

Computation of the first vertex of CO-PI index of $TUC_4C_8(S)$ nanotubes

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In this paper, at first we introduce a new index with the name CO-PI index and obtain some properties related to this new index. Then we compute this new index for $TUC_4C_8(S)$ nanotubes.

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1. Introduction

Let G be a simple molecular graph without directed and multiple edges and without loops. The graph G consists of the set of vertices $V(G)$ and the set of edges $E(G)$. In molecular graph, each vertex represented an atom of the molecule and bonds between atoms are represented by edges between corresponding vertices.

Khadikar and co-authors in [1-4] defined a new topological index and named it Padmakar-Ivan index. They abbreviated this new topological index as PI .

The distance between to vertices $x, y \in V(G)$ is equal to the number of edges on shortest path between them and it is shown with $d(x, y)$. The vertex version of PI index is defined in [5], as follow:

$$PI_v(G) = \sum_{e \in E(G)} [n_e(u) + n_e(v)] \quad (1)$$

where

$$n_e(u) = |C| = \left| \{x \in V(G) \mid d(x, u) < d(x, v)\} \right| \text{ and}$$

$$n_e(v) = |D| = \left| \{x \in V(G) \mid d(x, v) < d(x, u)\} \right|$$

And we can restate it as follow:

$$PI_v(G) = \sum_{e \in E(G)} (|V(G)| - n(e)) \quad (2)$$

where $n(e)$ is the number of edges which have equal to distance from u and v .

In this paper, we introduce the new index same as vertex version of PI index and obtain some properties related this new index. Then we compute this new index for $TUC_4C_8(S)$ nanotubes.

2. Results and discussion

In [6], the distance of a vertex x , $d(x)$, of a connected graph defined as follows:

$$d(x) = \sum_{y \in V(G)} d(x, y),$$

where $d(x, y)$ is the distance between x and y .

A useful relation concerning distances of two vertices which are adjacent stated in [4] that we state it as a lemma.

Lemma 2-1. [6] Suppose $x, y \in V(G)$ are two adjacent vertices of a connected graph G and suppose $xy = e \in E(G)$. Then $d(x) - d(y) = n_e(y) - n_e(x)$.

We restate PI index in the following Theorem.

Theorem 2-2. The vertex version of PI index according to distances is :

$$PI_v(G) = \sum_{e \in E(G)} \sum_{x \in V(G)} |d(u, x) - d(v, x)| \quad (I)$$

Proof. We prove the following relation for obtain the above formula :

Suppose

$$uv = e \in E(G).$$

then

$$n_e(u) + n_e(v) = \sum_{x \in V(G)} |d(u, x) - d(v, x)| \quad (a)$$

We can obtain easily the relation (I) from the relations (a) and (1).

Let $uv = e \in E(G)$, then for each $x \in V(G)$, we have

$$|d(u, x) - d(v, x)| = \begin{cases} 1 & , x \notin n(e) \\ 0 & , x \in n(e) \end{cases}$$

Therefore, $\sum_{x \in V(G)} |d(u, x) - d(v, x)| = V(G) - n(e) = n_e(u) + n_e(v)$ and

the proof is completed. Now, we are ready to introduce a new index similar to the vertex version of PI index.

Definition 2-3. Let G be a connected graph. The first vertex version of Co-PI index is define as follows:

$$Co-PI_v(G) = \sum_{e \in E(G)} |n_e(u) - n_e(v)|$$

In following theorem, we restate the first vertex version of Co-PI index :

Theorem 2-4. The first vertex version of Co-PI index according to distances is:

$$Co-PI_v(G) = \sum_{e \in E(G)} \left| \sum_{x \in V(G)} (d(u, x) - d(v, x)) \right| \quad (II)$$

Proof. It is sufficient we prove the following relation for obtain the relation (II).

Suppose $uv = e \in E(G)$. Then

$$n_e(u) - n_e(v) = \sum_{x \in V(G)} d(v, x) - d(u, x)$$

We can obtain easily the relation (II) from the above formula.

Let $uv = e \in E(G)$, then for each $x \in V(G)$, we have

$$d(v, x) - d(u, x) = \begin{cases} 1 & , x \in C \\ 0 & , x \in n(e) \\ -1 & , x \in D \end{cases}$$

Therefore, $\sum_{x \in V(G)} d(v, x) - d(u, x) = n_e(u) - n_e(v)$.

3. Conclusions

In this section, we compute the first vertex version of co-PI index for carbon nanotube $TUC_4C_8(S)$. Carbon nanotubes (CNTs) are allotropes of carbon with a cylindrical nanostructure. The vertex-PI index of $TUC_4C_8(S)$ nanotube has been computed in [7]. Also, in [8-16], some topological indices of $TUC_4C_8(S)$ are computed. For computing this index, the quantities of $n_e(u)$ and $n_e(v)$ have been computed for this nanotube in [7] that we recall them at following.

According to Fig. 1, we denote the number of squares in one row by p and the number of rows by k . These notations are standard only in this section of our paper.

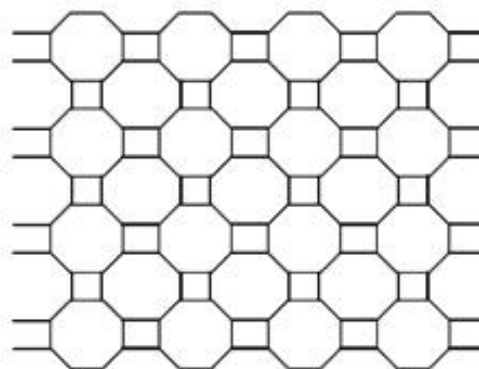


Fig. 1. Two dimensional lattice of $TUC_4C_8(S)$ nanotube, $p = 4, k = 8$.

Lemma 3-1. [7] Let G be the molecular graph of $TUC_4C_8(S)$ nanotube. Therefore,

(i) If e is a horizontal edge of G , then: $n_e(u) = n_e(v) = 2kp$.

(ii) If e is a vertical edge between rows m and $(m+1)$, $(1 \leq m \leq k-1)$, then: $n_e(u) = 4pm$ and $n_e(v) = 4p(k-m)$.

(iii) If e is an oblique edge in row m , $(1 \leq m \leq k)$, then:

$$n_e(u) = \begin{cases} 4p^2 - 4pm - k^2 + 2km + k - 2p & , m \leq p, k-m \leq p \\ 4p^2 - 4pm + m^2 + m - 2p & , m \leq p, k-m > p \\ 4pm - k^2 + 2km - m^2 + k - m - 2p & , m > p, k-m \leq p \\ 4pm - 2p & , m > p, k-m > p \end{cases}$$

and $n_e(v) = 4pk - n_e(u)$.

Lemma 3-2. Let G be the molecular graph of $TUC_4C_8(S)$ nanotube. Then, we have $n_e(u) = 4pk - n_e(v)$ for all edges of G . Therefore, $n_e(u) - n_e(v) = 4pk - 2n_e(v)$.

Proof. According to Lemma (3-1), the desire results can be obtained.

Theorem 3-3. The first vertex version of co-PI index for the molecular graph G of $TUC_4C_8(S)$ nanotubes is

$$co - PI_v(G) = \begin{cases} 16kp^3 + 8k^2p - 16k^2p^2 - 16p^2k + 16p^2k\left[\frac{k}{2}\right] - 16p^2\left[\frac{k}{2}\right] - 16p^2\left[\frac{k}{2}\right]^2, & k \leq p \\ \frac{8}{3}kp - \frac{16}{3}p^2 + 8p^2k + 8p^3 - 4k^2p + 4kp^3 - 4k^2p^2 + \frac{4}{3}pk^3 - \frac{8}{3}p^4 + \\ 16p^2k\left[\frac{k}{2}\right] - 16p^2\left[\frac{k}{2}\right] - 16p^2\left[\frac{k}{2}\right]^2, & p < k \leq 2p \\ 12p^3 - 4p^2 + 16p^2k\left[\frac{k}{2}\right] - 16p^2\left[\frac{k}{2}\right] - 16p^2\left[\frac{k}{2}\right]^2, & k > 2p \end{cases}$$

Proof. Let G be the molecular graph of $TUC_4C_8(S)$ nanotube. The graph G has three types of edges which are horizontal, vertical and oblique edges. The quantity $n_e(u) - n_e(v)$ is equal to zero for horizontal edges and equal to $4pk - 2n_e(v)$ for vertical and oblique edges.

Therefore, we have for vertical edges

$$\begin{aligned} \sum_{e \in \text{vertical edges}} |n_e(u) - n_e(v)| &= \\ 2p \sum_{m=1}^{k-1} |4pk - 8pm| &= \\ 8p^2 \left(\sum_{m=1}^{\left[\frac{k}{2}\right]} (k - 2m) + \sum_{m=\left[\frac{k}{2}\right]+1}^{k-1} (2m - k) \right) &= \\ 8p^2 \left(2k \left[\frac{k}{2}\right] - 2 \left[\frac{k}{2}\right] - 2 \left[\frac{k}{2}\right]^2 \right) \end{aligned} \quad (III)$$

Also, for oblique edges we have

$$\begin{cases} 2p \sum_{m=1}^k |4kp - 2(4p^2 - 4pm - k^2 + 2km + k - 2p)|, & k \leq p \\ 2p \sum_{m=1}^p |4kp - 2(4p^2 - 4pm + m^2 + m - 2p)| + \\ 2p \sum_{m=p+1}^k |4kp - 2(4pm - k^2 + 2km - m^2 + k - m - 2p)|, & p < k \leq 2p \\ 2p \sum_{m=1}^p |4kp - 2(4p^2 - 4pm + m^2 + m - 2p)| + 2p \sum_{m=p+1}^{k-p-1} |4kp - 2(4pm - 2p)| + \\ 2p \sum_{m=k-p}^k |4kp - 2(4pm - k^2 + 2km - m^2 + k - m - 2p)|, & k > 2p \end{cases}$$

Therefore, we can obtain the desire result only with summation of relations (III) and above relation..

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