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Eccentric connectivity polynomial of an infinite family of fullerenes

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The eccentricity connectivity polynomial of a molecular graph G is defined as $EC(G,x) = \Sigma_{a\in V(G)}x^{ecc(a)}$, 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 class of fullerenes.

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1. Introduction

Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms. 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} [1,2].

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 [3,4]. This theory had an important effect on the development of the chemical sciences. This paper reflects an attempt for studying fullerenes by using graph theory.

We now recall some algebraic definitions that will be used in the paper. 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 [5]. 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) | $x \in V(G)$}, see [6] 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 $x = 1$.

Our notation is standard and mainly taken from standard books of graph theory. We encourage the reader to consult [9–14] for background material, as well as, basic computational techniques.

2. Main results and discussion

The aim of this section is to compute ECP(G,x), for an infinite family of fullerenes. Before going to calculate this polynomial for fullerenes, we must compute ECP(G,x), for some well-known class of graphs.

Example 1. Consider the fullerene graph C_{20}, Fig. 1. One can see that the for every $x \in V(G)$, ecc(x) = 5 and so $ECP(C_{20},x) = 60x^5$.

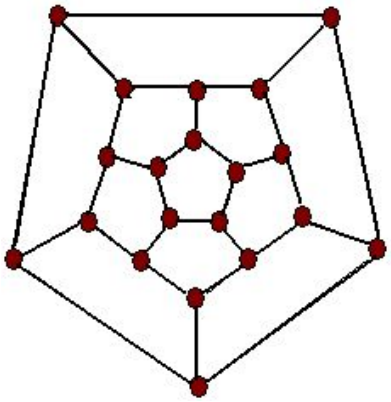

Fig. 1. The fullerene graph C_{20}.

A molecular graph G is said to be k-regular, if for every vertex x of G, $deg_G(x) = k$. It is easy to see that the EC polynomial of a k- regular graph G is equal to $ECP(G,x) = k\Sigma_{a\in V(G)}x^{ecc(a)}$. So, the EC polynomial of a fullerene graph G is $ECP(G,x) = 3\Sigma_{a\in V(G)}x^{ecc(a)}$. On the other hand, ECP(G, 1) = 2|E(G)| and ECP(G,0) = 0.

Example 2. Suppose K_n denotes the complete graph on *n* vertices. Then For every $v \in V(K_n)$, $deg(v) = n-1$ and so ecc(v)=1. This implies that $ECP(K_n,x) = n(n-1)x$.

Example 3. Let C_n denotes the cycle of length n. If n is even then for every i, the i-th row of distance matrix of C_n is $1,2,...,\overset{\}}{0},...,(n-1)/2,\ n/2,\ (n-1)/2,...,2,1$. Also, if n is

odd then the i-th row of distance matrix is equal to
$\{1,2,...,0,...,(n-1)/2,(n-1)/2,...,2,1\}$. Thus,

$$ECP(C_n,x)=\begin{cases}2nx^{n/2} & 2\mid n\\ 2nx^{(n-1)/2} & 2\nmid n\end{cases}.$$

Example 4. Let S_n be the star graph with n + 1 vertices, Fig. 2. The central vertex is denoted by x and others vertices by $u_1, u_2, \ldots, u_n$. Then for every $1 \le i, j \le n$, we have $d(x, u_i) = 1$ and $d(u_i, u_j) = 2$. So, $ECP(S_n, x)=nx^2+nx$.

Example 5. A wheel W_n is a graph of order n which contains a cycle of order n, and for which every vertex in the cycle is connected to other graph vertices, Figure 3. Suppose the central vertex is denoted by x and the others by $u_1,u_2,\ldots,u_n$. Then for every $1 \le i, j \le n$ we have $d(x, u_i) = 1$, $d(u_i, u_{i-1}) = 1$, $d(u_i, u_{i+1}) = 1$ and $d(u_i, u_j) = 2j(j \ne i - 1, i+1$. So, $ECP(W_n,x) = 3nx^2 + nx$.

Example 6. Consider a complete n-partite graph $G = M_{m_1,m_2,\ldots,m_n}$ containing $v = |V(G)|$ vertices. By definition of this graph, Fig. 4, V = V (G) can be partitioned into subsets $V_1, V_2, \ldots V_n$ of V such that for every i, $1 \le i \le n$, there is no edge between the vertices of V_i. By a direct calculation, one can see that

$$ECP(M_{m_1,m_2,\ldots,m_n})=\sum_{i=1}^{n} m_i \sum_{j=1,j\ne i}^{n} m_j x^2.$$

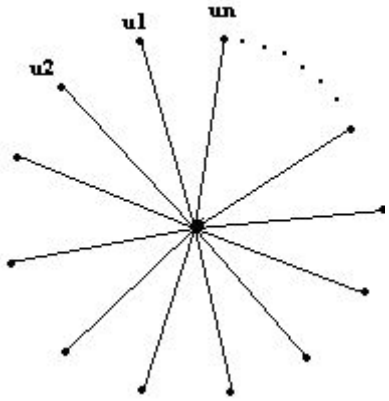

Fig. 2. The star graph with n+1 vertices.

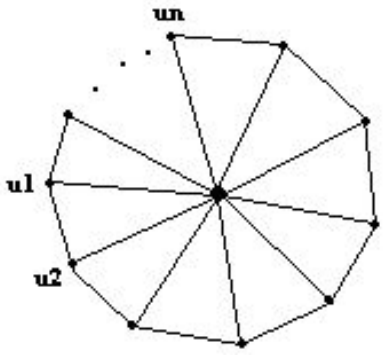

Fig. 3. The wheel graph with n+1 vertices.

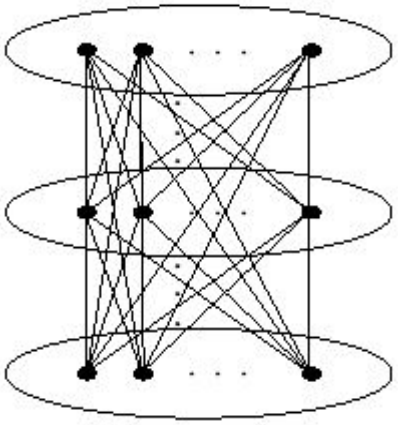

Fig. 4. The complete n-partite graph.

In Table 1, the EC polynomials of C_{10n} fullerenes, Fig. 5, are computed, $2 \le n \le 7$. If $n \ge 8$ then we have the following general formula for the EC polynomial of this class of fullerenes.

Theorem. The EC polynomial of C_{10n}, $n \ge 8$, fullerenes are computed as follows:

$$ECP(C_{10n},x) = 30\,x^n\,\frac{x^n-1}{x-1}.$$

Proof. From Fig. 5, one can see that there are two types of vertices of fullerene graph C_{10n}. These are the vertices of the central and outer pentagons, and, other vertices of C_{10n}. Obviously, we have:

Vertices	ecc(x)	No.
The Type 1 Vertices	2n – 1	10
Other Vertices	2n–i ($2 \le i \le n$)	10

By using these calculations and Fig. 6, the theorem is proved.

Some exceptional case are given in the following table:

Fullerenes	EC Polynomials
C_{20}	$60x^5$
C_{30}	$90x^6$
C_{40}	$30x^6+60x^7+30x^8$
C_{50}	$60x^7+60x^8+30x^9$
C_{60}	$72x^8+72x^9+36x^{10}$
C_{70}	$60x^8+30x^9+30x^{10}+30x^{11}+30x^{12}+30x^{13}$

Table 1. Some exceptional cases of the fullerenes C_{10n}..

3. Conclusions

Our calculation was done by a combination of HyperChem [15], TopoCluj [16] and GAP [17]. We first draw the molecule by HyperChem and them load it into TopoCluj. We compute its distance matrix by TopoCluj and then upload this matrix into a GAP program given in the end of this paper. In this way, we obtain a very fast method for our calculations.

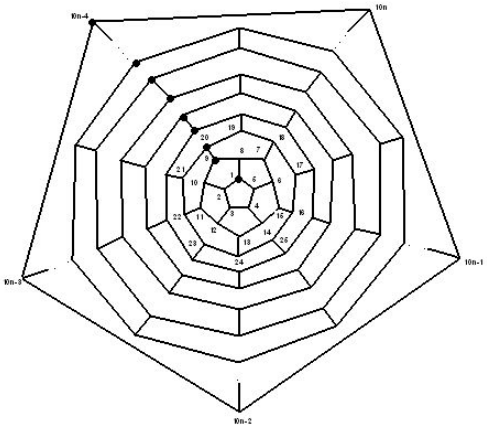

Fig. 5. The molecular graph of the fullerene C_{10n}.

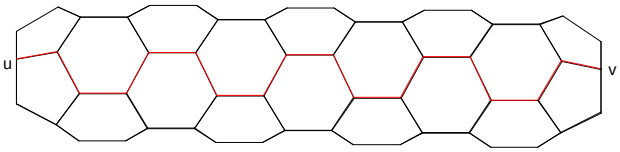

Fig. 6. The value of ecc(x) for vertices of central and outer pentagons.

A GAP Program for Computing EC Polynomial of a Graph

```
f=function(M)
        local s, t, g, gg, u, i, j, a, N;
                s:=[]; t:=0; g:=[]; gg:=[]; u:=[], N:=[];
for i in M do
                Add(N, Maximum(i));
od;
Sort(N);
for i in N do
        for j in N do
                 if j=i then
                        Add(g,j);
                fi;
        od;
        AddSet(gg,g);g:=[];
od;
Print("AM Polynomial = ");
for i in [1..Length(gg)-1] do
        Print(Length(gg[i]),"x^");Print(gg[i][1]);Print("+");
                u:=u+Length(gg[i])*(gg[i][1]);
od;
a:=Length(gg); Print(Length(gg[a]),"x^");Print(gg[a][1],"\n");
                                u:=u+Length(gg[a])*(gg[a][1]);
                        Print("\n");
                return;
end;
```

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