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Connective eccentric index of fullerenes

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ABSTRACT. Fullerenes are carbon-cage molecules in which a number of carbon atoms are bonded in a nearly spherical configuration. The connective eccentric index of graph G is defined as $C^{\xi}(G)= \Sigma_{a\in V(G)} \deg(a)\varepsilon(a)^{-1}$, where $\varepsilon(a)$ is defined as the length of a maximal path connecting a to another vertex of G. In the present paper we compute some bounds of the connective eccentric index and then we calculate this topological index for two infinite classes of fullerenes.

Keywords: Connective eccentric index, Eccentric connectivity index, Fullerene graphs.

1. INTRODUCTION

In theoretical chemistry molecular structure descriptor or topological indices, are used to compute properties of chemical compounds. 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, $\xi(G)$, was proposed by Sharma, Goswami and Madan [1]. It is de ined as $\xi(G) = \Sigma_{u\in V(G)}\deg(u)\,\varepsilon(u)$, where $\deg(x)$ denotes the degree of the vertex x in G and $\varepsilon(u) = \max\{d(x, u) \mid x \in V(G)\}$, [2-6]. The radius $r(G)$ and diameter $d(G)$ of G are defined as the minimum and maximum eccentricity among vertices of G, respectively. The total eccentricity index define as $\theta(G) = \sum_{u\in V(G)}\varepsilon(u)$.

The connective eccentric index was de ined by Gupta, Singh and Madan [7] as follows:

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$$C^{\xi}(G) = \sum_{u \in V(G)} \frac{\deg(u)}{\varepsilon(u)}.$$

Fullerenes are carbon-cage molecules in which a number of carbon atoms are 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 [8, 9]. Throughout this paper, our notations are standard and mainly taken from the standard book of graph theory such as [10]. We encourage reader to references [11 – 16] to study some properties of connective eccentric index of some nanostructures.

2. RESULT AND DISCUSSION

In this section at first we obtain some bounds of the connective eccentric index and then we compute this topological index for vertex – transitive graphs. Finally, we compute this topological index for two infinite classes of fullerenes. We begin this section by a Lemma related to the regular graphs:

Lemma 1. The connective eccentric index of a k- regular graph is:

$$C^{\xi}(G) = k\sum_{a \in V(G)} \varepsilon(a)^{-1}.$$

This Lemma implies for a fullerene graph F, $C^{\xi}(F) = 3\sum_{a \in V(F)} \varepsilon(a)^{-1}$.

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 $\varepsilon(v)$=1. Hence, $C^{\xi}(G) = (n-1)\sum_{a \in V(G)} 1 = n(n-1)$.

Theorem 3. Let G be a (n, m) graph. Then

$$C^{\xi}(G) \geq \frac{2m}{\theta(G)}.$$

Proof. Let a, b, c and d be positive integers. Then one can see that easily $\frac{a}{b} + \frac{c}{d} \geq \frac{a+c}{b+d}$.

By using this non – equality we have the following lower bound for connective eccentric index:

$$C^{\xi}(G) = \sum_{u \in V(G)} \frac{\deg(u)}{\varepsilon(u)} \geq \frac{\sum_{u \in V(G)} \deg(u)}{\sum_{u \in V(G)} \varepsilon(u)} = \frac{2m}{\theta(G)}.$$

Theorem 4. Let G be a (n, m) graph. Then

$$2m / d(G) \leq C^{\xi}(G) \leq n(n-1)$$

With right equality if and only if $G \cong K_n$.

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Proof. Four upper bound, since for every vertex u of graph, $\varepsilon(u) \geq 1$ and $\deg(u) \leq n$-1, so we have $C^{\xi}(G) \leq n(n-1)$. Clearly equality holds for complete graph K_n. Conversely, if $C^{\xi}(G) = n(n-1)$ then, for every vertex u, $\varepsilon(u) = 1$ and $\deg(u) = n$-1. Hence, $G \cong K_n$.
For lower bound it is easy to see that for every vertex u of G, $\varepsilon(u) \leq d(G)$. Thus,

$$C^{\xi}(G) \geq \sum_{u \in V(G)} \frac{\deg(u)}{d(G)} = 2m / d(G).$$

Let C_n be a fullerene graph on n vertices. For every vertex u in fullerene C_{20}, $\varepsilon(u) = 5$, (Fig. 1). Since C_{20} is the smallest fullerene, then for every vertex in C_n, $\varepsilon(u) \geq 5$. This implies $C^{\xi}(C_n) \leq \sum_{u \in V(G)} \frac{3}{5} = 3n / 5$.

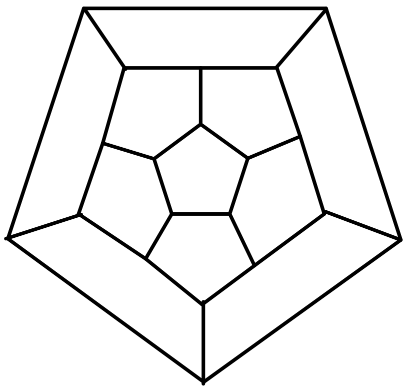

Fig. 1. 2 – dimensional graph of fullerene C_{20}.

3. Vertex - Transitive Graphs

A bijection σ on vertices set of graph G is named an automorphism of graph if it preserves the edge set. In other words, σ is an automorphism if $e = uv$ is an edge, then $\sigma(e)=\sigma(u)\sigma(v)$ is an edge of E. Let $Aut(G) = \{\alpha : V \to V, \alpha \text{ is bijection}\}$, then $Aut(G)$ under the 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 $\alpha(u) = v$.

Lemma 5. Suppose G is a graph, $A_1, A_2, ..., A_t$ are the orbits of $Aut(G)$ under its natural action on $V(G)$ and $x_i \in A_i$, $1 \leq i \leq t$. Then $C^{\xi}(G) = \sum_{j=1}^{t} |A_j| \deg(x_j)\varepsilon(x_j)^{-1}$. In particular, if G is vertex transitive then $C^{\xi}(G) = k.|V(G)|.r(G)^{-1}$ 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 φ such that $\varphi(u) = v$. choose a vertex x such that $\varepsilon(u) = d(u, x)$. Since φ

is onto, for every vertex y there exists the vertex w such that $y = \varphi(w)$. Thus $d(v, y) = d(\varphi(u), \varphi(w)) = d(u,w)$ and so

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

On the other hand, it is a trivial fact that the vertices of a given orbit have equal degrees. Therefore, $C^{\xi}(G) = \sum_{j=1}^{t} |A_j| \deg(x_j)\varepsilon(x_j)^{-1}$. If G is vertex transitive then it is k – regular graph, for some k and $C^{\xi}(G) = k.|V(G)| / r(G)$. This completes our proof.

Lemma 6 [16]. The molecular graph of a polyhex nanotorus (Fig. 2) is vertex transitive.

Theorem 7. $C^{\xi}(T[p,q]) = 3pq / ([p/2] + q)$.

Proof. By Fig. 2, it can easily seen that $|V(T[p,q])| = pq$. By Lemma 6, $T[p, q]$ is vertex transitive and by Lemma 5, $C^{\xi}(T[p,q]) = 3pq / \varepsilon(x)$, for a vertex x. Now the proof is follows from this fact that $\varepsilon(x) = [p/2] + q$, proving the result.

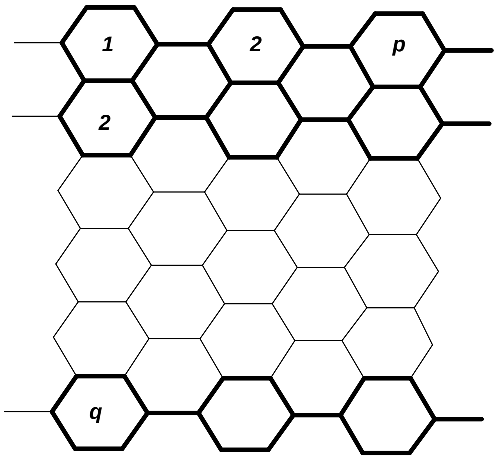

Fig. 2. A 2 –dimensional lattice for $T[p, q]$.

4. Connective eccentric index of two classes of fullerenes

The goal of this section is computing the connective eccentric 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 Fig. 3. In Table 1, the eccentricity of every vertex of C_{12n+2} fullerenes is computed for $1 \le n \le 9$. If $n \ge 10$ then a general formula for the connective eccentric index of C_{12n+2} is as follows:

Theorem 8.

$$C^{\xi}(C_{12n+2}) = 36\sum_{i=1}^{n}\frac{1}{n+i} + \frac{30}{n}.$$

Proof. By Fig. 2 and by using GAP [15] 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	ε(x)	No.
The Type 1 Vertices	$2n$	8
The Type 2 Vertices	n	6
Other Vertices	$n+i$ $(1 \le i \le n)$	12

Some exceptional cases are given in the Table 1:

Table 1. Some exceptional cases of C_{12n+20} fullerenes.

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

By using these calculations and Fig. 3, the Theorem is proved.

Consider now an in inite 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 $1 \le n \le 10$. If $n \ge 11$ then a general formula for the connective eccentric index of C_{20n+40} is as follows:

Theorem 9.

$$C^{\xi}(C_{20n+40}) = 60\sum_{i=0}^{n}\frac{1}{n+4+i} + 30\left(\frac{1}{2n+5}+\frac{1}{2n+6}\right).$$

Proof. Similar to proof of Theorem 8, from Fig. 4, one can see that there are three types of vertices of fullerene graph C_{20n+40}.

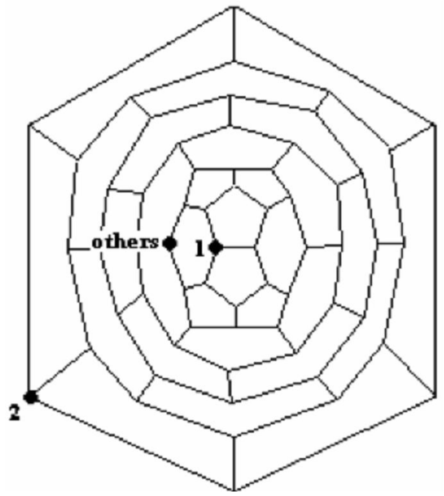

Fig. 3. The molecular graph of the fullerene C_{12n+2} for $n = 4$.

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	ε(*x*)	No.
The Type 1 Vertices	$2n + 6$	10
The Type 2 Vertices	$2n + 5$	10
Other Vertices	$n+4+i$ $(0 \le i \le n+1)$	20

Some exceptional cases are given in the Table 2:

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

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

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By using these calculations and Fig. 4, the Theorem is proved.

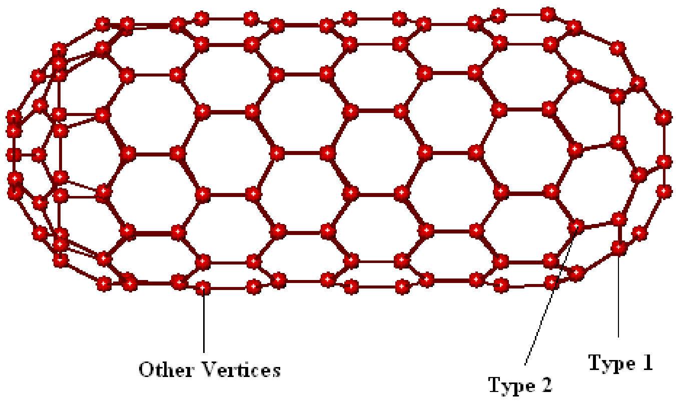

Fig. 4. The molecular graph of the fullerene C_{20n+40} for $n = 3$.

5. Conclusion

Topological descriptors are very important tools in chemical graph theory. Among them topological indices role a fundamental map in predicting chemical phenomena. The connective eccentric index is a topological index was defined by Gupta, Singh and Madan. In this paper this topological index of two infinite classes of fullerene graphs were computed.

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