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Augmented eccentric connectivity index of Fullerenes

REZA SHARAFDINI

Department of Mathematics, Faculty of Science, Persian Gulf University

sharafdini@pgu.ac.ir

ABSTRACT. Fullerenes are carbon-cage molecules in which a number of carbon atoms are bonded in a nearly spherical configuration. The augmented eccentric connectivity index of graph G is defined as ${}^{A}\xi(G)=\sum_{u\in V(G)}M(u)\varepsilon(u)^{-1}$ where $\varepsilon(u)$ is defined as the length of a maximal path connecting u to another vertex of G and $M(u)$ denotes the product of degrees of all neighbors of vertex u. In the present paper, we compute the augmented eccentric connectivity index of two classes of fullerenes C_{12n+2} and C_{20n+40}.

Keywords: Augmented eccentric connectivity index, Eccentricity, Fullerene graphs.

1. INTRODUCTION

Throughout this article G denotes a simple connected graph. We denote the vertex and the edge set of G by $V(G)$ and $E(G)$, respectively. For two vertices u and v of $V(G)$, we define their distance $d(u,v)$ as the length of any shortest path connecting u and v in G. The eccentricity $\varepsilon(u)$ of the vertex u of G is the distance from u *to* any vertex farthest away from it in G, i.e., $\varepsilon(u)=\max\{d(u,v)\mid v\in V(G)\}$. The maximum eccentricity over all vertices of G is called the diameter of G and denoted by $D(G)$; the minimum eccentricity among the vertices of G is called the radius of G and denoted by $r(G)$.

A molecular graph is a simple connected graph such that its vertices correspond to the atoms and the edges to the bonds.

A fullerene is a cubic carbon molecule in which each carbon atom is chemically bonded to three other carbon atoms and they are arranged on a sphere in pentagons and hexagons. Fullerene molecule was discovered experimentally in 1985 [2,13]. Since then, fullerenes have attracted the interest of scientists in many fields all over the world. The molecular graph of a fullerene (or a fullerene graph) is a cubic planar

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3-connected graph with pentagonal and hexagonal faces. Such graphs are suitable models for fullerene molecules: carbon atoms are represented by vertices of the graph, whereas the edges represent bonds between adjacent atoms. Considering the molecular graph of fullerenes many properties of these nanomaterials can be investigated using mathematical tools and methods.

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. The augmented eccentric connectivity index ${}^{A}\xi(G)$ of a graph G is defined as ${}^{A}\xi(G)=\sum_{u\in V(G)}M(u)\varepsilon(u)^{-1}$, where $M(u)$ denotes the product of degrees of all neighbors of the vertex u. It was introduced in [1] concerned with various modifications of some eccentric-based topological indices. Interested readers are encouraged to consult references [3–11] for more mathematical and chemical properties of eccentric-based indices of some nanostructures. In the present paper, we compute the augmented eccentric connectivity index of two classes of fullerene graphs C_{12n+2} and C_{20n+40}.

2. VERTEX-TRANSITIVE GRAPHS

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A bijection α on $V(G)$ is called an automorphism of graph G if it preserves $E(G)$. In the other words, α is an automorphism if for each edge $e = uv$ of G, $\alpha(e)=\alpha(u)\alpha(v)$ is an edge of G. Assume that $Aut(G)=\{f \mid f:V\rightarrow V \text{ is bijection}\}$. Then $Aut(G)$ forms a group under the composition of mappings. $Aut(G)$ acts transitively on $V(G)$ if for any vertices u and v in $V(G)$ there exists $\alpha\in Aut(G)$ such that $\alpha(u)=v$.

Lemma 1. Suppose G is a k-regular graph and $A_1,A_2,\cdots,A_t$ are the orbits of $Aut(G)$ under its natural action on $V(G)$ and $x_i\in A_i$, for $1\le i\le t$. Then ${}^{A}\xi(G)=k^k\sum_{i=1}^{t}|A_i|\,\varepsilon(x_i)^{-1}$. In particular, if G is vertex-transitive, then ${}^{A}\xi(G)=k^k\,|V(G)|\,r(G)^{-1}$ 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 α such that $\alpha(u)=v$. Choose a vertex x such that $\varepsilon(u)=d(u,x)$, since it is onto, for every vertex y there exists a vertex w such that $y=\alpha(w)$. Thus

$$d(v,y)= d(\alpha(u),\alpha(w))= d(u,w).$$

It follows that

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

So the vertices of a given orbit have the same eccentricities. On the other hand, it is known that the vertices of a given orbit have equal degrees. In the case that G is vertex-transitive, it is a k–regular graph, for some k and ${}^{A}\xi(G)=k^k\,|V(G)|\,r(G)^{-1}$. This completes our proof.

It is known that the molecular graph of a polyhex nanotorus, $T[p,q]$, (Figure 1) is vertex-transitive [1]. Therefore the following theorem follows from Lemma 1.

Theorem 2. ${}^{A}\xi(T[p,q])=9pq/[p/2]q$.

Proof. As it is easily seen in Figure 1, we have that $|V(T[p,q])| = pq$. Since $T[p, q]$ is vertex-transitive, it follows from Lemma 1 that ${}^{A}\xi(T[p,q]) = 9pq/[p/2]q$ due to the fact that eccentricity of each vertex of $T[p,q]$ is $[p/2]q$.

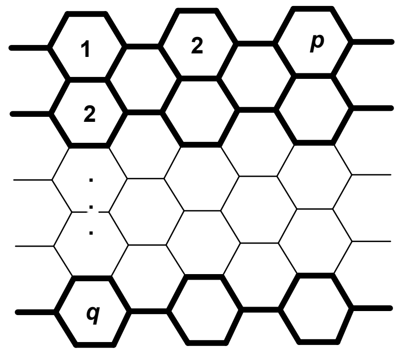

Figure 1. 2-dimensional lattice for $T[p,q]$.

3. AUGMENTED ECCENTRIC CONNECTIVITY INDEX OF TWO CLASSES OF FULLERENES

The goal of this section is to compute the augmented eccentric connectivity index of two infinite classes of fullerenes, namely C_{12n+2} and C_{20n+40}.

At first consider an infinite class of fullerene with exactly $12n + 2$ vertices and $18n + 3$ edges, depicted in Figure 2. In Table 1, the eccentricity of every vertex of C_{12n+2} fullerenes is computed for $2 \le n \le 9$.

Table 1. Some exceptional cases of C_{12n+2} fullerenes.

Fullerenes	Augmented eccentric connectivity index for $2 \le n \le 9$
C_{26}	9(72/5+1)
C_{38}	9(114/7)
C_{50}	9(36/7 + 102/8 + 12/9)
C_{62}	9(72/8 + 72/9 + 42/10)
C_{74}	9(36/8 + 72/9 + 54/10 + 36/11 + 24/12)
C_{86}	9(72/9 + 54/10 + 36/11 + 36/12 + 36/13 + 24/14)
C_{98}	9(12/9 + 18/10 + 12/11 + 12/12 + 12/13 + 12/14 + 12/15 + 8/16)
C_{110}	9(18/10 + 12/11 + 12/12 + 12/13 + 12/14 + 12/15 + 12/16 + 12/17 + 8/18)

A general formula for the augmented eccentric connectivity index of C_{12n+2}, for $n \ge 10$ is as follows:

Theorem 3.

$${}^{A}\xi(C_{12n+2}) = \frac{270}{n} + 324\sum_{i=1}^{n-1}\frac{1}{n+i}.$$

Proof. By Figure 2 and by using GAP [12] software, one can see that there are three types of vertices of fullerene graph C_{12n+2}. These are the vertices of the central and outer pentagons and other vertices of C_{12n+2}. By computing the eccentricity of these vertices we have the following table:

Vertices	Eccentricity	Number
The type 1 of vertices	$2n$	8
The type 2 of vertices	n	6
Other vertices	$n+i$ $(1 \le i \le n-1)$	12

By using these calculations and Figure 2, the Theorem is proved.

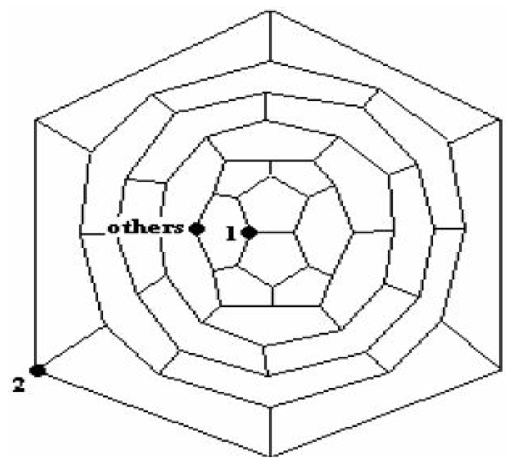

Figure 2. The molecular graph of the fullerene C_{12n+2} for n = 4.

Consider now an in infinite class of fullerene with exactly $20n + 40$ vertices and $30n + 60$ edges, depicted in Figure 3. In Table 2, the eccentricity of vertices of C_{20n+40} fullerenes are computed for $1 \le n \le 10$.

Table 2. Some exceptional cases of C_{20n+40} fullerenes.

Fullerenes	Augmented eccentric connectivity index for $1 \le n \le 10$
C_{60}	180
C_{80}	9(240/11)
C_{100}	9(60/11+240/12)
C_{120}	9(120/12+210/13+30/14)
C_{140}	9(60/12+120/13+180/14+30/15+30/16)
C_{160}	9(120/13+120/14+120/15+60/16+30/17+30/18)
C_{180}	9(60/13+120/14+120/15+90/16+60/17+60/18+30/19)
C_{200}	9(60/14+120/15+90/16+60/17+90/18+60/19+60/20+60/21+30/22+30/23)
C_{220}	9(120/15+90/16+60/17+90/18+60/19+60/20+60/21+60/22+60/23+30/24 +30/25)
C_{240}	9(60/25+90/16+20/17+90/18+60/19+60/20+60/21+60/22+60/23+60/24 +60/25+30/26+30/27)

A general formula for the augmented eccentric connectivity index of C_{20n+40}, for $n \geq 11$, is as follows:

Theorem 4.

$$ {}^{A}\xi(C_{20n+40}) = \frac{270(4n+11)}{(2n+5)(2n+6)} + 540\sum_{i=0}^{n}\frac{1}{n+4+i}. $$

Proof. Similar to proof of Theorem 3, by using Figure 3, one can see that there are three types of vertices of fullerene graph C_{20n+40}. These are the vertices of the central and outer pentagons and other vertices of C_{20n+40}. By computing the eccentricity of these vertices we have the following table:

Vertices	Eccentricity	Number
The type 1 of vertices	$2n + 6$	10
The type 2 of vertices	$2n + 5$	10
Other vertices	$n + 4 + i$ $(0 \leq i \leq n)$	20

By using these calculations and Figure 3, the theorem is proved.

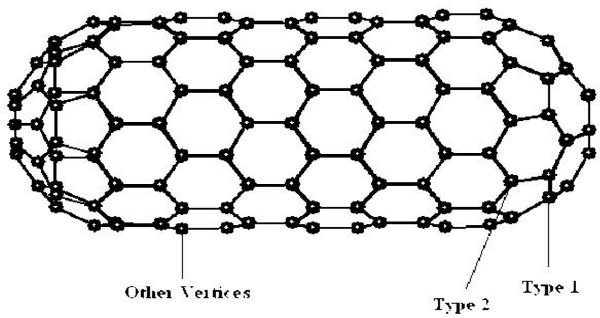

Figure 3. The molecular graph of the fullerene C_{20n+40} for $n = 3$.

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