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

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

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 $|V(G)| = 4pk$.

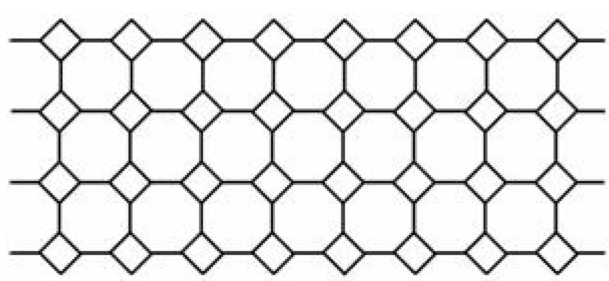

Figure 1. Two dimensional lattice of $TUC_4C_8(R)$ nanotube, $k = 4, p = 8$.

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:

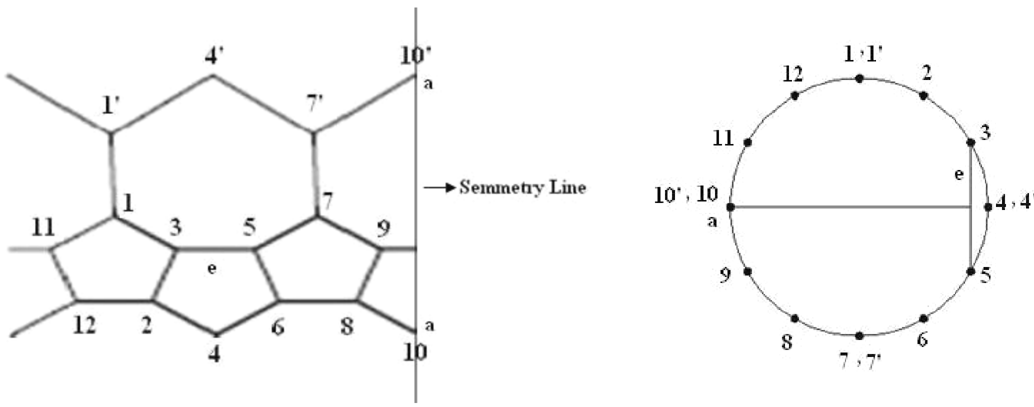

Figure 2. Symmetry Line of $HAC_5C_7[4,2]$

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,

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

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

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

1. If p is odd then

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

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 :

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

2. If p is odd, then we have:

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

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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