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Eccentricity Sequence and the Eccentric Connectivity Index of Two Special Categories of Fullerenes

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ABSTRACT. In this paper, we calculate the eccentric connectivity index and the eccentricity sequences of two infinite classes of fullerenes with 50 + 10k and 60 + 12k ($k \in N$) carbon atoms.

Keywords: Eccentricity sequence, Eccentric connectivity index, Fullerene.

1. INTRODUCTION

In mathematical chemistry a molecule can be modeled by a graph in which vertices are the atoms and two vertices are adjacent if and only if there is a bond between the two corresponding atoms.

Suppose u and v are two vertices of a graph G. Define $d_G(u,v)$ to be the length of a shortest path connecting u and v in G. The eccentricity $ec_G(u)$ is the largest distance between u and any other vertex in G. The maximum eccentricity over all vertices of G is called the diameter of G, D(G), and the minimum eccentricity is called the radius of G and denoted by R(G). The set of all vertices whose eccentricities are equal to R(G) is called the center of G. Furthermore, the eccentric connectivity index of a graph G is defined as $\xi^c(G) = \sum_{v\in V(G)} ec_G(v)deg_G(v)$, where $deg_G(v)$ is the degree of the vertex v in G [9]. This index has been widely studied by many authors. We refer the reader to [1, 2, 4, 7], for more information on this topic. For a connected graph G with vertex set $V(G) = \{v_1, v_2, ..., v_n\}$ the eccentricity sequence of G, ec(G), is defined as $ec(G) = \{ec_G(v_1), ec_G(v_2), \dots, ec_G(v_n)\}$ [3, 8].

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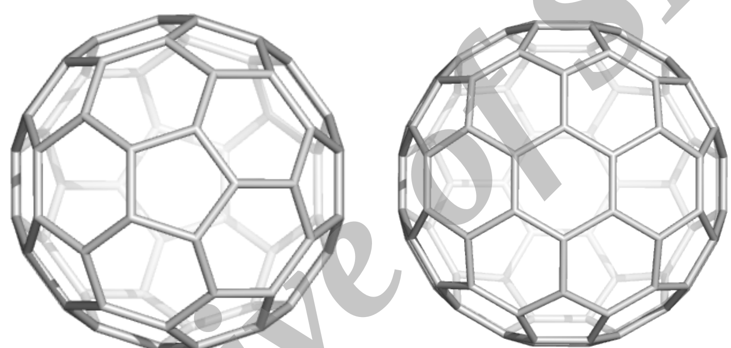
The fullerene C_{60} is first discovered by Harry Kroto in 1985. Since these molecules have several commercial applications, they are of great importance. A fullerene with n vertices is a planner, 3–regular and 3–connected graph containing 12 pentagonal and n/2 + 10 hexagonal faces.

The aim of this paper is to compute the eccentricity sequence and the eccentric connectivity index of fullerenes with exactly 50 + 10k and 60 + 12k ($k\in N$) carbon atoms. The notations used in the whole paper are standard and derived from [10].

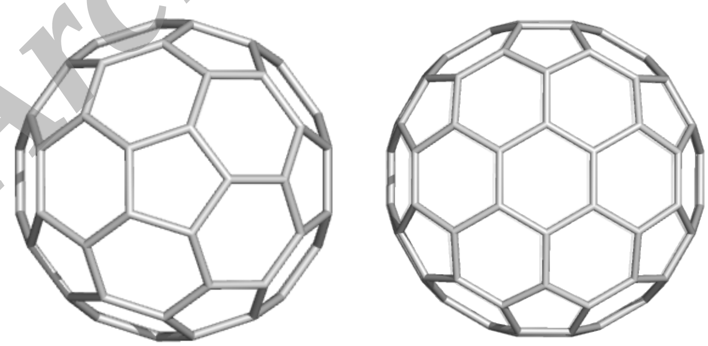
2. MAIN RESULTS

Here, we present some results for the eccentric connectivity index and the eccentricity sequence of fullerenes with exactly 50 + 10k and 60 + 12k ($k \in N$) carbon atoms. Some examples of these fullerenes are depicted in Figures 1 and 2.



C_{100} C_{120}

Figure 1: Fullerenes of type C_{50+10k} and C_{60+12k} for k = 5.



C_{110} C_{132}

Figure 2: Fullerenes of type C_{50+10k} and C_{60+12k} for k = 6.

Theorem 1. Consider the fullerene molecule C_{50+10k}, $k \geq 7$. Then the following holds:

- If k is even, then there are k/2 + 3 different classes of eccentricities in which k/2 + 6 is the lower bound and k + 8 is the upper bound.
- If k is odd, then there are $\lfloor k/2 \rfloor$ + 3 different classes of eccentricities in which the lower and the upper bounds are $\lceil k/2 \rceil$ + 6 and k + 8 respectively.

Proof. In [6] it is proved that the automorphism group of C_{50+10k} is isomorphic to dihedral group of order 20, D_{20}. In the action of the automorphism group on the set of all vertices, when k is even, there are k/2 + 4 different orbits and when k is odd, then $\lfloor k/2 \rfloor$ + 4 different orbits exist. It is clear that all of the vertices of an arbitrary orbit have the same eccentricity. Furthermore, two of these orbits have the same eccentricity. Therefore, the number of different eccentricities of the vertices of C_{50+10k} is k/2+3 when k is even and is $\lfloor k/2 \rfloor$ + 3 when k is odd.

In C_{50+10k} there are two pentagons opposite to each other and the diameter is obtained by the length of the shortest path connecting two vertices of these pentagons. Notice that there are 12 pentagons in such molecules. By increasing k, the number of octagons goes up and as a results, the fullerene becomes in a shape of a tube. In fact, the fullerenes of type C_{50+10k} are constructed of two caps and a tube. In each cap, there is a path of length four from a vertex of one of the mentioned opposite pentagons into a vertex of the tube. Moreover, the length of the tube is twice the number of its hexagons. Since there are k/2 hexagons in the tube, the length of the path in the tube is k. As a result, the diameter is k + 8. Similarly, the same method can be applied for the radius of C_{50+10k}. □

Theorem 2. If k ≥ 9, in the fullerenes of type C_{60+12k} the following results hold:

- If k is even, then there are k/2 + 3 different classes of eccentricities in which k/2 + 7 is the lower bound and k + 9 is the upper bound.
- If k is odd, then there are (k +3)/2 different classes of eccentricities in which the lower and the upper bounds are (k+15)/2 and k + 8, respectively.

Proof. By using [5] and the same method as Theorem 1, the result can be proved. □

In what follows, the eccentricity sequence of these two types of fullerenes is calculated:

Theorem 3. In the C_{50+10k} fullerenes, k ≥ 7, the eccentricity sequence can be obtained as follows:

- If k is even, then

$$ec(G)=\left\{\overbrace{0.5k+6,\dots,0.5k+6}^{10},\overbrace{\dots}^{20},\overbrace{k+7,\dots,k+7}^{30},\overbrace{k+8,\dots,k+8}^{10}\right\}.$$

- If k is odd, then

$$ec(G)=\left\{\overbrace{\left\lceil\frac{k}{2}\right\rceil+6,\dots,\left\lceil\frac{k}{2}\right\rceil+6}^{20},\overbrace{\dots}^{20},\overbrace{k+8,\dots,k+8}^{20}\right\}.$$

Proof. For k even, the orbits in which 1, 6 and 5k+21 are the representatives of orbits of size 10 and the size of all other orbits is 20. Each orbit has its own eccentricity and the first and the last orbits (orbits with 1 and 5k + 21 as the representatives) have the minimum and the maximum number of eccentricities. Moreover, the orbits in which 6 and 11 are representatives have the same eccentricities. Similarly, when k is odd, numbers 1, 6, 11, ..., 5k + 16 are representatives of the orbits. Since all of orbits have the same size, by considering Theorem 1 the result is obtained. □

Theorem 4. In the C_{60+12k} fullerenes, $k \geq 9$, the eccentricity sequence can be obtained as follows:

- If k is even then,

$$ec(G)=\left\{\overbrace{0.5k+7,\dots,0.5k+7}^{12},\overbrace{\dots}^{24},\overbrace{k+9,\dots,k+9}^{24}\right\}$$

- If k is odd then,

$$ec(G)=\left\{\overbrace{\frac{k+15}{2},\dots,\frac{k+15}{2}}^{24},\overbrace{\dots}^{24},\overbrace{k+8,\dots,k+8}^{48}\right\}.$$

Proof. In the action of the automorphism group on the set of all vertices, the following holds:

- When k is even, then {1, 7, 13, 25, …, 6k + 13, 6k + 25} is the set of all representatives of the orbits. As it can be seen, numbers 7 and 13 are obtained by adding 6 to their previous numbers and the others are found by adding 12 to their previous numbers. Moreover, in the first, second and the last orbits there are 12 elements and the other orbits have size 24.

- When k is odd, {1, 7, 13, 25, .., 6k + 19} is the set of all representatives of the orbits. Numbers 7 and 13 are obtained by adding 6 to their previous numbers and the others are obtained by adding 24. In addition, the number of elements in the first and second orbits is 12 and it is 24 in the others. Now by the same method as Theorem 3, the result is obtained. □

Now we compute the eccentric connectivity index of these fullerenes:

Theorem 5. In the fullerene molecules of type C_{50+10k}, $k \geq 7$, the eccentric connectivity index is computed as follows:

- If k is even, then

$$\xi^c(G) = \sum_{v \in V(G)} deg_G(v) ec_G(v) = 22.5k^2 + 330k + 1050$$

- If k is odd, then

$$\xi^c(G) = \sum_{v \in V(G)} deg_G(v) ec_G(v) = 22.5k^2 + 330k + 1087.5$$

Proof. Since C_{50+10k} is a 3−regular graph, the degree of each vertex is 3. Also, in the Theorem 3, the eccentricity of the vertices has been presented. □

Also we can write:

Theorem 6. In the fulleren molecules of type C_{60+12k}, $k \geq 7$, the eccentric connectivity index is as follows:

- If k is even, then

$$\xi^c(G) = \sum_{v \in V(G)} deg_G(v) ec_G(v) = 27n^2 + 432n + 1413$$

- If k is odd, then

$$\xi^c(G) = \sum_{v \in V(G)} deg_G(v) ec_G(v) = 27n^2 + 432n + 1476$$

Proof. It suffices to apply the same method as Theorem 5 and also use Theorem 4. □

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