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# Vertex-$PI$ Index of Some Nanotubes

Ali Sousaraei[a], Anehgaldi Mahmiani[b] and Omid Khormali[c1]

[a] Islamic Azad University Branch of Azadshaher, Azadshaher, Iran.
[b] University of Payame Noor, Gonbad-e-Kavoos, Iran.
[c] Academic Center for Education, Culture and Research TMU
P.O.Box: 14115-343, Tehran, Iran.

Email: ali_Sousaraei@yahoo.com
Email: Mahmiani @pnu.ac.ir
Email: o_khormali@modares.ac.ir

Abstract. The vertex version of $PI$ index is a molecular structure descriptor which is similar to vertex version of Szeged index. In this paper, we compute the vertex-$PI$ index of $TUC_4C_8(S)$, $TUC_4C_8(R)$ and $HAC_5C_7[r,p]$.

**Keywords**: Vertex-$PI$ Index, Vertex-Szeged index, Molecular Graph, Nanotubes.
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## 1. Introduction

Let $G$ is 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.

[1]Correspondence author

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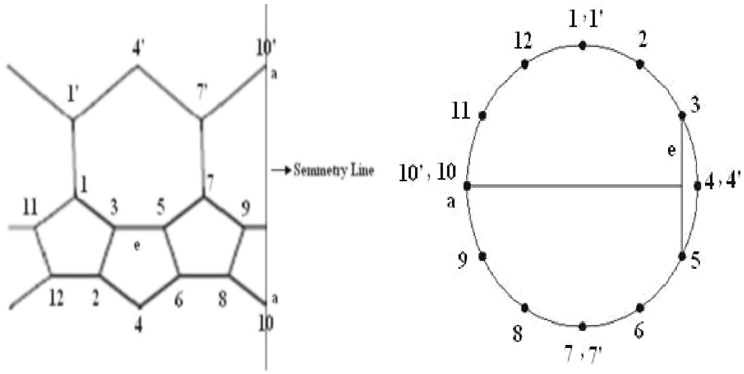


FIGURE 1. Symmetry Line of $HAC_5C_7[4,2]$

Carbon Nanotubes are tubes containing carbon and hydrogen atoms of diameter between 1 and 100 nanometers. Topological indices are integer numbers which can computed with relations on graph parameters (vertex degree, distance between vertices, etc.), which have been defined during studies on molecular graphs in chemistry.

Khadikar and Co-authors [5-8] defined a new topological index and named it Padmakar-Ivan index. They abbreviated this new topological index as $PI$. If $e = uv$ is an edge of $G$, it is defined as $PI_e(G) = \sum_{e\in E(G)}[m_1(e\,|G)+m_2(e\,|G)]$, where $m_1(e\,|G)$ is the number of edges of G lying closer to $u$ than to $v$ and $m_2(e\,|G)$ is the number of edges of G lying closer to $v$ than to $u$. This is the edge version of $PI$ index and in [1-3], the edge-$PI$ index has been computed for some graphs.

The vertex version of $PI$ index was also considered [9], defined as $PI_v(G) = \sum_{e\in E(G)}[n_1(e\,|G) + n_2(e\,|G)]$, such that $n_1(e\,|G)$ is the number of vertices of G lying closer to $u$ than to $v$ and $n_2(e\,|G)$ Is the number of vertices of G lying closer to $v$ than to $u$.

In this paper, we compute the vertex-$PI$ index of $TUC_4C_8(S)$,$TUC_4C_8(R)$ and $HAC_5C_7[r,p]$ nanotubes.

At first, we define the symmetry line which exists in every nanotube [4].

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 1, we show that the symmetry line for $HAC_5C_7[4,2]$:

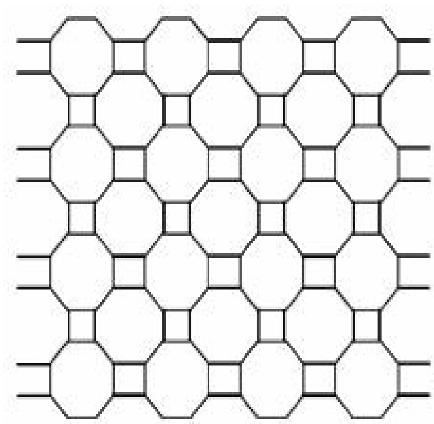

FIGURE 2. Two dimensional lattice of $TUC_4C_8(S)$ nanotube, $p = 4, k = 8$.

## 2. Vertex-$PI$ index of $TUC_4C_8(S)$

According to Figure 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.

**Observation 2.1.** *If $e$ is a horizontal edge of $G$, then:* $n_1(e\,|G) = n_2(e\,|G) = \frac{|V(G)|}{2} = 2kp$.

**Observation 2.2.** *If $e$ is a vertical edge in row $m, (1 \leq m \leq k)$, then:* $n_1(e\,|G) = 4pm$ *and* $n_2(e\,|G) = 4p(k-m)$.

**Observation 2.3.** *If $e$ is an oblique edge in row $m, (1 \leq m \leq k)$, then:*

$$n_1(e|G) = \begin{cases} 4p^2 - 4pm - k^2 + 2km + k - 2p & , m \leq p, k-m \leq p \\ 4p^2 - 4pm + m^2 + m - 2p & , m \leq p, k-m > p \\ 4pm - k^2 + 2km - m^2 + k - m - 2p & , m > p, k-m \leq p \\ 4pm - 2p & , m > p, k-m > p \end{cases} \quad \text{and}$$

$$n_2(e|G) = 4pk - n_1(e|G).$$

*Proof.* We compute only $n_1(e\,|G)$ due to the fact that the computation of $n_2(e\,|G)$ is similar to the computation of $n_1(e\,|G)$.

If we consider the shape of $TUC_4C_8(S)$ and the position of a fixed oblique edge, we can see:

The row $m-1$ has 2 vertices more than row $m$ and row $m-2$ has 2 vertices more than row $m-1$ and so on.

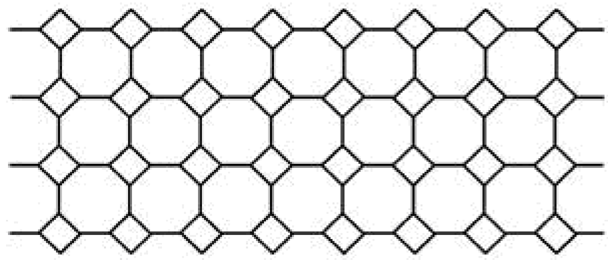

FIGURE 3. Two dimensional lattice of $TUC_4C_8(R)$ nanotube, $k = 4, p = 8$.

The row $m + 1$has 2 vertices less than row $m$ and row $m + 2$ has 2 vertices less than row $m + 1$ and so on.

Then:

$$n_1(e\,|G) = \begin{cases} \sum_{i=0}^{p-m-1}(2p+2i) + \sum_{i=k-m}^{p-1} 2i & , m \le p, k-m \le p \\ \sum_{i=0}^{p-m-1}(2p+2i) + \sum_{i=1}^{p-1} 2i & , m \le p, k-m > p \\ \sum_{i=0}^{p}(2p+2i) + \sum_{i=1}^{m-p-1} 4p + \sum_{i=k-m}^{p-1} 2i & , m > p, k-m \le p \\ \sum_{i=0}^{p}(2p+2i) + \sum_{i=1}^{m-p-1} 4p + \sum_{i=1}^{p-1} 2i & , m > p, k-m > p \end{cases},$$

and $n_2(e\,|G) = 4pk - n_1(e\,|G)$. □

**Observation 2.4.** *In according to Observations (2-1, 2-2 and 2-3),* $n_1(e\,|G) + n_2(e\,|G) = 4pk$*, for every edge in* $E(G)$.

**Theorem 2.1.** *The vertex-*$PI$ *index of* $TUC_4C_8(S)$ *is equal to:*

$$PI_v(G) = \sum_{e \in E(G)} [n_1(e\,|G) + n_2(e\,|G)] = \sum_{e \in E(G)} 4pk = (4pk).(4pk)$$

## 3. VERTEX-$PI$ INDEX OF $TUC_4C_8(R)$

According to Figure 2, $k$ 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$i-throwandj-thcolumn$ with $S_{ij}$. Also, we have$|V(G)| = 4pk$. These notations are valid only in this section of our paper.

**Observation 3.1.** *If* $e$*is a horizontal edge of*$G$*, then:* $n_1(e\,|G) = n_2(e\,|G) = \frac{|V(G)|}{2} = 2kp$.

**Observation 3.2.** *If* $e$ *is a vertical edge between* $m-thand(m+1)-throws$, $(1 \le m \le k-1)$*, then:* $n_1(e\,|G) = 4pm$ *and*$n_2(e\,|G) = 4p(k-m)$.

**Observation 3.3.** *If $e$ is an oblique edge in rhombus $S_{ij}$, $(1 \le i \le k, 1 \le j \le p)$, then:*

(1) *If p is even,*

$$n_1(e\,|G) = \begin{cases} 2pk - 3k - 2k^2 + 4ki & , i \le \frac{p}{2}, k-i \le \frac{p}{2} \\ 2pi - 3i + 2i^2 + \frac{1}{2}p^2 - \frac{3}{2}p + 1 & , i \le \frac{p}{2}, k-i > \frac{p}{2} \\ -\frac{1}{2}p^2 + \frac{13}{2}p - 2 + 2pi + 2pk - 3k \\ \quad +3i - 2k^2 + 4ki - 2i^2 & , i > \frac{p}{2}, k-i \le \frac{p}{2} \\ 5p + 4pi - 1 & , i > \frac{p}{2}, k-i > \frac{p}{2} \end{cases}$$

(2) *If p is odd,*

$$n_1(e\,|G) = \begin{cases} 2pk - 3k - 2k^2 + 4ki & , i \le \left[\frac{p}{2}\right], k-i \le \left[\frac{p}{2}\right] \\ 2pi - 3i + 2i^2 + 2p\left[\frac{p}{2}\right] - 3\left[\frac{p}{2}\right] - 2\left[\frac{p}{2}\right]^2 & , i \le \left[\frac{p}{2}\right], k-i > \left[\frac{p}{2}\right] \\ -2p\left[\frac{p}{2}\right] - 2p + \left[\frac{p}{2}\right] - 1 + 2\left[\frac{p}{2}\right]^2 + 2pk + 2pi \\ \quad -3k + 3i - 2k^2 + 4ki - 2i^2 & , i > \left[\frac{p}{2}\right], k-i \le \left[\frac{p}{2}\right] \\ 4pi - 2p - 2\left[\frac{p}{2}\right] - 1 & , i > \left[\frac{p}{2}\right], k-i > \left[\frac{p}{2}\right] \end{cases}$$

*Proof.* Since the computation of $n_2(e\,|G)$ is similar to the computation of$n_1(e\,|G)$, we compute only $n_1(e\,|G)$.
If we consider the shape of $TUC_4C_8(R)$ and the position of a fixed oblique edge, we can see:
The row $m-1$ has 4 vertices more than row $m$ and row $m-2$ has 4 vertices more than row $m-1$ and so on.
The row $m+1$ has 4 vertices less than row $m$ and row $m+2$ has 4 vertices less than row $m+1$ and so on.
Then:

(1) If p is even,

$$n_1(e\,|G) = \begin{cases} \sum_{m=0}^{i-1}((2p-1)+4m) + \sum_{m=1}^{k-i}((2p-1)-4m) & , i \le \frac{p}{2}, k-i \le \frac{p}{2} \\ \sum_{m=0}^{i-1}((2p-1)+4m) + \sum_{m=1}^{\frac{p}{2}-1}((2p-1)-4m) & , i \le \frac{p}{2}, k-i > \frac{p}{2} \\ \sum_{m=0}^{\frac{p}{2}}((2p-1)+4m) + \sum_{m=1}^{i-\frac{p}{2}+1} 4p \\ \quad + \sum_{m=1}^{k-i}((2p-1)-4m) - 1 & , i > \frac{p}{2}, k-i \le \frac{p}{2} \\ \sum_{m=0}^{\frac{p}{2}}((2p-1)+4m) + \sum_{m=1}^{i-\frac{p}{2}+1} 4p \\ \quad + \sum_{m=1}^{\frac{p}{2}-1}((2p-1)-4m) - 1 & , i > \frac{p}{2}, k-i > \frac{p}{2} \end{cases},$$

and $n_2(e\,|G) = 4pk - n_1(e\,|G)$.

(2) If p is odd, We have a vertex on symmetry line in every row of rhombus. Then,

$$n_1(e\,|G) = \begin{cases} \sum_{m=0}^{i-1}((2p-1)+4m) + \sum_{m=1}^{k-i}((2p-1)-4m) & ,i \le \left[\frac{p}{2}\right], k-i \le \left[\frac{p}{2}\right] \\ \sum_{m=0}^{i-1}((2p-1)+4m) + \sum_{m=1}^{\left[\frac{p}{2}\right]-1}((2p-1)-4m) & ,i \le \left[\frac{p}{2}\right], k-i > \left[\frac{p}{2}\right] \\ \sum_{m=0}^{\left[\frac{p}{2}\right]}((2p-1)+4m) + \sum_{m=1}^{i-\left[\frac{p}{2}\right]+1} 4p + \sum_{m=1}^{k-i}((2p-1)-4m) & ,i > \left[\frac{p}{2}\right], k-i \le \left[\frac{p}{2}\right] \\ \sum_{m=0}^{\left[\frac{p}{2}\right]}((2p-1)+4m) + \sum_{m=1}^{i-\left[\frac{p}{2}\right]+1} 4p + \sum_{m=1}^{\left[\frac{p}{2}\right]-1}((2p-1)-4m) & ,i > \left[\frac{p}{2}\right], k-i > \left[\frac{p}{2}\right] \end{cases},$$

and $n_2(e\,|G) = 4pk - n_1(e\,|G)$.

□

**Observation 3.4.** *parallel oblique edges in a* $S_{ij}, (1 \le i \le k, 1 \le j \le p)$ *have the equal* $n_1(e\,|G)$ *and* $n_2(e\,|G)$.

**Observation 3.5.** *In according to Observations (3-1, 3-2, 3-3 and 3-4),*

(1) *If p is even,* $n_1(e\,|G) + n_2(e\,|G) = 4pk$, *for every edge in* $E(G)$.
(2) *If p is odd,* $n_1(e\,|G) + n_2(e\,|G) = 4pk - p$,

**Theorem 3.1.** *The vertex-PI index of* $TUC_4C_8(R)$ *is equal to:*

(1) *If p is even,*

$$PI_v(G) = \sum_{e \in E(G)} 4pk = (4pk)(6pk - p)$$

(2) *If p is odd,*

$$PI_v(G) = \sum_{e \in E(G)/\{e \in S_{ij} | 1 \le i \le k, 1 \le j \le p\}} 4pk + \sum_{\{e \in S_{ij} | 1 \le i \le k, 1 \le j \le p\}} (4pk - p) = (4pk)(2pk - p) + (4pk - p)(4pk).$$

## 4. Vertex-$PI$ index of

$HAC_5C_7[r,p]$ The vertex-Szeged index of $HAC_5C_7[r,p]$ was computed by A. Iranmanesh in 2007 [4]. And we only repeat the main results.
We denote the number of heptagons in one row by $p$, the number of the periods by k and each period consist of three rows as in figure 4, which shows the $m$-th period,$1 \le m \le k$.

Let e be an edge in Figure 5. Denote:
$E_1 = \{e \in E(G) \,|\, e$ is an oblique edge between two heptagons$\}$
$E_2 = \{e \in E(G) \,|\, e$ is a horizontal edge$\}$
$E_3 = \{e \in E(G) \,|\, e$ is a vertical edge$\}$

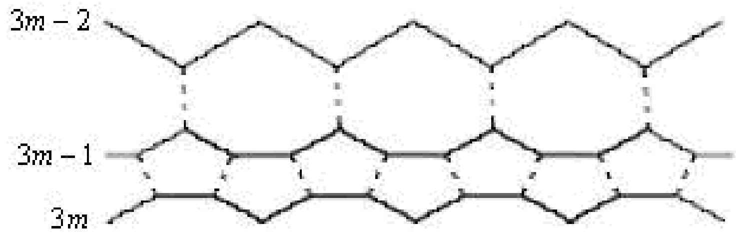


FIGURE 4. $m$-th period

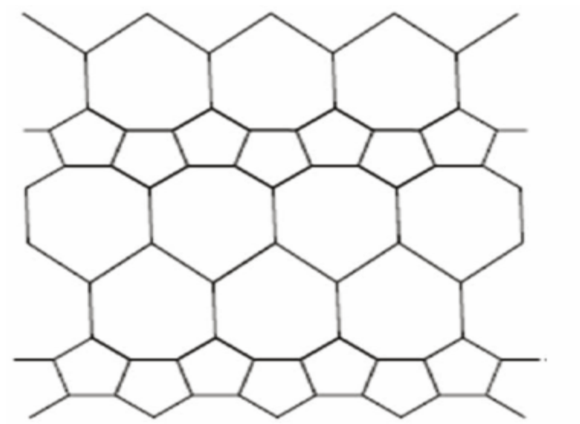

FIGURE 5. Two dimensional lattice of HAC5C7[8,4].

$E_4 = \{e \in E(G) \mid e$ is an oblique edge between heptagon and pentagon$\}$
$E_5 = \{e \in E(G) \mid e$ is an oblique edge between two pentagons$\}$.
Also, we can define some subsets of $E_i$'s as follows:
$E_{2'} = \{e \in E_2 \mid e$ is an edge in $(3m-1)-th$ row$\}$
$E_{2''} = \{e \in E_2 \mid e$ is an edge in $3m-th$ row$\}$ so that $E_2 = E_{2'} \bigcup E_{2''}$.
$E_{3'} = \{e \in E_3 \mid e$ is an edge between $(3m-1)-th$ and $(3m-2)-th$ rows$\}$
$E_{3''} = \{e \in E_3 \mid e$ is an edge between $3m-th$ and $(3(m+1)-2)-th$ rows$\}$
so that $E_3 = E_{3'} \bigcup E_{3''}$. $E_{4'} = \{e \in E_2 \mid e$ is an edge in $(3m-1)-th$ row$\}$
$E_{4''} = \{e \in E_2 \mid e$ is an edge in $3m-th$ row$\}$so that $E_4 = E_{4'} \bigcup E_{4''}$.
And the number of vertices in each period of this nanotube is equal to $8p$.
For computing the vertex-$PI$ index, we must discus in two cases: **Case 1:** $p$ is even.
If $p = 2$, then: $PI_v(HAC_5C_7[4,2]) = 288k^2 - 68k + 5$.

If $p=4$, then: $PI_v(HAC_5C_7[8,4])=\begin{cases}876k^2+868k+10 & ,k\le 2\\ 896k^2+2344k-3790 & ,2<k\le 4\\ 1280k^2-264k+498 & ,k>4\end{cases}$.

Now, let $p\ge 6$.

a) $e\in E_1$:

$$n_e(u)=\begin{cases}8km-4k^2-9k+4pk-1 & ,m\le\frac{p}{2},k-m\le\frac{p}{2}-1\\ 4pm-9m+4m^2+p^2-\frac{9}{2}p+4 & ,m\le\frac{p}{2},k-m>\frac{p}{2}-1\\ \begin{array}{l}8km-\frac{9}{2}p-6-p^2+4pk+4pm+9m\\ -4k^2-4m^2-9k\end{array} & ,m>\frac{p}{2},k-m\le\frac{p}{2}-1\\ 8pm-9p-1 & ,m>\frac{p}{2},k-m>\frac{p}{2}-1\end{cases}$$

$$n_e(v)=\begin{cases}-8km-4k^2+5k+4pk-1 & ,m\le\frac{p}{2},k-m\le\frac{p}{2}-1\\ 8pk-4pm+5m-4m^2-p^2+\frac{5}{2}p-2 & ,m\le\frac{p}{2},k-m>\frac{p}{2}-1\\ \begin{array}{l}-8km+\frac{5}{2}p+p^2+4pk-4pm-5m\\ +4k^2+4m^2+5k\end{array} & ,m>\frac{p}{2},k-m\le\frac{p}{2}-1\\ 8pk-8pm+5p-1 & ,k-m>\frac{p}{2}-1\end{cases}$$

b) $e\in E_2$:

We have $n_e(u)=n_e(v)$ in this case. Then:

I) $e\in E_{2'}$:

$$n_e(u)=\begin{cases}8km-4k^2-7k+4pk-4-8m^2+12m & ,m\le\frac{p}{2},k-m\le\frac{p}{2}-1\\ 4pm+5m-4m^2+p^2-\frac{7}{2}p-1 & ,m\le\frac{p}{2},k-m>\frac{p}{2}-1\\ \begin{array}{l}8km+\frac{5}{2}p-4+p^2+4pk-4pm+7m\\ -4k^2-4m^2-7k\end{array} & ,m>\frac{p}{2},k-m\le\frac{p}{2}-1\\ 2p^2-p-1,m>\frac{p}{2} & ,k-m>\frac{p}{2}-1.\end{cases}$$

II) $e\in E_{2''}$:

$$n_e(u)=\begin{cases}8km-4k^2-k+4pk+1-8m^2 & ,m\le\frac{p}{2},k-m\le\frac{p}{2}-1\\ 4pm-m-4m^2+p^2-\frac{1}{2}p-2 & ,m\le\frac{p}{2},k-m>\frac{p}{2}-1\\ \begin{array}{l}8km-\frac{1}{2}p+1+p^2+4pk-4pm\\ +m-4k^2-4m^2-k\end{array} & ,m>\frac{p}{2},k-m\le\frac{p}{2}-1\\ 2p^2-p-2 & ,m>\frac{p}{2},k-m>\frac{p}{2}-1\end{cases}$$

d) $e\in E_4$:

I) $e \in E_{4'}$:

$$n_e(u) = \begin{cases} 4pm - m - \frac{p}{2} - 2 + 4m^2 & , m \leq \frac{p}{2}, k-m \leq \frac{p}{2} - 1 \\ 4pm - m + 4m^2 - \frac{1}{2}p - 2 & , m \leq \frac{p}{2}, k-m > \frac{p}{2} - 1 \\ 8pm + 1 - p^2 + 7p & , m > \frac{p}{2}, k-m \leq \frac{p}{2} - 1 \\ 8pm - p^2 + 7p + 1 & , m > \frac{p}{2}, k-m > \frac{p}{2} - 1 \end{cases}$$

$$n_e(v) = \begin{cases} k + 4k^2 - 8km + 4pk - 4pm - m + \frac{5p}{2} + 1 + 4m^2 & , m \leq \frac{p}{2}, k-m \leq \frac{p}{2} - 1 \\ 8pk - p^2 + 3p + 4 - 8pm & , m \leq \frac{p}{2}, k-m > \frac{p}{2} - 1 \\ k + 4k^2 - 8mk + 4pk - 4pm - m + \frac{5p}{2} + 1 + 4m^2 & , m > \frac{p}{2}, k-m \leq \frac{p}{2} - 1 \\ 8pm - p^2 + 3p + 4 - 8pm & , m > \frac{p}{2}, k-m > \frac{p}{2} - 1 \end{cases}$$

II) $e \in E_{4''}$:

$$n_e(u) = \begin{cases} 4pm - 13m - \frac{p}{2} + 11 + 4m^2 & , m \leq \frac{p}{2}, k-m \leq \frac{p}{2} - 1 \\ 4pm - 13m + 4m^2 - \frac{1}{2}p + 11 & , m \leq \frac{p}{2}, k-m > \frac{p}{2} - 1 \\ 8pm + 2 - p^2 + p & , m > \frac{p}{2}, k-m \leq \frac{p}{2} - 1 \\ 8pm - p^2 + p + 2 & , m > \frac{p}{2}, k-m > \frac{p}{2} - 1 \end{cases}$$

$$n_e(v) = \begin{cases} 9k + 4p(k-m) - 9m + \frac{p}{2} + 4(k-m)^2 & , m \leq \frac{p}{2}, k-m \leq \frac{p}{2} - 1 \\ 8pk - p^2 + 7p - 6 - 8pm & , m \leq \frac{p}{2}, k-m > \frac{p}{2} - 1 \\ 9k + 4p(k-m) - 9m + \frac{p}{2} + 4(k-m)^2 & , m > \frac{p}{2}, k-m \leq \frac{p}{2} - 1 \\ 8pm - p^2 + 7p - 6 - 8pm & , m > \frac{p}{2}, k-m > \frac{p}{2} - 1 \end{cases}$$

e) $e \in E_5$:

$$n_e(u) = 8p(m-1) + 5p - 9$$
$$n_e(v) = 8p(k-m) + 3p - 9.$$

For simplicity of computations, we define: For subcase a:

$$a_1 = 8km - 4k^2 - 9k + 4pk - 1$$
$$b_1 = 4pm - 9m + 4m^2 + p^2 - \frac{9}{2}p + 4$$
$$c_1 = 8km - \frac{9}{2}p - 6 - p^2 + 4pk + 4pm + 9m - 4k^2 - 4m^2 - 9k$$
$$d_1 = 8pm - 9p - 1$$
$$a_2 = -8km - 4k^2 + 5k + 4pk - 1$$
$$b_2 = 8pk - 4pm + 5m - 4m^2 - p^2 + \frac{5}{2}p - 2$$
$$c_2 = -8km + \frac{5}{2}p + p^2 + 4pk - 4pm - 5m + 4k^2 + 4m^2 + 5k$$
$$d_2 = 8pk - 8pm + 5p - 1$$

For subcase b:

$$a_3 = 8km - 4k^2 - 7k + 4pk - 4 - 8m^2 + 12m$$
$$b_3 = 4pm + 5m - 4m^2 + p^2 - \frac{7}{2}p - 1$$
$$c_3 = 8km + \frac{5}{2}p - 4 + p^2 + 4pk - 4pm + 7m - 4k^2 - 4m^2 - 7k$$
$$d_3 = 2p^2 - p - 1$$
$$a_4 = 8km - 4k^2 - k + 4pk + 1 - 8m^2$$
$$b_4 = 4pm - m - 4m^2 + p^2 - \frac{1}{2}p - 2$$
$$c_4 = 8km - \frac{1}{2}p + 1 + p^2 + 4pk - 4pm + m - 4k^2 - 4m^2 - k$$
$$d_4 = 2p^2 - p - 2$$

For subcase c:

$$z_1 = 8pm - 28$$
$$t_1 = 8p(k - m) + 14$$
$$z_2 = 8pm - 6p + 14$$
$$t_2 = 8(k - m) + 6p - 2$$

For subcase d:

$$a_5 = 4pm - m - \frac{p}{2} - 2 + 4m^2$$
$$b_5 = a_5$$
$$c_5 = 8pm + 1 - p^2 + 7p$$
$$d_5 = c_5$$
$$a_6 = k + 4k^2 - 8km + 4pk - 4pm - m + \frac{5p}{2} + 1 + 4m^2$$
$$b_6 = 8pk - p^2 + 3p + 4 - 8pm$$
$$c_6 = a_6$$
$$d_6 = b_6$$
$$a_7 = 4pm - 13m - \frac{p}{2} + 11 + 4m^2$$
$$b_7 = a_7$$
$$c_7 = 8pm + 2 - p^2 + p$$
$$d_7 = c_7$$
$$a_8 = 9k + 4p(k - m) - 9m + \frac{p}{2} + 4(k - m)^2$$
$$b_8 = 8pk - p^2 + 7p - 6 - 8pm$$
$$c_8 = a_8$$
$$d_8 = b_8$$

For subcase e:

$$z_3 = 8p(m-1) + 5p - 9$$
$$t_3 = 8p(k-m) + 3p - 9.$$

Then:

$$S_1 = 2p(a_1+a_2)+2pa_3+2pa_4+p(z_1+t_1)+2p(a_5+a_6)+2p(a_7+a_8)+2p(z_3+t_3)$$
$$S_2 = 2p(b_1+b_2)+2pb_3+2pb_4+p(z_1+t_1)+2p(b_5+b_6)+2p(b_7+b_8)+2p(z_3+t_3)$$
$$S_3 = 2p(c_1+c_2)+2pc_3+2pc_4+p(z_1+t_1)+2p(c_5+c_6)+2p(c_7+c_8)+2p(z_3+t_3)$$
$$S_4 = 2p(d_1+d_2)+2pd_3+2pd_4+p(z_1+t_1)+2p(d_5+d_6)+2p(d_7+d_8)+2p(z_3+t_3)$$

Then we have:

**Theorem 4.1.** *The vertex-$PI$ index of nanotube $HAC_5C_7[r,p]$, for even $p \geq 6$, is:*

$$PI_v(G) = \begin{cases} \sum_{m=1}^{k} S_1 + \sum_{m=1}^{k-1} p(z_2+t_2) & , k \leq \frac{p}{2} \\ \sum_{m=1}^{\frac{p}{2}} S_2 + \sum_{m=\frac{p}{2}+1}^{k} S_3 + \sum_{m=1}^{\frac{p}{2}} p(z_2+t_2) \\ + \sum_{m=\frac{p}{2}+1}^{k-1} p(z_2+t_2) & , \frac{p}{2} < k < p \\ \sum_{m=1}^{\frac{p}{2}} S_2 + \sum_{m=k-\frac{p}{2}+1}^{k} S_3 + \sum_{m=\frac{p}{2}+1}^{k-\frac{p}{2}} S_4 \\ + \sum_{m=1}^{\frac{p}{2}} p(z_2+t_2) + \sum_{m=\frac{p}{2}+1}^{k-\frac{p}{2}} p(z_2+t_2) & , k > p \\ + \sum_{m=k-\frac{p}{2}+1}^{k-1} p(z_2+t_2) \end{cases}$$

**Case 2:** $p$ is odd number.
If $p = 1$, then: $PI_v(HAC_5C_7[2,1]) = 72k^2 - 52k + 1$.
If $p = 3$, then: $PI_v(HAC_5C_7[6,3]) = 720k^2 - 90k - 139$.

If $p = 5$, then: $PI_v(HAC_5C_7[10,5]) = \begin{cases} 1370k^2 + 1510k + 13 & , k \leq 2 \\ 1400k^2 + 3770k - 5807 & , 2 < k \leq 4 \\ 2000k^2 - 420k + 1353 & , k > 4 \end{cases}$.

For $p \geq 7$, we can compute vertex-$PI$ as the same way which $p$ is even number. There are only some differences between the cases which $p$ is odd or even number. For example, we must use $\left[\frac{p}{2}\right]$ instead of $\frac{p}{2}$.

a) $e \in E_1$:

$$n_e(u) = \begin{cases} 8km - 4k^2 - 9k + 4pk - 2 + m & , m \leq \left[\frac{p}{2}\right], k-m \leq \left[\frac{p}{2}\right] - 1 \\ 4pm - 8m + 4m^2 - 4\left[\frac{p}{2}\right]^2 + 4p\left[\frac{p}{2}\right] \\ -\left[\frac{p}{2}\right] - 4p + 4 & , k-m > \left[\frac{p}{2}\right] - 1 \\ 8km - 4p - 6 + 4\left[\frac{p}{2}\right]^2 - 4p\left[\frac{p}{2}\right] + 4pk \\ +4pm + 9m - 4k^2 - 4m^2 - 9k & , m > \left[\frac{p}{2}\right], k-m \leq \left[\frac{p}{2}\right] - 1 \\ 8pm - 8p - \left[\frac{p}{2}\right] & , m > \left[\frac{p}{2}\right], k-m > \left[\frac{p}{2}\right] - 1 \end{cases}.$$

$$n_e(v)=\begin{cases}-8km+4k^2+6k+4pk-1 & ,m\le\left[\frac{p}{2}\right],k-m\le\left[\frac{p}{2}\right]-1\\ 8pk-4pm+6m-4m^2+4\left[\frac{p}{2}\right]^2-4p\left[\frac{p}{2}\right] \\ -2\left[\frac{p}{2}\right]+4p-4 & ,m\le\left[\frac{p}{2}\right],k-m>\left[\frac{p}{2}\right]-1\\ -3+4p\left[\frac{p}{2}\right]-4\left[\frac{p}{2}\right]^2-2\left[\frac{p}{2}\right]+4p(k-m+1) \\ -2k+2m+4(k-m+1)^2 & ,m>\left[\frac{p}{2}\right],k-m\le\left[\frac{p}{2}\right]-1\\ 8pk-8pm+8p-2-4\left[\frac{p}{2}\right] & ,m>\left[\frac{p}{2}\right],k-m>\left[\frac{p}{2}\right]-1\end{cases}.$$

b) $e\in E_2$:
In this subcase $n_e(u)=n_e(v)$.
I) $e\in E_{2'}$:

$$n_e(u)=\begin{cases}8km-4k^2-7k+4pk-4+12m-8m^2 & ,m\le\left[\frac{p}{2}\right],k-m\le\left[\frac{p}{2}\right]-1\\ 4pm+5m+4m^2-4\left[\frac{p}{2}\right]^2+4p\left[\frac{p}{2}\right]+\left[\frac{p}{2}\right]-4p & ,m\le\left[\frac{p}{2}\right],k-m>\left[\frac{p}{2}\right]-1\\ 8km+1-4\left[\frac{p}{2}\right]^2+4p\left[\frac{p}{2}\right]+5\left[\frac{p}{2}\right]+4pk-4pm \\ +7m-4k^2-4m^2-7k & ,m>\left[\frac{p}{2}\right],k-m\le\left[\frac{p}{2}\right]-1\\ 8p\left[\frac{p}{2}\right]-4p+6\left[\frac{p}{2}\right]-8\left[\frac{p}{2}\right]^2+5 & ,m>\left[\frac{p}{2}\right],k-m>\left[\frac{p}{2}\right]-1\end{cases}.$$

II) $e\in E_{2''}$:

$$n_e(u)=\begin{cases}8km-4k^2-k+4pk+1-8m^2 & ,m\le\left[\frac{p}{2}\right],k-m\le\left[\frac{p}{2}\right]-1\\ 4pm-m-4m^2-4\left[\frac{p}{2}\right]^2+4p\left[\frac{p}{2}\right]-\left[\frac{p}{2}\right]+1 & ,m\le\left[\frac{p}{2}\right],k-m>\left[\frac{p}{2}\right]-1\\ 8km+1-4\left[\frac{p}{2}\right]^2+4p\left[\frac{p}{2}\right]-\left[\frac{p}{2}\right]+4pk \\ -4pm+m-4k^2-4m^2-k & ,m>\left[\frac{p}{2}\right],k-m\le\left[\frac{p}{2}\right]-1\\ 8p\left[\frac{p}{2}\right]-2\left[\frac{p}{2}\right]-8\left[\frac{p}{2}\right]^2+1 & ,m>\left[\frac{p}{2}\right],k-m>\left[\frac{p}{2}\right]-1\end{cases}.$$

c) $e\in E_3$: I) $e\in E_{3'}$:

$$n_e(u)=8pm-28$$

$$n_e(v)=8p(k-m)+14$$

II) $e\in E_{3''}$:

$$n_e(u)=8pm-6p+14$$

$$n_e(v)=8(k-m)+6p-2$$

d) $e\in E_4$: I) $e\in E_{4'}$:

$$n_e(u)=\begin{cases}pm-\left[\frac{p}{2}\right]+6m\left[\frac{p}{2}\right]+7-7m+4m^2 & ,m\le\left[\frac{p}{2}\right],k-m\le\left[\frac{p}{2}\right]-1\\ pm-7m+4m^2+6m\left[\frac{p}{2}\right]-\left[\frac{p}{2}\right]+7 & ,m\le\left[\frac{p}{2}\right],k-m>\left[\frac{p}{2}\right]-1\\ 8pm+10\left[\frac{p}{2}\right]^2-7p\left[\frac{p}{2}\right]+6\left[\frac{p}{2}\right]+p+1 & ,m>\left[\frac{p}{2}\right],k-m\le\left[\frac{p}{2}\right]-1\\ 8pm+p+6\left[\frac{p}{2}\right]-7p\left[\frac{p}{2}\right]+10\left[\frac{p}{2}\right]+1 & ,m>\left[\frac{p}{2}\right],k-m>\left[\frac{p}{2}\right]-1\end{cases}.$$

$$n_e(v)=\begin{cases} -\left[\frac{p}{2}\right]+6\left[\frac{p}{2}\right](k-m+1)+p(k-m+1) & ,m\leq\left[\frac{p}{2}\right],k-m\leq\left[\frac{p}{2}\right]-1\\ +5m-5k-p+4(k-m+1)^2 & \\ 8pk-8pm+10\left[\frac{p}{2}\right]^2-7p\left[\frac{p}{2}\right]-5\left[\frac{p}{2}\right]+7p+9 & ,m\leq\left[\frac{p}{2}\right],k-m>\left[\frac{p}{2}\right]-1\\ 5m+6\left[\frac{p}{2}\right](k-m+1)-\left[\frac{p}{2}\right]+p(k-m+1) & ,m>\left[\frac{p}{2}\right],k-m\leq\left[\frac{p}{2}\right]-1\\ +4(k-m+1)^2-5k-p & \\ 8pk-8pm+10\left[\frac{p}{2}\right]^2-7p\left[\frac{p}{2}\right]-5\left[\frac{p}{2}\right]+7p+9 & ,m>\left[\frac{p}{2}\right],k-m>\left[\frac{p}{2}\right]-1 \end{cases}.$$

II) $e\in E_{4''}$:

$$n_e(u)=\begin{cases} pm-\left[\frac{p}{2}\right]+6m\left[\frac{p}{2}\right]+15-14m+4m^2 & ,m\leq\left[\frac{p}{2}\right],k-m\leq\left[\frac{p}{2}\right]-1\\ pm-14m+4m^2+6m\left[\frac{p}{2}\right]-\left[\frac{p}{2}\right]+15 & ,m\leq\left[\frac{p}{2}\right],k-m>\left[\frac{p}{2}\right]-1\\ 8pm+10\left[\frac{p}{2}\right]^2-7p\left[\frac{p}{2}\right]-\left[\frac{p}{2}\right]+p & ,m>\left[\frac{p}{2}\right],k-m\leq\left[\frac{p}{2}\right]-1\\ 8pm+p-\left[\frac{p}{2}\right]-7p\left[\frac{p}{2}\right]+10\left[\frac{p}{2}\right] & ,m>\left[\frac{p}{2}\right],k-m>\left[\frac{p}{2}\right]-1 \end{cases}$$

$$n_e(v)=\begin{cases} -\left[\frac{p}{2}\right]+6\left[\frac{p}{2}\right](k-m+1)+p(k-m+1)-1 & ,m\leq\left[\frac{p}{2}\right],k-m\leq\left[\frac{p}{2}\right]-1\\ +4(k-m+1)^2-p & \\ 8pk-8pm+10\left[\frac{p}{2}\right]^2-7p\left[\frac{p}{2}\right]-\left[\frac{p}{2}\right]+7p-4 & ,m\leq\left[\frac{p}{2}\right],k-m>\left[\frac{p}{2}\right]-1\\ 6\left[\frac{p}{2}\right](k-m+1)-\left[\frac{p}{2}\right]+p(k-m+1) & ,m>\left[\frac{p}{2}\right],k-m\leq\left[\frac{p}{2}\right]-1\\ +4(k-m+1)^2-p-1 & \\ 8pk-8pm+10\left[\frac{p}{2}\right]^2-7p\left[\frac{p}{2}\right]-\left[\frac{p}{2}\right]+7p-4 & ,m>\left[\frac{p}{2}\right],k-m>\left[\frac{p}{2}\right]-1 \end{cases}.$$

e) $e\in E_5$:

$$n_e(u)=8p(m-1)+5p-9$$

$$n_e(v)=8p(k-m)+3p-9$$

For odd case, we do same way for simplicity of computations. Then:

**Theorem 4.2.** *The vertex-$PI$ index of nanotube $HAC_5C_7[r,p]$ for odd $p\geq 7$, is:*

$$PI_v(G)=\begin{cases} \sum_{m=1}^{k}S_1+\sum_{m=1}^{k-1}p(z_2+t_2) & ,k\leq\left[\frac{p}{2}\right]\\ \sum_{m=1}^{\left[\frac{p}{2}\right]}S_2+\sum_{m=\left[\frac{p}{2}\right]+1}^{k}S_3 & ,\left[\frac{p}{2}\right]<k<p\\ +\sum_{m=1}^{\left[\frac{p}{2}\right]}p(z_2+t_2)+\sum_{m=\left[\frac{p}{2}\right]+1}^{k-1}p(z_2+t_2) & \\ \sum_{m=1}^{\left[\frac{p}{2}\right]}S_2+\sum_{m=k-\left[\frac{p}{2}\right]+1}^{k}S_3 & \\ +\sum_{m=\left[\frac{p}{2}\right]+1}^{k-\left[\frac{p}{2}\right]}S_4+\sum_{m=1}^{\left[\frac{p}{2}\right]}p(z_2+t_2) & ,k>p\\ +\sum_{m=\left[\frac{p}{2}\right]+1}^{k-\left[\frac{p}{2}\right]}p(z_2+t_2)+\sum_{m=k-\left[\frac{p}{2}\right]+1}^{k-1}p(z_2+t_2) & \end{cases}$$

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