

The eccentric connectivity index of one pentagonal carbon nanocones

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Let G be a graph. The eccentric connectivity index $\xi(G)$ is defined as $\xi(G) = \sum_{u,v \in V(G)} \deg(u) \varepsilon(u)$, where $\deg(u)$ denotes the degree of vertex u and $\varepsilon(u)$ is the largest distance between u and any other vertex v of G . In this paper, exact formulas for the eccentric connectivity index of one pentagonal carbon nanocones are given.

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1. Introduction

One pentagonal carbon nanocones, Fig. 1, originally discovered by Ge and Sattler in 1994 [1]. These are constructed from a graphene sheet by removing a 60° wedge and joining the edges produces a cone with a single pentagonal defect at the apex.

We now recall some algebraic definitions that will be used in the paper. Topological indices are graph invariants and are used for Quantitative Structure- Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies, [2,3]. Many topological indices have been defined and several of them have found applications as means to model physical, chemical, pharmaceutical and other properties of molecules.

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by $V(G)$ and $E(G)$, respectively. A topological index of a graph G is a numeric quantity related to G . The oldest topological index is the Wiener index which introduced by Harold Wiener [4]. The name of topological index was introduced by Haro Hosoya [5]. We encourage the reader to consult [6-8] for historical background material as well as basic computational techniques.

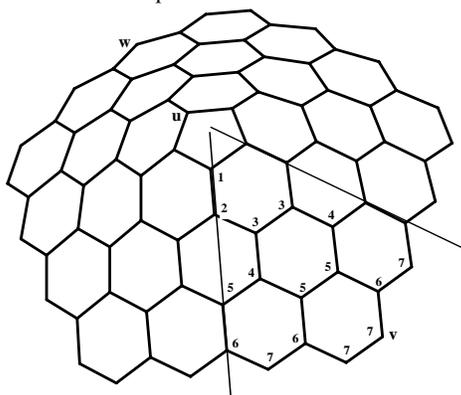


Fig. 1. The one-pentagonal carbon nanocone $CnC_5[3]$.

The distance $d(u,v)$ between two vertices u and v of a graph G is defined as the length of a shortest path connecting them. The summation of these numbers over all edges of G is called the Wiener index of G [4]. For a given vertex u of $V(G)$ its eccentricity, $\varepsilon(u)$, is the largest distance between u and any other vertex v of G . The maximum eccentricity over all vertices of G is called the diameter of G and denoted by $D(G)$ and the minimum eccentricity among the vertices of G is called radius of G and denoted by $R(G)$. The eccentric connectivity index $\xi(G)$ of is defined as $\xi(G) = \sum_{u,v \in V(G)} \deg(u) \varepsilon(u)$, [9-11]. The mathematical properties of this topological index are studied in some recent papers [12-18].

This paper addresses the problem of computing the eccentric connectivity index of one pentagonal carbon nanocones. We encourage the readers to consult papers [19-21] for computational techniques related to carbon nanocones, as well as [22-28] for background materials. Our notation is standard and taken mainly from the standard books of graph theory.

2. Main results and discussion

In [19-21], one of the present authors (ARA) computed some distance based topological indices of nanocones. So, it is natural to ask about other graph invariants of these nanotubes. In this section the eccentric connectivity index of one-pentagonal carbon nanocone $C[n] = CNC_5[n]$ containing $2n + 1$ layers is computed. From Fig. 1, it is clear that

$$|V(C[n])| = 5[1 + 1 + 2 + 2 + \dots + n + n + (n + 1)] = 5(n + 1)^2,$$

$$|E(C[n])| = 5[1 + 3 + 5 + \dots + (2n + 1) + 1 + 2 + 3 + \dots + n]$$

$$= 5[(n + 1)^2 + n(n + 1)/2] = 5/2(n + 1)(3n + 2).$$

In the following lemma, the diameter of this nanocone is computed.

Lemma 1. $R(C[n]) = 2n + 2$ and $D(C[n]) = 4n + 2$.

Proof. Suppose u is a vertex of the central pentagon of $C[n]$. Then from Fig. 1, one can see that there exists a vertex v of degree 2 such that $d(u,v) = 2n + 2$ and so $\varepsilon(u) = 2n + 2$. On the other hand, there exists another vertex w of degree 2 such that $d(u,w) = 2n$. Therefore, the shortest path with maximum length is connecting two vertices of degree 2 in $C[n]$. This implies that $D(G) = \text{Max}\{d(x,y) \mid \text{deg}(x) = \text{deg}(y) = 2\} = 4n + 2$ and $R(G) = 2n + 2$.

The proof of lemma 1, shows that the eccentricities of vertices of $C[n]$ are varied between $2n + 2$ and $4n + 2$. From Fig. 1, we can see that if P is the central pentagon of $C[n]$ and a and b are two vertices of $C[n]$ such that $d(a,P)$

$= d(b,P)$ then $\varepsilon(a) = \varepsilon(b)$, where $d(x,P) = \text{Min}\{d(x,y) \mid y \in V(P)\}$. Define $A_i = \{x \in C[n] \mid d(x,P) = i\}$, $1 \leq i \leq 2n + 1$.

From Fig. 1, it is clear that $|A_i| = 5 \left(1 + \left\lfloor \frac{i-1}{2} \right\rfloor\right)$, where $\lfloor x \rfloor$ denotes the greatest integer less than or equal to x . On the other hand, the eccentricity of vertices in each layer is constant and the number of vertices in the layers $2k$ and $2k + 1$ are the same, $1 \leq k \leq n$. Thus, the summation of eccentricities in the layers $2j$ and $2j + 1$ is $t_j = [2n + 2 + 2(j - 1)] + [2n + 2 + (2(j - 1) + 1)] = 4(n + j) + 1$, $1 \leq j \leq n$. Therefore,

$$\xi(C[n]) = 5 \sum_{j=1}^n [3j(4n + 4j + 1)] + 10(n + 1)(4n + 2) = 5 \left(10n^3 + \frac{48}{5}n^2 + \frac{34}{5}n + 4\right).$$

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