

## Computation of Co-PI index of $TUC_4C_8(R)$ nanotubes

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### ABSTRACT

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

**Keywords:** Vertex-PI index, Co-PI index,  $TUC_4C_8(R)$  Nanotube.

### 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 [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 was also defined in [5], as follow:

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

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where  $n_e(u) = |C| = \left| \left\{ x \in V(G) \mid d(x,u) < d(x,v) \right\} \right|$  and  $n_e(v) = |D| = \left| \left\{ x \in V(G) \mid d(x,v) < d(x,u) \right\} \right|$ , and we can restate it as follows:

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

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

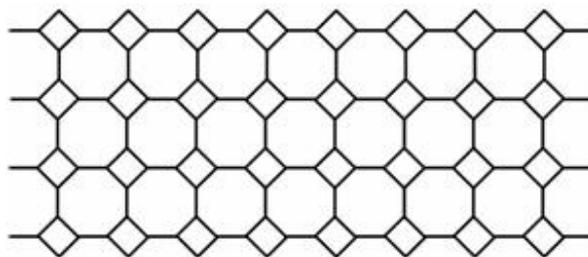
Iranmanesh *et al.* introduced the new index similar to the vertex version of PI index recently [6]. This index is the vertex version of Co-PI index which is  $Co-PI_v(G) = \sum_{e \in E(G)} |n_e(u) - n_e(v)|$ .

In this paper, we compute the new index, vertex version of Co-PI index, for  $TUC_4C_8(R)$  nanotubes.

## 2 DISCUSSION AND RESULT

In this section, we compute the first vertex version of co-PI index for carbon nanotube  $TUC_4C_8(R)$ . Carbon nanotubes (CNTs) are allotropes of carbon with a cylindrical nanostructure. The vertex-PI index of  $TUC_4C_8(R)$  nanotube has been computed in [7]. Also, in [8-16], some topological indices of  $TUC_4C_8(R)$  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 as follows.

According to Figure 1,  $k$  is the number of rows of rhombus and  $p$  is the number of rhombus in a row (that  $p$  indicates the number of columns of rhombus in Figure 2). Therefore, we indicate the rhombus which located in  $i$ -th row and  $j$ -th column with  $S_{ij}$ . Also, we have  $|V(G)| = 4pk$ .



**Figure 1.** Two dimensional lattice of  $TUC_4C_8(R)$  nanotube,  $k = 4, p = 8$ .

At first, we define the symmetry line which exists in every nanotube [8]. We can show all vertices in a row on a circle, let  $e$  be an arbitrary edge on this row. This edge is connecting two points on the circle. Consider a line perpendicular at the mid point to this edge passed a vertex or an edge, say  $a$ , in the opposite side of the circle. A line trough the

point  $a$  and parallel to height of nanotube is called a symmetry line of the nanotube. For example in Figure 2, we show that the symmetry line for  $HAC_5C_7[4,2]$  nanotube:

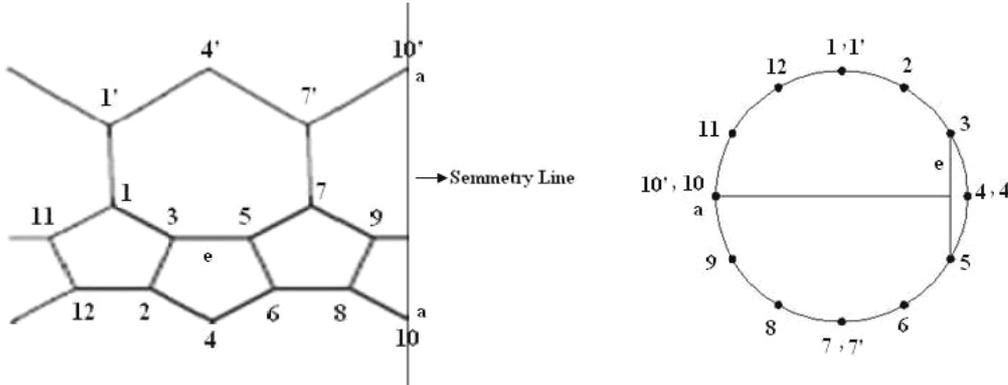


Figure 2. Symmetry Line of  $HAC_5C_7[4,2]$

**Lemma 2.1-** If  $e$  is a horizontal edge of  $G$ , then  $|n_e(u) - n_e(v)| = 0$ .

**Proof.** Due to the Figure 1, the desire result can be concluded. ■

**Lemma 2.2-** If  $e$  is a vertical edge of  $G$ , then,

$$|n_e(u) - n_e(v)| = \begin{cases} 4p(k - 2m) & , m \leq \frac{k}{2} \\ 4p(2m - k) & , m > \frac{k}{2} \end{cases}$$

**Proof.** Due to the Figure 1, the desire result can be concluded. ■

**Lemma 2.3-** If  $e$  is an oblique edge of  $G$ , then,

1. If  $p$  is even then

$$|n_e(u) - n_e(v)| = \begin{cases} |4(k - 2m) + 2| & , m \leq \frac{p}{2} + 1, k - m \leq \frac{p}{2} \\ |4(pk - pm - m) + 2p^2 + 2p + 2| & , m \leq \frac{p}{2} + 1, k - m > \frac{p}{2} \\ |4(k - pm - m) + 2p^2 + 2p - 6| & , m > \frac{p}{2} + 1, k - m \leq \frac{p}{2} \\ |4p(k - 2m) + 4p - 6| & , m > \frac{p}{2} + 1, k - m > \frac{p}{2} \end{cases}$$

1. If  $p$  is odd then

$$|n_e(u) - n_e(v)| = \begin{cases} |4(k - 2m) + 3| & , m \leq \left\lfloor \frac{p}{2} \right\rfloor + 1, k - m \leq \left\lfloor \frac{p}{2} \right\rfloor \\ \left| 4(pk - pm - m) + 2p^2 + 2p + 3 - (k - m - \left\lfloor \frac{p}{2} \right\rfloor) \right| & , m \leq \left\lfloor \frac{p}{2} \right\rfloor + 1, k - m > \left\lfloor \frac{p}{2} \right\rfloor \\ \left| 4(k - pm - m) + 2p^2 + 2p - 5 - (m - \left\lfloor \frac{p}{2} \right\rfloor - 1) \right| & , m > \left\lfloor \frac{p}{2} \right\rfloor + 1, k - m \leq \left\lfloor \frac{p}{2} \right\rfloor \\ \left| 4p(k - 2m) + 4p - 5 - (k - m - \left\lfloor \frac{p}{2} \right\rfloor) - (m - \left\lfloor \frac{p}{2} \right\rfloor - 1) \right| & , m > \left\lfloor \frac{p}{2} \right\rfloor + 1, k - m > \left\lfloor \frac{p}{2} \right\rfloor \end{cases}$$

**Proof.** Let  $e = uv$  be an oblique edge of  $G$ . According to the symmetry line of edge  $e$ , we can identify the region which contains the vertices closer to  $u$  and another region which contains the vertices closer to  $v$ . The vertices which are on symmetry line are not in regions. If  $p$  is an odd number, there are some vertices which are on the symmetry line. By considering Figure 1 and counting the vertices of regions, the result can be proved. ■

**Theorem 2-3.** The vertex version of co-PI index for molecular graph  $G$  of  $TUC_4C_8(R)$  nanotube is:

1. If  $p$  is even, then we have :

$$co - PI_v(G) = \begin{cases} 2k^2p^2 + 8k^2p + 8pk & , k \leq \frac{p}{2} \\ 8kp^3 - 8p^4 - 16p^3 + 6k^2p^2 + 4pk^2 + 8p^2k - 24kp + 16p^2 + 32p & , \frac{p}{2} < k \leq p \\ -8kp^3 + 4p^4 - 12p^3 + 10k^2p^2 + 24p^2k - 24kp + 16p^2 + 16p & , k > p \end{cases}$$

2. If  $p$  is odd, then we have:

$$co - PI_v(G) = \begin{cases} 2k^2p^2 + 8k^2p + 12pk & , k \leq \left\lfloor \frac{p}{2} \right\rfloor \\ 8kp^3 - 16p^3 + 6k^2p^2 - pk^2 + 8p^2k - 12kp + 28p + 28p \left\lfloor \frac{p}{2} \right\rfloor + 8pk \left\lfloor \frac{p}{2} \right\rfloor - 16p^3 \left\lfloor \frac{p}{2} \right\rfloor & , \left\lfloor \frac{p}{2} \right\rfloor < k \leq p \\ 10k^2p^2 - 8p^3 - 3pk^2 + 16p^2k - 18kp + 8p^2 + 16p + 16p^2 \left\lfloor \frac{p}{2} \right\rfloor^2 - 24p \left\lfloor \frac{p}{2} \right\rfloor^2 - 16p^2k \left\lfloor \frac{p}{2} \right\rfloor + 24pk \left\lfloor \frac{p}{2} \right\rfloor + 16p \left\lfloor \frac{p}{2} \right\rfloor & , k > p \end{cases}$$

**Proof.** Let  $G$  be the molecular graph of  $TUC_4C_8(R)$  nanotube. By using the Lemmas (2-1, 2-2 and 2-3) and the fact that there are  $p$  horizontal edge,  $p$  vertical edge and  $4p$  oblique edge in each row of rhombus, we can get the desire results. ■

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