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Poster Presentation

Revised Augmented Eccentric Connectivity Index of Fullerenes

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Abstract

In theoretical chemistry, molecular structure descriptors are used for modeling physio-chemical, pharmacologic, toxicological, biological and other properties of chemical compound. 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. Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms bonded in a nearly spherical configuration. In this paper we compute some bounds of the augmented eccentric connectivity index and then we calculate this topological index for two infinite classes of fullerenes.

Keywords: Augmented eccentric connectivity index, fullerenes, topological index, eccentricity.

MSC(2010): Primary: 65F05; Secondary: 46L05, 11Y50.

1 Introduction

In theoretical chemistry, molecular structure descriptors are used for modeling physico-chemical, pharmacologic, toxicological, biological and other properties of chemical compound.

Let G be any simple connected graph with vertex set $V(G)$ and edge set $E(G)$ and $n = |V(G)|$. For two vertices u and v in $V(G)$ their distance $d_G(u,v)$ is defined as the length of a shortest path connecting u and v in G. For a given vertex u of G its eccentricity $\varepsilon_G(u)$ is the largest distance between u and any other vertices of G, i.e., $\varepsilon_G(u) = \max_{v\in V(G)} d(u,v)$. The maximum eccentricity over all vertices of G is called the diameter of G and is denoted by $D(G)$; the minimum eccentricity among the vertices of G is called radius of G and is denoted by $R(G)$. The set of all vertices of minimum eccentricity is called the center of G.

The eccentric connectivity index of a graph G is defined as

$$\xi^c(G) = \sum_{u\in V(G)} d_G(u)\varepsilon_G(u),$$

where $d_G(u)$ denotes the degree of vertex u, i. e., the number of its neighbors in G. The eccentric connectivity index was introduced by Madan *et al.* and used in a series of papers concerned with QSAR/QSPR studies [8, 7, 5]. This index was successfully used for mathematical models of biological activities of diverse nature. In fact, this index has been shown to give a high degree of predictability of pharmaceutical properties, and may provide leads for the development of safe and potent anti-HIV compounds.

The augmented eccentric connectivity index ${}^\star\xi^A(G)$ of a graph G is defined as [2]

$${}^\star\xi^A(G) = \sum_{u\in V(G)} \frac{M(u)}{\varepsilon_G(u)},$$

where $M(u)$ denotes the product of degrees of all neighbors of vertex u. From above definition it is clear that, as the degrees are taken over the neighborhoods and then multiplied, so the contribution of a vertex to this index is non-local and again since the reciprocal of eccentricity is considered for a vertex so the contribution of a vertex is also non-linear.

A revised version of augmented eccentric connectivity index, under the name Ediz eccentric connectivity index, has been defined as

$${}^\star\xi^A(G) = \sum_{u\in V(G)} \frac{S(u)}{\varepsilon(u)},$$

where $S(u)$ denotes the sum of degrees of all neighbors of vertex u.

Fullerenes, discovered experimentally in 1985, are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms bonded in a nearly spherical configuration. It is well-known fact that fullerenes made entirely of n carbon atoms, have 12 pentagonal and (n/2-10) hexagonal faces, while $n \neq 22$ is a natural number equal or greater than 20 [12,13]. The most important member of the family of fullerenes is C_{60} (See Fig.1). In this paper we aim to compute revised augmented eccentric connectivity index for two infinite classes of fullerene graphs C_{12n+2} and C_{20n+40}. Throughout this paper, our notations are standard and mainly taken from standard books of graph theory such as [19].

2 Main Results

In this section we aim to compute the revised augmented eccentric connectivity index of two infinite classes of fullerenes, namely C_{12n+2} and C_{20n+40}. First consider an infinite class of fullerene with exactly $12n+2$ vertices and $18n+3$ edges, depicted in Fig. 3. In Table 1, the augmented eccentric connectivity index of C_{12n+2} fullerenes is computed for $1 \leq n \leq 9$.

Fullerenes	Exceptional augmented eccentric connectivity index for $1 \leq n \leq 9$
C_{26}	$3 \times 72/5 + 1$
C_{38}	$3 \times 114/7$
C_{50}	$3 \times 36/7 + 3 \times 102/8 + 3 \times 12/9$
C_{62}	$3 \times 72/8 + 3 \times 72/9 + 3 \times 42/10$
C_{74}	$3 \times 36/8 + 3 \times 72/9 + 3 \times 54/10 + 3 \times 36/11 + 3 \times 24/12$
C_{86}	$3 \times 72/9 + 3 \times 54/10 + 3 \times 36/11 + 3 \times 36/12 + 3 \times 36/13 + 24/14$
C_{98}	$3 \times (12/9 + 18/10 + 12/11 + 12/12 + 12/13 + 12/14 + 12/15 + 8/16)$
C_{110}	$3 \times (18/10 + 12/11 + 12/12 + 12/13 + 12/14 + 12/15 + 12/16 + 12/17 + 8/18)$

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

Theorem 2.1.

$$^{A}\xi(C_{12n+2}) = \frac{90}{n} + 108\sum_{i=1}^{n}\frac{1}{n+i}.$$

Proof. Using GAP [20] 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	$\varepsilon(u)$	Number
The Type 1 Vertices	2	8
The Type 1 Vertices	n	6
Other Vertices	$n+i(1 \leq i \leq n)$	12

Consider now an infinite class of fullerene with exactly $20n+40$ vertices and $30n+60$ edges, depicted in Fig. 4. In Table 2, the eccentricity of vertices of C_{20n+40} fullerenes are computed for $1 \leq n \leq 10$. If $n11$ then a general formula for the augmented eccentric connectivity index of C_{20n+40} is obtained as follows:

Theorem 2.2.

$$^{A}\xi(C_{20n+40}) = 180\sum_{i=0}^{n}\frac{1}{n+4+i} + 90(\frac{1}{2n+5} + \frac{1}{2n+6}).$$

Proof. Similar to proof of Theorem 2.1, one can see that there are three types of vertices in the fullerene graph (See Fig. 4). These are the vertices of the central and outer pentagons and other vertices of C_{20n+40}. Computing the eccentricity of these vertices we have the following table:

Vertices	$\varepsilon(u)$	Number
The Type 1 Vertices	$2n+6$	10
The Type 1 Vertices	$2n+5$	10
Other Vertices	$n+4+i(0 \leq i \leq n+1)$	20

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