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Eccentric Connectivity Polynomial of C_{18n+10} Fullerenes

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The fullerene era was started in 1985 with the discovery of a stable C_{60} cluster and its interpretation as a cage structure with the familiar shape of a soccer ball by Kroto and co-authors. The eccentric connectivity polynomial of a molecular graph G is defined as $ECP(G, x) = \Sigma_{a\in V(G)} deg_G(a)x^{ecc(a)}$, where $ecc(a)$ is defined as the length of the maximum path connecting to another vertex of G. In this paper this polynomial is computed for C_{18n+10} fullerenes.

Keywords: Eccentric Connectivity Index, Eccentric Connectivity Polynomial, Fullerene, Diameter of graph.

INTRODUCTION

We first recall some algebraic definitions that will be kept throughout. A pair $G = (V, E)$ such that V is a non-empty set and E is a subset of 2-element subsets of V is called a simple graph (graph for short). G is said to be connected if for arbitrary vertices x and y of G, there exists a sequence $x = x_0, x_1, x_2, \ldots, x_n = y$ such that x_i and x_{i+1} are adjacent in G. 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 the minimum path connecting x and y. The eccentric connectivity index of G, $\xi^c(G)$, was proposed by Sharma, Goswami and Madan [1]. 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 $ecc(u) = \mathrm{Max}\{d(x, u) \mid x \in V(G)\}$ [2–6]. The radius and diameter of G are defined as the minimum and maximum eccentricity among vertices of G, respectively.

A fullerene is a molecule composed entirely of carbon atoms. The fullerene era was started in 1985 with the discovery of a stable C_{60} cluster [7, 8]. Let F be a fullerene graph with exactly p, h, n and m pentagons, hexagons, vertices and edges between them, respectively. Since each vertex lies in exactly 3 faces and each edge lies in 2 faces, the number of vertices 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 Euler's formula $n - m + f = 2$, one can deduce that $(5p + 6h)/3 – (5p + 6h)/2 + p + h = 2$, and therefore $p = 12$, $v = 2h + 20$ and $e = 3h + 30$. Therefore, such molecules are made up entirely of n carbon atoms having 12 pentagonal and $(n/2 - 10)$ hexagonal faces, where $n \neq 22$ is a natural number equal or greater than 20.

We now define the eccentric connectivity polynomial of a graph G, as

$$\Xi(G,x)=\Sigma_{a\in V(G)} deg_G(a)x^{ecc(a)}.$$

Then the eccentric connectivity index is the first derivative of $\Xi(G,x)$ evaluated at $x = 1$. Herein, our notation is standard and taken from the standard book of graph theory [9–14].

RESULTS AND DISCUSSION

This paper describes significant updates to the fullerene chemistry. In other words, this is a synthesis of knowledge. The research is based on our earlier works [9, 11–14] on constructing new classes of fullerenes and providing good computer programs for discovering their topological properties. Our research in this field started with the classification of fullerenes by their molecular graphs [9]. In the field, it is generally observed that there are more than 20 infinite families of fullerene graphs. This problem has been known to partly arise from the stability of fullerenes. The aim of this section was to compute eccentric connectivity index of an infinite family of these series of

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fullerenes, namely, C_{18n+10}. To do this, we first drew these compounds by HeperChem [15] and then computed their adjacency and distance matrices by TopoCluj [16]. Next, we applied some GAP [17] programs to compute the $ecc(u)$ for a given vertex u of these nano-materials. The final step of this process is the analysis of the data obtained by our GAP programs. These programs are accessible from the authors upon request.

An automorphism of the graph $G = (V, E)$ is a bijection σ on V which preserves the edge set E, i.e., if $e = uv$ is an edge, then $\sigma(e)=\sigma(u)\,\sigma(v)$ is an edge of E, where $\sigma(u)$ is the image of the vertex u. Thus Aut(G), the set of all automorphisms of G, under composition of mappings, forms a group. Aut(G) acts transitively on V if for any vertices u and v in V there is $\alpha \in Aut(G)$ such that.$\alpha(u) = v$.

To explain our method, we computed the eccentric connectivity polynomial of an icosahedral fullerene C_{20} with 20 vertices and a cube H_3 with 8 vertices. Since for every, $v \in V(C_{20})$, $ecc(v)= 5$, $\Xi(C_{20}, x) = 60x^5$. On the other hand, H_3 is 3-regular and so for every $v \in V(H_3)$, $ecc(v)= 3$. Hence $\Xi(H_3, x) = 24x^3$.

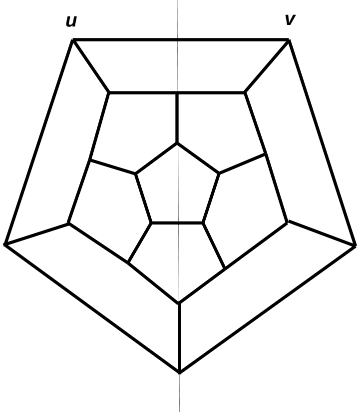

Fig. 1: The molecular graph of fullerene C_{20}.

We began by the following simple Lemma:

Lemma 1. Let $G = (V, E)$ be a graph. If Aut(G) acts transitively on V, then G is k-regular, where $|E| = k|V|/2$. Moreover, for every u in $V(G)$, $\Xi(G, x) = k|V|\times x^{ecc(u)}$.

The hypercube H_n is a graph consisting of all n-tuples $b_1b_2b_n$, $b_i \in \{0,1\}$, as vertices. Two vertices are adjacent if the corresponding tuples differ in precisely one place, so for every vertex a in $V(G)$, $ecc(a) = n$ and H_n is n - 1 regular. Darafsheh [14] proved that H_n is transitive. We now applied Lemma 1 to compute the eccentric connectivity polynomial of a hypercube H_n. We have $\Xi(H_n,x) = (n-1)2^n.x^{n-1}$. On the other hand, by considering the fullerene graph C_{20} shown in Figure 1, one can see that C_{20} is vertex transitive. But $ecc(u) = 5$, for every u in $V(C_{20})$. This implies that $\Xi(C_{20},x) = 60x^5$. The fullerenes C_{20} and C_{60} are the only vertex transitive fullerenes. So it is important how to compute $\Xi(G, x)$ polynomial for other fullerenes.

Lemma 2. Let $G = (V, E)$ be a graph. If orbits of Aut(G) under its action on V are V_1, V_2, V_s and u_i is a vertex of V_i, then:

$$\Xi(G,x)=\sum_{i=1}^{s} k_i\,|V_i|\,x^{ecc(u_i)}.$$

Proof. Suppose V_i's ($1 \le i \le s$) are orbits of Aut(G) on the set V. Clearly, for every u_i in V_i $deg_G u_i = k_i$ and Aut(G) acts transitively on V_i ($1 \le i \le s$). By using Lemma 1 the proof is completed.

Now we used Lemma 2 to compute the polynomial $\Xi(G,x)$ for the fullerene graph C_{18n+10}. In Table 1, the $\Xi(G,x)$ polynomials of C_{18n+10} fullerenes (Figures 2 and 3) are computed, $4 \le n \le 13$. For $n \ge 14$ we have the following general formula for the $\Xi(G,x)$ polynomial of this class of fullerenes:

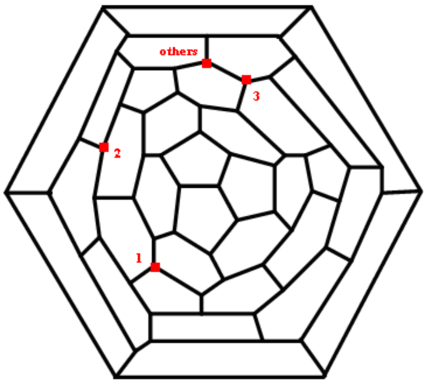

Fig. 2. The molecular graph of the fullerene C_{18n+10}.

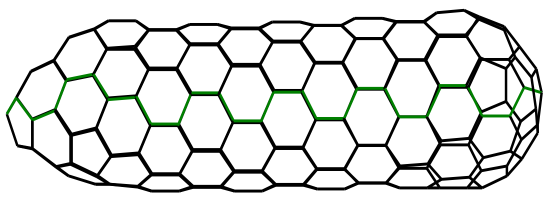

Fig. 3. The value of $ecc(x)$ for vertices of central and outer polygons.

Theorem 1. The $\Xi(G,x)$ polynomial of the fullerene C_{18n+10} ($n \ge 14$), is computed as follows:

$$\Xi(C_{18n+10}, x) = 54x^{n+2}\times\frac{x^{n-2}-1}{x-1} + 45(x^{2n} + x^{2n+1}) + 27x^{2n+2} + 21x^{2n+3}.$$

Proof. From Figure 2, one can see that Aut(G) has exactly four orbits on the vertices of C_{18n+10}. We named the representatives of these orbits as type 1, type 2, type 3 and type 4. In Table 1, we recorded our calculations:

Table 1: The type of vertices and their eccentricities

Vertices	ecc(x)	No.
Type 1 Vertices	$2n+3$	7
Type 2 Vertices	$2n+2$	9
Type 3 Vertices	$2n$, $2n+1$	15
Type 4 Vertices	$n+i$ $(2 \le i \le n-1)$	18

By the calculations given in Table 1, and Figure 2, the theorem is proved.

Some exceptional cases are given in Table 2.

Corollary 1. The diameter of C_{18n+10} fullerene, $n \ge 4$, is $2n + 3$.

Table 2. Some exceptional cases of C_{18n+10} fullerenes.

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

CONCLUSION

This paper contains information about the topological property of an infinite class of fullerenes. The area of fullerene chemistry is relatively young and received a strong boost after the discovery of the C_{60} fullerene molecule by Kroto and his team. Our results are related to the mathematical properties of this new allotrope of carbon.

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ПОЛИНОМ НА ЕКСЦЕНТРИЧНА СВЪРЗАНОСТ НА C_{18N+10} ФУЛЕРЕНИ

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(Резюме)

Епохата на фулерените започва през 1985г. с откриването на стабилен C_{60} клъстер и неговата интерпретация като клетъчна структура с познатата форма на футболна топка от Крото и съавтори. Полиномът на ексцентрична свързаност на молекулен граф G, определен като $ECP(G, x) = \Sigma_{a\varepsilon\, V(G)} deg_G(a)x^{ecc(a)}$, където $ecc(a)$ е дължината на максималния път до друг възел от G. В настоящата статия този полиномът е изчислен за C_{18n+10} фулерени.