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PI Index of $TUC_4C_8(R)$ Nanotubes

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Abstract

A C_4C_8 net is a trivalent decoration made by alternating squares C_4 and octagons C_8. It can cover either a cylinder or a torus.

In this paper we compute Padmakar-Ivan index, abbreviated (PI) index, of $TUC_4C_8(R)$ nanotube where PI index of a graph G is defined as $PI(G) = \sum [n_{eu}(e|G) + n_{ev}(e|G)]$, where $n_{eu}(e|G)$ is the number of edges of G lying closer to u than to v, $n_{ev}(e|G)$ is the number of edges of G lying closer to v than to u and summation goes over all edges of G .This topological index is developed recently.

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1. Introduction

A graph G consists of a set of vertices $V(G)$ and a set of edges $E(G)$. The vertices in G are connected by an edge if there exists an edge $U_iU_j \in E(G)$ connecting the vertices U_i and U_j in G such that $U_i, U_j \in V(G)$. In chemical graphs, each vertex represents an atom of the molecule, and covalent bonds between atoms are represented by edges between the corresponding vertices. This shape derived from a chemical compound is often called its molecular graph, and can be a path, a tree, or in general a graph.

A real number that describes a molecular graph is called a topological index. Usage of topological indices in biology and chemistry began in 1947 when chemist Harold Wiener [1] introduced Wiener index to demonstrate correlations between physico-chemical properties of organic compounds and the index of their molecular graphs. Wiener originally defined his index (W) on trees and studied its use for correlations of physico chemical properties of alkanes, alcohols, amines and their analogous compounds [2].

Another topological index was introduced by Gutman and called the Szeged index, abbreviated as Sz [2]. For the reason of the coincidence of Wiener and Szeged indices in case of trees the authors in [3,4] introduced another Szeged/Wiener-like topological index and named it Padmakar-Ivan index, abbreviated as PI. Unlike Szeged index (Sz), PI index is very different for trees as well as for cyclic graphs, and not much is known about the applicability of PI index in chemistry [2].

The distance between a pair of vertices u and v of G is denoted by $d_G(u,v)$ or $d(u,v)$. We define for $e = uv$ two quantities $n_{eu}(e|G)$ and $n_{ev}(e|G)$ where $n_{eu}(e|G)$ is the number of edges of G lying closer to u than to v and $n_{ev}(e|G)$ is the number of edges of G lying closer to v than to u. Edges equidistant from both ends of the edges are not counted.

If $G_{u,e} = \{x \mid d(u,x) < d(v,x)\}, G_{v,e} = \{x \mid d(u,x) > d(v,x)\}$, and G_e represents the vertices of edges that equidistant from two vertices u and v, then

$n_{eu}(e \mid G) = |E(G_{u,e})|$, $n_{ev}(e \mid G) = |E(G_{v,e})|$ and $N(e) = |E(G_e)|$. Here for any subset U of the vertex set $V = V(G)$, $|E(U)|$, denotes the number of edges of G between the vertices of U . In a series of papers, some people computed the Wiener index and the PI index of some nanotubes [5-12].

In this paper, PI index of $TUC_4C_8(R)$ nanotubes is computed. We denote the number of rhombs on the level 1 by p and the length of tube by q . Therefore we have $2q$ rows of edges and $3q$ rows of vertices in $TUC_4C_8(R)$ nanotube.

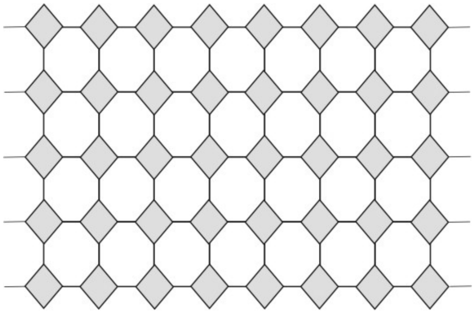

Figure 1- The $TUC_4C_8(R)$ Nanotube with p=8 and q=5

2. PI index of $TUC_4C_8(R)$ Nanotubes

In this section, we compute the PI index of the graph $T = TUC_4C_8(R)$ nanotube. To do this, we assume that $E = E(T)$ is the set of all edges of T and $N(e) = |E| - (n_{eu}(e|G) + n_{ev}(e|G))$ .Then $PI(T) = |E|^2 - \sum_{e \in E} N(e)$.

But $|E(T)| = p(6q-1)$ and so $PI(T) = p^2(6q-1)^2 - \sum_{e \in E} N(e)$. Therefore, for computing the PI index of T , it is enough to calculate $N(e)$, for every $e \in E$.

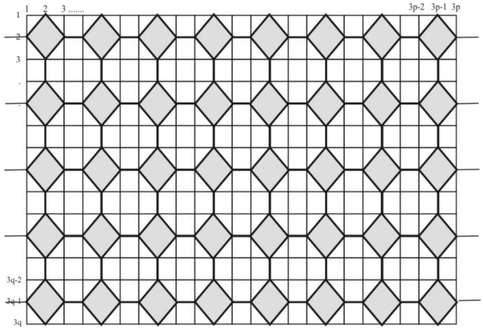

Figure 2- The TUC_4C_8(R) Nanotube with 3q rows and 3p columns of vertices

At first, we assume that p is even . Therefore, we have the following lemmas:

Lemma 2.1. If e is a horizontal edge in Figure 2, then $N(e)=2q$.

Proof. Suppose $e=U_{ij}U_{i(j+1)}$ is an arbitrary horizontal edge of i^{th} row of vertices in $TUC_4C_8(R)$ nanotube. In this case for every k, $k=2,5,\ldots,3q-1$ we have $d(U_{ij},U_{kj})=d(U_{i(j+1)},U_{k(j+1)})$ and also $d(U_{ij},U_{kj})<d(U_{kj},U_{i(j+1)})$ and $d(U_{k(j+1)},U_{i(j+1)})<d(U_{k(j+1)},U_{ij})$.Therefore if we suppose

$$A=\{U_{kj},U_{k(j+1)}\mid K=2,5,\ldots,3q-1\}$$

we have $|E(A)|=q$ and $A\subseteq T_e$. For founding the remained edges that belong to T_e we consider three cases:

i) If $j=\frac{3p}{2}$, then for every $k=2,5,\ldots,3q-1$ we have

$$d(U_{ij},U_{k(3p)})=d(U_{i(j+1)},U_{k1}).$$

ii) If $j=3p$, then for every $k=2,5,\ldots,3q-1$ we have:

$$d(U_{i(3p)},U_{k(\frac{3p}{2}+1)})=d(U_{i1},U_{k(\frac{3p}{2})})$$

iii) If $j\neq 3p,\frac{3p}{2}$, then we have $d(U_{ij},U_{kl})=d(U_{i(j+1)},U_{k(1+1)})$ where

$$l=\begin{cases} j+\frac{3}{2}p & j<\frac{3p}{2} \\ j-\frac{3p}{2} & \frac{3p}{2}<j<3p \end{cases}.$$

Hence in all cases q edges are equidistant from both ends of the edge e. So if we insert these q edges in the set B, we have $N(e) \geq |E(A)| + |E(B)| = 2q$. Now, we prove that $N(e) = |E(A)| + |E(B)| = 2q$. Suppose $U_{m\,n}U_{(m+1)\,n}$ is a vertical edge. Hence for $j \leq \frac{3p}{2}$, we have:

$$\begin{cases} d\left(U_{m\,n}, U_{i\,(j+1)}\right) < d\left(U_{m\,n}, U_{i\,j}\right), d\left(U_{(m+1)\,n}, U_{i\,(j+1)}\right) < d\left(U_{(m+1)\,n}, U_{i\,j}\right) & \text{if} \quad j \leq n < j + \frac{3p}{2} \\ d\left(U_{m\,n}, U_{i\,(j+1)}\right) > d\left(U_{m\,n}, U_{i\,j}\right), d\left(U_{(m+1)\,n}, U_{i\,(j+1)}\right) > d\left(U_{(m+1)\,n}, U_{i\,j}\right) & \text{if} \quad n < j \text{ or } n > j + \frac{3p}{2} \end{cases}$$

and for $j > \frac{3p}{2}$, we have:

$$\begin{cases} d\left(U_{m\,n}, U_{i\,j}\right) < d\left(U_{m\,n}, U_{i\,(j+1)}\right), d\left(U_{(m+1)\,n}, U_{i\,j}\right) < d\left(U_{(m+1)\,n}, U_{i\,(j+1)}\right) & \text{if} \quad j - \frac{3p}{2} \leq n < j \\ d\left(U_{m\,n}, U_{i\,(j+1)}\right) < d\left(U_{m\,n}, U_{i\,j}\right), d\left(U_{(m+1)\,n}, U_{i\,(j+1)}\right) < d\left(U_{(m+1)\,n}, U_{i\,j}\right) & \text{if} \quad n \geq j \text{ or } n < j - \frac{3p}{2} \end{cases}$$

The proof for any horizontal edge which neither in $E(A)$ nor in $E(B)$ and also for any oblique edge is the same as above and therefore $N(e) = 2q$. ∎

Lemma 2.2. If e is a vertical edge in Figure 2, then $N(e) = p$.

Proof. Let $e = U_{i\,j}U_{(i+1)\,j}$ be a vertical edge. Therefore for every k, $k = 2, 5, \ldots, 3p-1$, we have $d\left(U_{i\,j}, U_{i\,k}\right) = d\left(U_{(i+1)\,j}, U_{(i+1)\,k}\right)$. If we suppose $A = \left\{U_{i\,k}, U_{(i+1)\,k} \mid k = 2, 5, \ldots, 3p-1\right\}$, then $E(A)$ has exactly p elements which are parallel to e. We prove that $|E(A)| = N(e)$. Suppose $e = U_{mn}U_{(m+1)n}$ is a vertical edge that not belongs to A. We have two cases:

Case1. If $i < m$, then $d\left(U_{mn}, U_{(i+1)\,j}\right) < d\left(U_{mn}, U_{i\,j}\right)$ and $d\left(U_{(m+1)n}, U_{(i+1)\,j}\right) < d\left(U_{(m+1)n}, U_{i\,j}\right)$.

Case2. If $i > m$, then $d\left(U_{mn}, U_{i\,j}\right) < d\left(U_{mn}, U_{(i+1)\,j}\right)$ and $d\left(U_{(m+1)n}, U_{i\,j}\right) < d\left(U_{(m+1)n}, U_{(i+1)\,j}\right)$.

Now suppose that $U_{sl}U_{s\,(l+1)}$ is a horizontal edge. Then for $s \le i$, $d(U_{sl},U_{ij}) < d(U_{sl},U_{(i+1)j})$ and $d(U_{s(l+1)},U_{ij}) < d(U_{s(l+1)},U_{(i+1)j})$, else $d(U_{sl},U_{(i+1)j}) < d(U_{sl},U_{ij})$ and $d(U_{s(l+1)},U_{(i+1)j}) < d(U_{s(l+1)},U_{ij})$.

Let $U_{m\,n}U_{k\,(n+1)}$ be an oblique edge where k is equal to $m+1$ or $m-1$. If $i > m$, then $d(U_{m\,n},U_{ij}) < d(U_{m\,n},U_{(i+1)j})$ and $d(U_{k(n+1)},U_{ij}) < d(U_{k\,(n+1)},U_{(i+1)j})$. If $i < m$, then $d(U_{m\,n},U_{(i+1)j}) < d(U_{m\,n},U_{ij})$ and $d(U_{k(n+1)},U_{(i+1)j}) < d(U_{k\,(n+1)},U_{ij})$. Therefore we proved that $|E(A)| = N(e)$ and the proof is completed. █

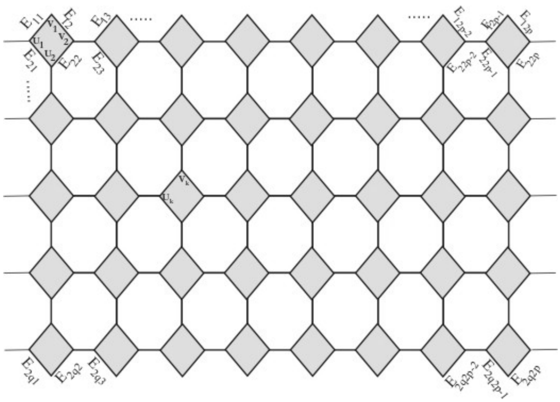

Figure 3- The $TUC_4C_8(R)$ Nanotube with p=8 and q=5

Lemma 2.3. Let e be an oblique edge in the k^{th} row of edges in Figure 3, then:

1) If $2q \le p$, then $N(e) = 4q$

2) If $2q \ge p$, then we have the following cases:

Case1: If $2p-1 > 2q$, then

$$N(e) = \begin{cases} 2p+2(k-1) & 1 \le k \le 2q-p+1 \\ 4q & 2q-p+2 \le k \le p-1 \\ 2p+2(2q-k) & p \le k \le 2q \end{cases}$$

Case2: If $2p-1 \le 2q$, then

$$N(e)=\begin{cases} 2p+2(k-1) & 1\le k\le p \\ 4p-2 & p+1\le k\le 2q-p \\ 2p+2(2q-k) & 2q-p+1\le k\le 2q \end{cases}$$

Proof: At first we denote the oblique edges $E_{ij}, 1\le i\le 2q, 1\le j\le 2p$ of $TUC_4C_8(R)$ as be described in Figure 3. It is obvious that $N(E_{k1})=N(E_{k2})=\ldots=N(E_{k(2p)})$, for every k, so it is enough to calculate $N(E_{11}), N(E_{21}),\ldots,N(E_{(2q)1})$. Suppose $2q\le p$. For computing of $N(E_{11})$, we consider $A=\{E_{11},E_{22},\ldots,E_{(2q)(2q)},E_{1(p+1)},\ldots,E_{(2q)(p+1)}\}$. Suppose that $E_{ii}=u_iv_i$, $1\le i\le 2q$. Then, we have

$d(u_1,u_i)=d(v_1,v_i), d(u_1,u_i)<d(v_1,u_i), d(v_1,v_i)<d(u_1,v_i)$ for $1\le i\le 2q$.As a similar way, $E_{i(p+1)}\in E(T_{E_{11}})$ for $1\le i\le 2q$ and therefore $N(E_{11})\ge |A|=4q$.With the same proof in the Lemma 2.1, we can prove that $N(E_{11})=4q$. We continue our argument by considering the edge E_{22}. If we consider $B=\{E_{11},E_{22},\ldots,E_{(2q)(2q)},E_{1(p+2)},E_{2(p+2)},\ldots,E_{2q(p+2)}\}$, then $N(E_{22})\ge |B|=4q$ and again we can show that $N(E_{22})=4q$. Now we consider the edge E_{31}. To find $N(E_{31})$, we delete the first and the second row of edges of the $TUC_4C_8(R)$ and obtain a new $TUC_4C_8(R)$ nanotube with $2q-2$ rows of edges. Since E_{31} is the $(1,1)$ entry of this lattice and $2q-2\le p$, we have $N(E_{31})=R+4q-4$, where R is the number of edges $E(T_{E_{31}})$ in the first and the second row of edges of $TUC_4C_8(R)$ nanotube. On the other hand, $E_{1(2p-1)},E_{2(2p)},E_{1(p+1)},E_{2(p+1)}$ are only edges of $TUC_4C_8(R)$ in the first and the second row of edges that belong to $N(E_{31})$. Therefore $N(E_{31})=4q$. If we continue this method, we have $N(E_{11})=N(E_{21})=\ldots=N(E_{(2q)1})=4q.$

Now suppose $2q>p$ and $2p>2q+1$. For computing of the value $N(E_{11})$, we consider $A=\{E_{11},E_{22},\ldots,E_{(pp)},E_{1(p+1)},\ldots,E_{p(p+1)}\}$. Suppose that $E_{ii}=u_iv_i$, $1\le i\le p$, we have $d(u_1,u_i)=d(v_1,v_i), d(u_1,u_i)<d(v_1,u_i), d(v_1,v_i)<d(u_1,v_i)$ for $1\le i\le p.$ As a similar way $E_{i(p+1)}\in E(T_{E_{11}})$ for $1\le i\le p$, and therefore $N(E_{11})\ge |A|=2p$ and as the same above, we have $N(E_{11})=2p$. We consider the edge E_{22}. If $2q\ge p+1$, then with considering,

$$B = \{E_{11}, E_{22}, \ldots, E_{(p+1)(p+1)}, E_{1(p+2)}, E_{2(p+2)}, \ldots, E_{(p+1)(p+2)}\}$$

we have $N(E_{21}) \geq |B| = 2p+2$ and again we can show that $N(E_{21}) = 2p+2$. Now we consider the edge E_{31} .If $2q \geq p+2$, then to find $N(E_{31})$, we delete the first and the second row of edges of the $TUC_4C_8(R)$ and obtain a new $TUC_4C_8(R)$ nanotube with $2q-2$ rows of edges. Since E_{31} is the $(1,1)$ entry of this lattice, we have $N(E_{31}) = R + 2p$, where R is the number of edges $E(T_{E_{31}})$ in the first and second row of edges of T. $E_{1(2p-1)}, E_{2(2p)}, E_{1(p+1)}, E_{2(p+1)}$ are the only edges of $TUC_4C_8(R)$ in the first and the second row of edges that belong to $N(E_{31})$. Therefore $N(E_{31}) = 2p+4$. If we continue this method, then we have $N(E_{k1}) = 2p + 2(k-1)$ for $k \leq 2q - p + 1$. Let e be an oblique edge in the k-th row of edges in Figure3 and $2q - p + 2 \leq k \leq p - 1$. A part of the elements of $N(e)$ can be in $p-1$ rows of edges before k and since $k \leq p-1$, this elements exist in all of the rows of edges before k. Also since there exist two elements of $N(e)$ in each row of edges, $2k-2$ elements of $N(e)$ are in $k-1$ rows of edges before k. The other part of the elements of $N(e)$ can be in p rows of edges equal to or greater than to k. For $2q - p + 2 \leq k \leq p - 1$, we have $k + p - 1 > 2q$ and therefore all of rows of edges greater than or equal to k, contains some elements of $N(e)$. Since there exist two elements of $N(e)$ in each row of edges, we have $N(e) = 4q$. Now let e be in the k-th row of edges where $p \leq k \leq 2q$. By the symmetric property in the $TUC_4C_8(R)$ nanotube, we have $N(e) = 2p + 2(2q - k)$.

Let $2p - 1 \leq 2q$. If e is in the k-th row of edges, $1 \leq k \leq p$, similar to last case we have $N(e) = 2p + 2(k-1)$.

Let e be an oblique edge in the k-th row of edges in Figure3 and $p + 1 \leq k \leq 2q - p$. A part of the elements of $N(e)$ can be in $p-1$ rows of edges before k and since $p - 1 < k$, these elements exist in $p-1$ rows of edges before k. Also since there exist two elements of $N(e)$ in each row of edges, $2p-2$ elements of $N(e)$ are in $p-1$ rows of edges before k. The other part of the elements of $N(e)$ can be in p rows of edges equal to or greater than to k. For $p + 1 \leq k \leq 2q - p$, we have $k + p - 1 < 2q$ and therefore p rows of edges greater than or equal to k, contains some elements of $N(e)$.

Since there exist two elements of $N(e)$ in each row of edges, $2p$ elements of $N(e)$ are in p rows of edges equal to or greater than to k. Hence we have $N(e)=4p-2$. If e is in the k-th row of edges , $2q-p+1\le k\le 2q$ by the symmetric property in the $TUC_4C_8(R)$ nanotube, we have $N(e)=2p+2(2q-k)$. █

Now we assume that p is odd .Therefore, we have the following lemmas:

Lemma 2.4. If p is a horizontal edge, then $N(e)=q$.

Proof. Suppose $e=U_{ij}U_{i(j+1)}$ is an arbitrary horizontal edge of i-th row of vertices in $TUC_4C_8(R)$ nanotube. In this case, for every k, $k=2,5,\ldots,3q-1$, we have $d(U_{ij},U_{kj})=d(U_{i(j+1)},U_{k(j+1)})$ and also $d(U_{ij},U_{kj})<d(U_{i(j+1)},U_{kj})$ and $d(U_{i(j+1)},U_{k(j+1)})<d(U_{ij},U_{k(j+1)})$. Therefore if we suppose $A=\{U_{kj},U_{k(j+1)}\,|\,k=2,5,\ldots,3q-1\}$ we have $N(e)=|E(A)|=q$. █

Lemma 2.5. If e is a vertical edge, then $N(e)=p$.

Proof. The proof is similar to lemma 2.2. █

Lemma 2.6. If e is an oblique edge in the k th row of edges, then we have

1) If $2q\le p$, then $N(e)=2q$

2) If $2q\ge p$, then we have two cases:

Case1: If $2p-1>2q$, then

$$N(e)=\begin{cases} p+k-1 & 1\le k\le 2q-p+1 \\ 2q & 2q-p+2\le k\le p-1 \\ p+2q-k & p\le k\le 2q \end{cases}$$

Case2: If $2p-1\le 2q$, then

$$N(e)=\begin{cases} p+k-1 & 1\le k\le p \\ 2p-1 & p+1\le k\le 2q-p \\ p+2q-k & 2q-p+1\le k\le 2q \end{cases}$$

Proof. The proof is similar to Lemma 2.3. █

We now ready to prove the main result of the paper.

Main Theorem. The PI index of $TUC_4C_8(R)$ nanotube is as follows:

If p is even, then we have

$$PI(TUC_4C_8(R)) = \begin{cases} 36p^2q^2 - 13p^2q - 18pq^2 + 2p^2 & 2q \le p \\ 36p^2q^2 - 29p^2q + 8pq - 2pq^2 + 4p^3 - 3p^2 & 2q > p \end{cases}$$

If p is odd, then we have

$$PI(TUC_4C_8(R)) = \begin{cases} 36p^2q^2 - 13p^2q - 9pq^2 + 2p^2 & 2q \le p \\ 36p^2q^2 - 21p^2q + 4pq - pq^2 + 2p^3 & 2q > p \end{cases}$$

Proof. Since $PI(G) = |E|^2 - \sum_{e \in E} N(e)$, it is enough to compute $\sum_{e \in E} N(e)$. Suppose A, B and C are the sets of all horizontal, vertical and oblique edges of T, respectively. Thus we have $PI(TUC_4C_8(R)) = |E|^2 - \sum_{e \in A} N(e) - \sum_{e \in B} N(e) - \sum_{e \in C} N(e)$.

If p is even, then we have $\sum_{e \in A} N(e) = 2pq^2$ and $\sum_{e \in B} N(e) = p^2q - p^2$. Now if $2q \le p$, then we have $\sum_{e \in C} N(e) = 16pq^2$ and for $2q > p$ we have

$$\begin{aligned} \sum_{e \in C} N(e) &= 2p\left[2\sum_{i=1}^{2q-p+1}[2p + 2(i-1)] + \sum_{i=2q-p+2}^{p-1} 4q\right] \\ &= 2p\left[2\sum_{i=1}^{p}[2p + 2(i-1)] + \sum_{i=p+1}^{2q-p}(4p-2)\right] \\ &= 16p^2q + 4p^2 - 4p^3 - 8pq \end{aligned}$$

Assume that p is odd so $\sum_{e \in A} N(e) = pq^2$ and $\sum_{e \in B} N(e) = p^2q - p^2$. Now if $2q \le p$, then we have $\sum_{e \in C} N(e) = 8pq^2$. And for $2q > p$,

$$\begin{aligned} \sum_{e \in C} N(e) &= 2p\left[2\sum_{i=1}^{2q-p+1}[p + i - 1] + \sum_{i=2q-p+2}^{p-1} 2q\right] \\ &= 2p\left[2\sum_{i=1}^{p}[p + i - 1] + \sum_{i=p+1}^{2q-p}(2p-1)\right] \\ &= 8p^2q + 2p^2 - 2p^3 - 4pq \end{aligned}$$

So if p is even, then we have

$$PI(TUC_4C_8(R)) = \begin{cases} 36p^2q^2 - 13p^2q - 18pq^2 + 2p^2 & 2q \le p \\ 36p^2q^2 - 29p^2q + 8pq - 2pq^2 + 4p^3 - 3p^2 & 2q > p \end{cases}$$

If p is odd then, we have

$$PI\left(TUC_4C_8(R)\right)=\begin{cases} 36p^2q^2-13p^2q-9pq^2+2p^2 & 2q\le p \\ 36p^2q^2-21p^2q+4pq-pq^2+2p^3 & 2q>p \end{cases}$$

and the proof is completed. ∎

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