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The augmented eccentric connectivity index of nanotubes and nanotori

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ABSTRACT.

Let G be a connected graph, the augmented eccentric connectivity index is a topological index was defined as ${}^{A}\xi^{c}(G)=\sum_{i=1}^{n}M_i / E_i$ where M_i is the product of degrees of all vertices v_j, adjacent to vertex v_i, E_i is the largest distance between v_i and any other vertex v_k of G or the eccentricity of v_i and n is the number of vertices in graph G. In this paper exact formulas for the augmented eccentric connectivity index of $TUC_4C_8(S)$ nanotube and $TC_4C_8(R)$ nanotorus are given.

Keywords: Augmented eccentric connectivity index, Nanotube, Nanotorus.

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1. INTRODUCTION

A topological index is a numerical descriptor of the molecular structure derived from the corresponding (hydrogen-depleted) molecular graph. Various topological indices are widely used for quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies [1-4]. Throughout this paper, we only consider simple connected graphs. Consider a simple connected molecular graph G, and let $V(G)$ and $E(G)$

denote its vertex and edge sets, respectively. $|V(G)| = n$ is called the order of G. The distance between u and v in $V(G)$, $d_G(u,v)$, is the length of a shortest u-v path in G. If no ambiguity is possible, the subscript G may be omitted. The eccentricity, $\varepsilon(u)$ of a vertex $u \in V(G)$ is the maximum distance between u and any other vertex in G. The diameter of G, $diam(G)$, is defined as the maximum value of the eccentricities of the vertices of G. Similarly, the radius of G, $rad(G)$, is defined as the minimum value of the eccentricities of the vertices of G. A central vertex of G is any vertex whose eccentricity is equal to the radius of G. The subgraph induced by the central vertices of G is the center $Cen(G)$ of G. If $G = Cen(G)$, then G is called a self-centered graph. Finally, the degree of a vertex $v \in V(G)$, $\deg(v)$ is the number of edges incident to v.

Bajaj et al. [5] introduced a distance-based molecular structure descriptor, the augmented eccentric connectivity index defined as, ${}^{A}\xi^{c}(G) = \sum_{i=1}^{n} \left(\frac{M_i}{E_i} \right)$. In their study, they defined and investigated this topological index for discriminating power with regard to anti-HIV activity of 2-pyridinone derivatives. Ediz firstly computed this index for nano structures and find exact expression of the augmented eccentric connectivity index for an infinite class of nanostar dendrimers[6].

Carbon nanotubes form an interesting class of carbon nanomaterials. These can be imagined as rolled sheets of graphite about different axes. There are three types of nanotubes: armchair, chiral and zigzag structures. Further nanotubes can be categorized as single-walled and multi-walled nanotubes and it is very dif icult to produce the former. In 1991 Iijima [7] discovered carbon nanotubes as multi-walled structures. Carbon nanotubes show remarkable mechanical properties. Experimental studies have shown that they belong to the stiffest and elastic known materials. Diudea was the first chemist who considered the problem of computing topological indices of nanostructures [8-14]. A C_4C_8 net is a trivalent decoration made by alternating squares C_4 and octagons C_8. The $TUC_4C_8(S)$ nanotube is constructed from squares and octagons, Figure 1.

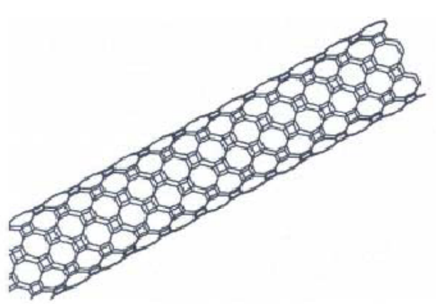

Figure 1. Three-dimensional perception of a $TUC_4C_8(S)$ nanotube.

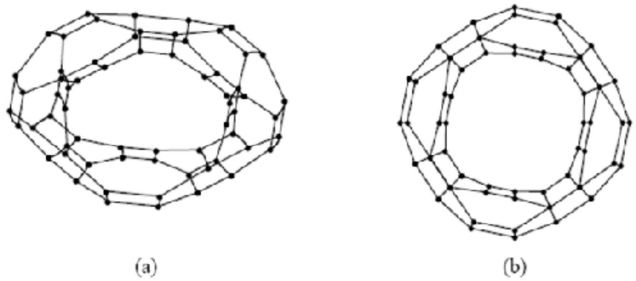

Figure 2. Three-dimensional perception of a $TC_4C_8(S)$ nanotorus (a) Side view (b) Top view.

Eccentric connectivity index of this nanotube and a nanotorus obtained from this nanotube by gluing its ends, Figure 2 was expressed by Ashra i et al.[15]. Also The Ediz eccentric connectivity index of this nanotube and nanotorus was determined by Ediz [16]. Saheli and Ashrafi found the exact formulae for the eccentric connectivity index of armchair polyhex nanotubes [17]. And Ashra i et al. investigated eccentric connectivity index of $TUC_4C_8(R)$ [18]. This article is the irst article to apply the augmented eccentric connectivity index for nano structures.

Throughout this paper $T = T[p,q]$ denotes an arbitrary $TUC_4C_8(S)$ nanotube in terms of the number of octagons in a fixed row (p) and the summation of the number of octagons and squares in a fixed column (q), in the two-dimensional lattice of T, Figure 3. We also denote a $TC_4C_8(S)$ nanotorus, Figure 2, by $S[p,q]$.

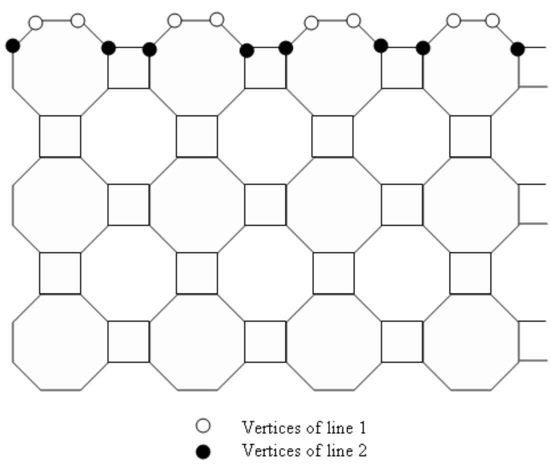

Fig.3. Two dimensional lattice of $TUC_4C_8(S)[4,5]$.

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2. Main results

In this section, the Augmented eccentric connectivity index of the molecular graph of an $TUC_4C_8(S)$ nanotube is computed. Sets in which this study are $E=E(T)$, $V=V(T)$ and X is the set of vertices of degree 2 and Y is the set of vertices of degree 3. It is easily seen that $|V|=4p(q+1)$, $|E|=2p(3q+2)$, $|X|=4p$ and $|Y|=4pq$.

Proposition 1. *If* $G=T[p,1]$ *then* ${}^{A}\xi^{c}(T[p,1])=\dfrac{96p}{2p+1}$.

Proof. It is obviously that $G=T[p,1]$ is self-centered and $rad(G)=diam(G)=2p+1$ (See in [19]). We know that $|X|=4p$. Consider the $G=T[p,1]$ given in Figure 4. One can see from Figure 4 that for any $v\in X$, the vertex v has exactly two neighbours with degree 2 and 3. Similarly $|Y|=4p$ and for any $v\in Y$, the vertex v has exactly three neighbours which two of them with degree 3 and the other vertex with degree 2. In the light of these observations we can write directly from the definition of the augmented eccentric connectivity index;

$$ {}^{A}\xi^{c}(T[p,1])=\sum_{i=1}^{n}\left(\frac{M_i}{E_i}\right)=4p\frac{6}{2p+1}+4p\frac{18}{2p+1}=\frac{96p}{2p+1}. $$

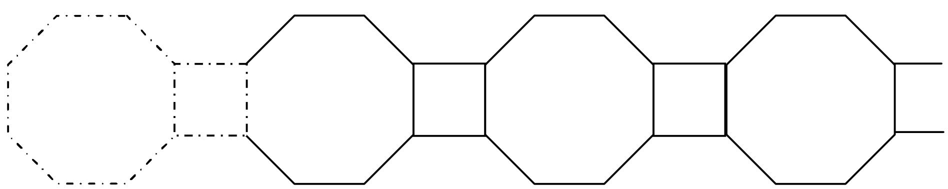

Figure 4. Two dimensional lattice of $TUC_4C_8(S)[p,1]$.

Obviously the eccentricity of a vertex in two dimensional lattice of $TUC_4C_8(S)[p,q]$ is the same as the eccentricity of its projected vertex under the horizontal plane symmetry. So, to compute the eccentricity of vertices of $TUC_4C_8(S)[p,q]$, it is enough to think one-half of its two dimensional lattice, say T_1. The following proposition was proved by Ashra i et al.[19] is extremely useful for to compute our parameter.

Proposition 2. (*Ashrafi et al.* [19]) *Suppose* $L=\{v_1,v_2,...,v_{q+1}\}$ *are vertices different lines of* T_1 *and* $K=\{e_1,e_2,...,e_{q+1}\}$, *where* $e_i=\varepsilon(v_i)$, $1\le i\le q+1$. *Then*

(a) *If* $p\le\left\lceil\dfrac{q+1}{2}\right\rceil$ *then* $e_i=p+2q+2-i, 1\le i\le q+1$.

(b) *If* $\left\lceil \frac{q+1}{2} \right\rceil < p \le q+1$ *then* $e_i = p+2q+2-i$, *when* $1 \le i \le 2(q-p+1)$ *and*

$$e_{i+2(q-p+1)} = 3p - \left\lceil \frac{i}{2} \right\rceil, \text{ for } 1 \le i \le 2p-q-1.$$

(c) *If* $p > q+1$ *then* $e_i = 2p+q+1-\left\lceil \frac{i}{2} \right\rceil$, *where* $1 \le i \le q+1$.

And now in the light of these results we can state our next three propositions.

Proposition 3. *If* $p \le \left\lceil \frac{q+1}{2} \right\rceil$ *then the Augmented eccentric connectivity index of* $T[p,q]$ *is computed as follows:*

$$^{A}\xi^{c}(T) = 4p\left(\frac{6}{p+2q+1} + \frac{18}{p+2q} + \frac{27}{p+2q-1} + \ldots + \frac{27}{p+q+1}\right).$$

Proof. Consider the $G = T[4,5]$ given in Fig.3. One can see from Fig.3. that for any $v \in X$ (vertices of line 1), the vertex v has exactly two neighbors with degree 2 and 3. Similarly for the vertices of line 2, $v \in Y$ and the vertex v has exactly three neighbors which two of them with degree 3 and the other vertex with degree 2. Analogously for the vertices of line 3 and remaining vertices of the other lines of T_1, $v \in Y$, and the vertex v has exactly three neighbors which all of them with degree 3.

In the light of these observations we can write directly from the definition of the Augmented eccentric connectivity index;

$$^{A}\xi^{c}(T) = \sum_{i=1}^{n} \left(\frac{M_i}{E_i}\right) = 2\left(2p\frac{6}{p+2q+1} + 2p\frac{18}{p+2q} + 2p\frac{27}{p+2q-1} + \ldots + 2p\frac{27}{p+q+1}\right)$$

$$^{A}\xi^{c}(T) = 4p\left(\frac{6}{p+2q+1} + \frac{18}{p+2q} + \frac{27}{p+2q-1} + \ldots + \frac{27}{p+q+1}\right).$$

This completes the proof.

Proposition 4. *If* $\left\lceil \frac{q+1}{2} \right\rceil < p \le q+1$ *then the Augmented eccentric connectivity index of* $T[p,q]$ *is computed as follows:*

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$$ {}^{A}\xi^{c}(T)=\begin{cases} 4p(\frac{6}{p+2q+1}+\frac{18}{p+2q}+\frac{27}{p+2q-1}+\ldots+\frac{27}{3p}+\frac{54}{3p-1} \\ +\ldots+\frac{54}{3p-\left\lceil\frac{2p-q-2}{2}\right\rceil}) \quad when\ q\ is\ odd. \\ 4p(\frac{6}{p+2q+1}+\frac{18}{p+2q}+\frac{27}{p+2q-1}+\ldots+\frac{27}{3p}+\frac{54}{3p-1} \\ +\ldots+\frac{54}{3p-\left\lceil\frac{2p-q-2}{2}\right\rceil}+\frac{27}{3p-\left\lceil\frac{2p-q-1}{2}\right\rceil}) \quad when\ q\ is\ even. \end{cases} $$

Proof. The proof can be done in the same way as in the proof of Proposition 3.

Proposition 5. *If* $p>q+1$ *then the Augmented eccentric connectivity index of* $T[p,q]$ *is computed as follows:*

$$ {}^{A}\xi^{c}(T)=\begin{cases} 4p(\frac{24}{2p+q}+\frac{54}{2p+q-1}+\ldots+\frac{54}{2p+q+1-\left\lceil\frac{q+1}{2}\right\rceil}) \ when\ q\ is\ odd. \\ 4p(\frac{24}{2p+q}+\frac{54}{2p+q-1}+\ldots+\frac{54}{2p+q+1-\left\lceil\frac{q}{2}\right\rceil}+\frac{27}{2p+q+1-\left\lceil\frac{q+1}{2}\right\rceil}) \quad when\ q\ is\ even. \end{cases} $$

Proof. The proof is similar to the proof of Proposition 3.

Now the molecular graph of a $TC_4C_8(S)[p,q]$ nanotorus is considered. Obviously the $TC_4C_8(S)[p,q]$ nanotorus has exactly $4p(q+1)$ vertices and $6p(q+1)$ edges. Ashrafi et al. [19] proved that the eccentricities of $S[p,q]$ as

$$ \varepsilon(S[p,q])=\begin{cases} p+q+1 & p\le\left\lceil\frac{q+1}{2}\right\rceil \\ \frac{4p+q}{2}+\frac{1-(-1)^{q}}{4} & p>\left\lceil\frac{q+1}{2}\right\rceil \end{cases} $$

Proposition 6. *The augmented eccentric connectivity index of* $S[p,q]$ *is computed as follows:*

$$ {}^{A}\xi^{c}(S[p,q]) = \begin{cases} \dfrac{108p(q+1)}{p+q+1} & p \le \left\lceil \dfrac{q+1}{2} \right\rceil \\ \\ \dfrac{432p(q+1)}{8p+2q+1-(-1)^{q}} & p > \left\lceil \dfrac{q+1}{2} \right\rceil \end{cases} $$

Proof. Notice that $S[p,q]$ is a self-centered and a 3-regular graph and therefore $S_v = 9$ for every vertex of $S[p,q]$. For $p \le \left\lceil \frac{q+1}{2} \right\rceil$ then $\varepsilon(S[p,q]) = p+q+1$. We can directly write from the definition of the augmented eccentric connectivity index as;

$$ {}^{A}\xi^{c}(S[p,q]) = \sum_{i=1}^{n} \left(\frac{M_i}{E_i} \right) = 4p(q+1)\frac{27}{p+q+1} = \frac{108p(q+1)}{p+q+1} $$

and for $p > \left\lceil \frac{q+1}{2} \right\rceil$ then $\varepsilon(S[p,q]) = \frac{4p+q}{2} + \frac{1-(-1)^{q}}{4}$. We can directly write from the definition of the Augmented eccentric connectivity index as;

$$ {}^{A}\xi^{c}(S[p,q]) = \sum_{i=1}^{n} \left(\frac{M_i}{E_i} \right) = 4p(q+1)\frac{27}{\frac{4p+q}{2} + \frac{1-(-1)^{q}}{4}} = \frac{432p(q+1)}{8p+2q+1-(-1)^{q}}. $$

3. Concluding remarks

The Augmented eccentric connectivity index is a connectivity index and in this paper exact formulas for the augmented eccentric connectivity index of $TUC_4C_8(S)$ nanotube and $TUC_4C_8(S)$ nanotorus are given. It would be interesting, the investigation of its mathematical properties and quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) for future study.

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