x^{17}+9x^{18}+7x^{19}$
F_{172}	$18x^{12}+27x^{13}+21x^{14}+18x^{15}+21x^{16}+18x^{17}+15x^{18}+15x^{19}+ 9x^{20}+7x21$
F_{190}	$27x^{13}+21x^{14}+18x^{15}+24x^{16}+18x^{17}+18x^{18}+18x^{19}+15x^{20}+15x^{21}+9x^{22}+7x^{23}$
F_{208}	$9x^{13}+21x^{14}+18x^{15}+24x^{16}+18x^{17}+18x^{18}+18x^{19}+ 18x^{20}+ 18x^{21}+ 15x^{22}+ 15x^{23} +9x^{24}+7x^{25}$
F_{226}	$21x^{14}+18x15+24x^{16}+18x^{17}+18x^{18}+18x^{19}+18x^{20}+18x^{21}+18x^{22}+18x^{23}+15x^{24}+15x^{25}+9x^{26}+7x^{27}$
F_{244}	$12x^{15}+24x^{16}+18x^{17}+18x^{18}+18x^{19}+18x^{20}+18x^{21}+18x^{22}+18x^{23}+18x^{24}+18x^{25}+15x^{26}+15x^{27}+9x^{28}+7x^{29}$

Table1. Some exceptional cases of F_{8n^2} fullerenes.

Corollary 5. The diameter of F_{8n^2}, $n \geq 2$, fullerenes is $4n - 1$.

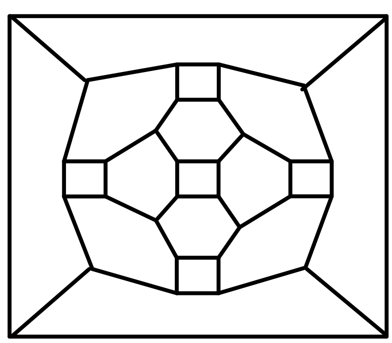

Figure 2. 2 – D graph of fullerene C_{8n^2} for $n = 2$.

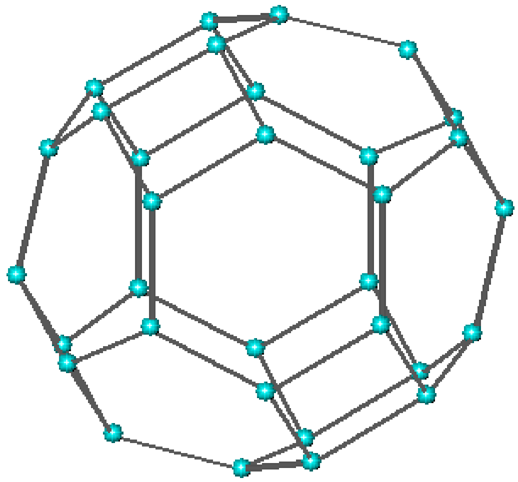

Figure 3. The molecular graph of the fullerene F_{8n^2} , for $n = 2$.

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