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The PI Index of $TUVC_6[2p, q]$

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Abstract

The PI index is a graph invariant defined as the summation of the sums of $n_{eu}(e|G)$ and $n_{ev}(e|G)$ over all the edges $e = uv$ of a connected graph G, i.e.,$PI(G) = \sum_{e\in E(G)}[n_{eu}(e|G) + n_{ev}(e|G)]$, where $n_{eu}(e|G)$ is the number of edges of G lying closer to u than to v and $n_{ev}(e|G)$ is the number of edges of G lying closer to v than to u. A formula for calculating the PI index of $TUVC_6[2p, q]$ is given.

1 Introduction

The structure of a molecule could be represented in a variety of ways. The information on the chemical constitution of molecule is conventionally represented by a molecular graph. And graph theory was successfully provided

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the chemist with a variety of very useful tools, namely, topological index. The first reported use of a topological index in chemistry was by Wiener [1] in the study of paraffin boiling points. Since then, in order to model various molecular properties, many topological indices have been designed [2]. Such a proliferation is still going on and is becoming counter productive.

In 1990s, Gutman [3] and coworkers [4] have introduced a generalization of the Wiener index (W) for cyclic graphs called Szeged index (Sz). The main advantage of the Szeged index is that it is a modification of W; otherwise, it coincides with the Wiener index. In [5,6] another topological index was introduced and it was named Padmakar-Ivan index, abbreviated as PI. This new topological index, PI, does not coincide with the Wiener index. Deng [9] gave a formula for calculating the PI index of catacondensed hexagonal systems and the extremal catacondensed hexagonal systems with the minimum or maximum PI index. Ashrafi and Loghman [10] computed the PI index of zig-zag polyhex nanotubes.

The primary aim of this article is to introduce the method for calculation of PI index for $TUVC_6[2p, q]$. Our notation is mainly taken from [7,8]. Throughout this paper $G = TUVC_6[2p, q]$ denotes an armchair polyhex nanotube, see Figure 1.

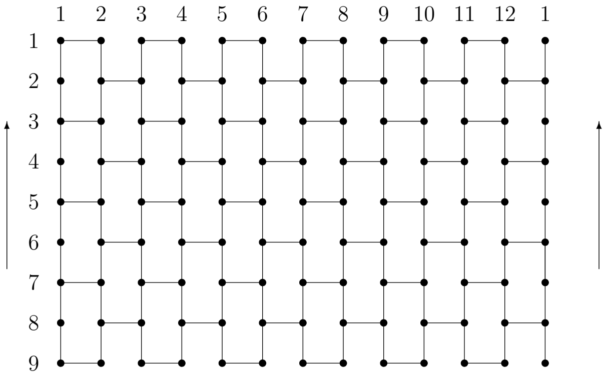

Figure 1. $G = TUVC_6[2p, q]$ with p=6 and q=9

2 The definition of PI index

Let G be a connected and undirected graph without multiple edges or loops. By $V(G)$ and $E(G)$ we denote the vertex and edge sets, respectively, of G.

If $G' = (V', E')$ is a subgraph of $G = (V, E)$ and contains all the edges of G that join two vertices in V', i.e., E' is the set of edges between vertices of

V', then G' is an induced subgraph of G by V' and is denoted by $G[V']$.

Let $e = xy$ be an edge of G, X is the subset of vertices of $V(G)$ which are closer to x than y and Y is the subset of vertices which are closer to y than x, i.e.,

$$X = \{v|v \in V(G), d_G(x,v) < d_G(y,v)\}$$
$$Y = \{v|v \in V(G), d_G(y,v) < d_G(x,v)\}$$

where $d_G(u,v)$ denotes the distance between vertices u and v of G. Let $G[X] = (X, E_1)$ and $G[Y] = (Y, E_2)$,

$$n_1(e) = |E_1|, \qquad n_2(e) = |E_2|$$

Here, $n_1(e)$ is the number of edges nearer to x than y and $n_2(e)$ is the number of edges nearer to y than x.

Then the PI index of G is defined as

$$PI(G) = \sum_{e \in E(G)} [n_1(e) + n_2(e)]$$

In all cases of cyclic graphs, there are edges equidistant to the both ends of the edges. Such edges are not taken into account. Let $[X, Y]$ denote the subset of edges between X and Y, $n(e) = |[X, Y]|$. Then $n(e) = |E(G)| - (n_1(e) + n_2(e))$ is the number of edges equidistant to the both ends of e for a bipartite connected graph G (It includes the current edge e in $n(e)$). And

$$PI(G) = |E(G)|^2 - \sum_{e \in E(G)} n(e)$$

Therefore, for computing the PI index of a bipartite connected graph G, it is enough to calculate $n(e)$ for each $e \in E(G)$.

To calculate $n(e)$, we consider two cases that e is horizontal or vertical.

Lemma 1. Let e be any horizontal edge between columns j and j+1 in $G = TUVC_6[2p, q]$, $1 \le j \le 2p$, where $2p + 1 \equiv 1(mod 2p)$.

(i)If q is odd, then $n(e) = \begin{cases} q, & \text{if p is odd;} \\ q+1, & \text{if p is even and j is odd;} \\ q-1, & \text{if p is even and j is even.} \end{cases}$

(ii) If q is even, then $n(e) = q$.

(iii) Let H be the sum of $n(e)$ over all horizontal edges in G. Then

$$H = \begin{cases} pq^2, & \text{q is even;} \\ pq^2 + p, & \text{q is odd and p is even;} \\ pq^2, & \text{q and p are odd.} \end{cases}$$

Proof. Let x_{ij} be the vertex on row i and column j, $e = x_{ij}x_{i,j+1}$. X is the subset of vertices of $V(G)$ which are closer to x_{ij} than $x_{i,j+1}$ and Y is the subset of vertices which are closer to $x_{i,j+1}$ than x_{ij}. It is obvious that X consists of the vertices on columns $j, j-1, \cdots, j-p+1$, and Y consists of the vertices on columns $j+1, j+2, \cdots, j+p$, where $j \pm k$ will be taken $j \pm k(mod 2p)$ if $j \pm k \notin \{1, 2, \cdots, 2p\}$. So, $[X, Y]$ is the set of the edges between columns j and j+1 and the edges between columns j-p+1 and j+p. Note that the number m_j of the edges between columns j and j+1 is

$$m_j = \begin{cases} \frac{q}{2}, & \text{if q is even;} \\ \frac{q+1}{2}, & \text{if q is odd and j is odd;} \\ \frac{q-1}{2}, & \text{if q is odd and j is even.} \end{cases}$$

So, we have

(i)if q is odd, then $n(e) = \begin{cases} q, & \text{if p is odd;} \\ q+1, & \text{if p is even and j is odd;} \\ q-1, & \text{if p is even and j is even.} \end{cases}$

(ii) if q is even, then $n(e) = q$.

(iii) Let H_j be the sum of $n(e)$ over all horizontal edges between columns j and j+1.

If q is even, then $H_j = \frac{q}{2} \times q = \frac{q^2}{2}$, and $H = \sum_{j=i}^{2p} H_j = 2p \times \frac{q^2}{2} = pq^2$.

If q is odd and p is even, then

$$H_j = \begin{cases} \frac{(q+1)^2}{2}, & \text{j is odd;} \\ \frac{(q-1)^2}{2}, & \text{j is even.} \end{cases}$$

and $H = \sum_{j=i}^{2p} H_j = p(q^2 + 1)$.

If q and p are all odd, then

$$H_j = \begin{cases} \frac{q(q+1)}{2}, & \text{j is odd;} \\ \frac{q(q-1)}{2}, & \text{j is even.} \end{cases}$$

and $H = \sum_{j=i}^{2p} H_j = pq^2$.

So, $H = \begin{cases} pq^2, & \text{q is even;} \\ pq^2 + p, & \text{q is odd and p is even;} \\ pq^2, & \text{q and p are odd.} \end{cases}$

To calculating $n(e)$ for the vertical edges e, we need only calculate $n(e)$ for $e = x_{11}x_{21}$, so is $n(e)$ for the vertical edges between rows 1 and 2 and the vertical edges between rows q-1 and q by the symmetry of G, and $n(e)$ can also be calculated for the vertical edges between rows i and i+1 by using two intersectional $TUVC_6$s.

3 The distances in $TUVC_6[2p, q]$

For $e = x_{11}x_{21}$, we will give a formula for calculating the distances from x_{11} (or x_{21}) in the following, and find the subset X of vertices of $V(G)$ which are closer to x_{11} than x_{21} and the subset Y of vertices which are closer to x_{21} than x_{11}.

We first consider two graphs G_1 and G_2, where G_1 is obtaining from $G = TUVC_6[2p, q]$ by deleting the horizontal edges between columns 1 and 2p (see Figure 2) and G_2 is obtaining from $G = TUVC_6[2p, q]$ by deleting the horizontal edges between columns 1 and 2 (see Figure 3), and the distances from x_{11} (or x_{21}) in G is the minimum of the ones in G_1 and in G_2.

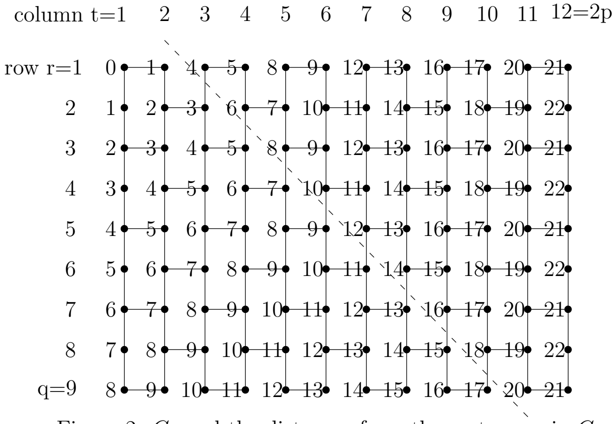

Figure 2. G_1 and the distances from the vertex x_{11} in G_1.

Table 1. The values of $d_1(x_{11}, x_{rt}) - t$.

	1	2	3	4	5	6	7	8	9	10	11	12
1	-1	-1	1	1	3	3	5	5	7	7	9	9
2	0	0	0	2	2	4	4	6	6	8	8	10
3	1	1	1	1	3	3	5	5	7	7	9	9
4	2	2	2	2	2	4	4	6	6	8	8	10
5	3	3	3	3	3	3	5	5	7	7	9	9
6	4	4	4	4	4	4	4	6	6	8	8	10
7	5	5	5	5	5	5	5	5	7	7	9	9
8	6	6	6	6	6	6	6	6	6	8	8	10
9	7	7	7	7	7	7	7	7	7	7	9	9

Now, we calculate the distances from x_{11} in G_1 as showing in Figure 2. And Table 1 lists the values of $d_1(x_{11}, x_{rt}) - t$, where $d_1(x_{11}, x_{rt})$ is the distance between x_{11} and x_{rt} in G_1.

From Table 1, we can see that

$$d_1(x_{11}, x_{rt}) - t = \begin{cases} r-2, & 1 \le t \le r+1; \\ 2[\frac{t}{2}] - 2, & t \ge r+2 \text{ and r is even}; \\ 2[\frac{t-1}{2}] - 1, & t \ge r+2 \text{ and r is odd}. \end{cases}$$

So, we have

Lemma 2. $d_1(x_{11}, x_{rt}) = \begin{cases} t+r-2, & 1 \le t \le r+1; \\ t-2+2[\frac{t}{2}], & t \ge r+2 \text{ and r is even}; \\ t-1+2[\frac{t-1}{2}], & t \ge r+2 \text{ and r is odd}. \end{cases}$

Lemma 2 can be easily proved by the inductive method on t, we omit here.

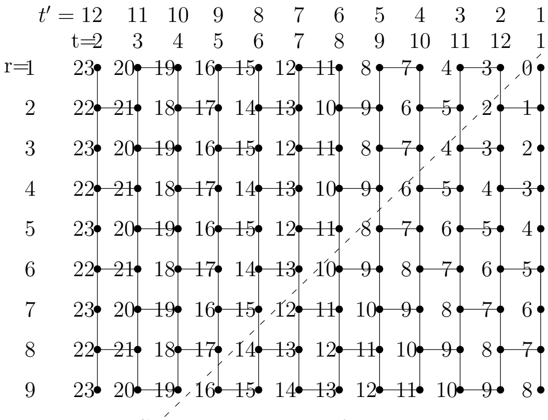

Figure 3. G_2 and the distances from the vertex x_{11} in G_2.

Table 2. The values of $d_2(x_{11}, x_{rt'}) - t'$.

	1	2	3	4	5	6	7	8	9	10	11	12
1	-1	-1	1	1	3	3	5	5	7	7	9	9
2	0	0	0	2	2	4	4	6	6	8	8	10
3	1	1	1	1	3	3	5	5	7	7	9	9
4	2	2	2	2	2	4	4	6	6	8	8	10
5	3	3	3	3	3	3	5	5	7	7	9	9
6	4	4	4	4	4	4	4	6	6	8	8	10
7	5	5	5	5	5	5	5	5	7	7	9	9
8	6	6	6	6	6	6	6	6	6	8	8	10
9	7	7	7	7	7	7	7	7	7	7	9	9

Similarly, we calculate the distances from x_{11} in G_2 as showing in Figure 3. And Table 2 lists the values of $d_2(x_{11}, x_{rt'}) - t'$, where $d_2(x_{11}, x_{rt'})$ is the distance between x_{11} and $x_{rt'}$ in G_2 and

$$t' = \begin{cases} 1, & t = 1 \\ 2p+2-t, & t \geq 2 \end{cases}$$

From Table 2, we can see that

$$d_2(x_{11}, x_{rt'}) - t' = \begin{cases} r-2, & 1 \leq t' \leq r; \\ 2[\frac{t'-1}{2}], & t' \geq r+1 \text{ and r is even;} \\ 2[\frac{t'}{2}]-1, & t' \geq r+1 \text{ and r is odd.} \end{cases}$$

So, we have

Lemma 3. $d_2(x_{11}, x_{rt'}) = \begin{cases} t'+r-2, & 1 \leq t' \leq r; \\ t'+2[\frac{t'-1}{2}], & t' \geq r+1 \text{ and r is even;} \\ t'-1+2[\frac{t'}{2}], & t' \geq r+1 \text{ and r is odd.} \end{cases}$

and

$$d_2(x_{11}, x_{rt}) = \begin{cases} 2p+r-t, & t \leq 2p+2-r (\text{t=1 if r=1}); \\ 2p+2-t+2[\frac{2p+1-t}{2}], & t \leq 2p+1-r \text{ and r is even;} \\ 2p+1-t+2[\frac{2p+2-t}{2}], & t \leq 2p+1-r \text{ and r is odd.} \end{cases}$$

Since the vertex x_{rt} in G_1 and the vertex $x_{rt'}$ in G_2 are identical, we have

Lemma 4. (i)If $t = 1$, then $d_1(x_{11}, x_{rt}) = d_2(x_{11}, x_{rt'})$;
(ii) If $2 \leq t \leq p+1$, then $d_1(x_{11}, x_{rt}) \leq d_2(x_{11}, x_{rt'})$;
(iii) If $p+2 \leq t \leq 2p$, then $d_1(x_{11}, x_{rt}) > d_2(x_{11}, x_{rt'})$.

Proof. (i) If $t = 1$, then $t' = 1$ and $d_1(x_{11}, x_{rt}) = d_2(x_{11}, x_{rt'})$ from Lemmas 2 and 3.

(ii) $2 \leq t \leq p+1$.

Case 1. $t \geq r+2$. Then $r+2 \leq t \leq p+1$ and $r \leq p-1$, $t' = 2p+2-t \geq p+1 \geq r+2$.

(a) If r is even, then by Lemmas 2 and 3

$$\begin{aligned} d_2(x_{11}, x_{rt'}) - d_1(x_{11}, x_{rt}) &= (t'+2[\tfrac{t'-1}{2}]) - (t-2+2[\tfrac{t}{2}]) \\ &= 4p+6-2t+2([\tfrac{-t-1}{2}]-[\tfrac{t}{2}]) \\ &\geq 4p+4-4t \geq 0 \end{aligned}.$$

(b) If r is odd, then by Lemmas 2 and 3

$$\begin{aligned} d_2(x_{11}, x_{rt'}) - d_1(x_{11}, x_{rt}) &= (t'-1+2[\tfrac{t'}{2}]) - (t-1+2[\tfrac{t-1}{2}]) \\ &= 4p+4-2t+2([\tfrac{-t}{2}]-[\tfrac{t-1}{2}]) \\ &\geq 4p+4-4t \geq 0 \end{aligned}.$$

Case 2. $2 \leq t \leq r+1$.

(a) If $t' \leq r$, then by Lemmas 2 and 3

$$\begin{aligned} d_2(x_{11}, x_{rt'}) - d_1(x_{11}, x_{rt}) &= (r+t'-2) - (r+t-2) \\ &= t'-t = 2p+2-2t \geq 0 \end{aligned}.$$

(b) If $t' \geq r+1$, i.e., $2p+2-t \geq r+1$, then $r+t \leq 2p+1$.

When r is even, by Lemmas 2 and 3 we have

$$\begin{aligned} d_2(x_{11}, x_{rt'}) - d_1(x_{11}, x_{rt}) &= (t'+2[\tfrac{t'-1}{2}]) - (r+t-2) \\ &\geq (r+1+2[\tfrac{r}{2}]) - (2r-1) > 0 \end{aligned}.$$

When r is odd, by Lemmas 2 and 3 we have

$$\begin{aligned} d_2(x_{11}, x_{rt'}) - d_1(x_{11}, x_{rt}) &= (t' - 1 + 2[\tfrac{t'}{2}]) - (r + t - 2) \\ &\geq (r + 2[\tfrac{r+1}{2}]) - (2r - 1) > 0 \end{aligned}.$$

(iii) $p + 2 \leq t \leq 2p$. Then $2 \leq t' = 2p + 2 - t \leq p$.

Case 1. $t' \geq r + 1$. Then $r + 1 \leq t' \leq p$, $r \leq p - 1$, $t = 2p + 2 - t' \geq p + 2 \geq r + 3$.

(a) If r is even, then by Lemmas 2 and 3

$$\begin{aligned} d_1(x_{11}, x_{rt}) - d_2(x_{11}, x_{rt'}) &= (t - 2 + 2[\tfrac{t}{2}]) - (t' + 2[\tfrac{t'-1}{2}]) \\ &= (2p - t' + 2([\tfrac{2p+2-t'}{2}]) - (t' + 2[\tfrac{t'-1}{2}]) \\ &= 4p + 2 - 2t' + 2([\tfrac{-t'}{2}] - [\tfrac{t'-1}{2}]) \\ &\geq 4p + 2 - 4t' > 0 \end{aligned}.$$

(b) If r is odd, then by Lemmas 2 and 3

$$\begin{aligned} d_1(x_{11}, x_{rt}) - d_2(x_{11}, x_{rt'}) &= (t - 1 + 2[\tfrac{t-1}{2}]) - (t' - 1 + 2[\tfrac{t'}{2}]) \\ &= 4p + 4 - 2t' + 2([\tfrac{-t'-1}{2}] - [\tfrac{t'}{2}]) \\ &\geq 4p + 2 - 4t' > 0 \end{aligned}.$$

Case 2. $2 \leq t' \leq r$.

(a) If $t \leq r + 1$, then by Lemmas 2 and 3

$$\begin{aligned} d_1(x_{11}, x_{rt}) - d_2(x_{11}, x_{rt'}) &= (r + t - 2) - (r + t' - 2) \\ &= t - t' = 2p + 2 - 2t' > 0 \end{aligned}.$$

(b) If $t \geq r + 2$, then by Lemmas 2 and 3

$$\begin{aligned} d_1(x_{11}, x_{rt}) - d_2(x_{11}, x_{rt'}) &= (t - 2 + 2[\tfrac{t}{2}]) - (r + t' - 2) \\ &\geq (r + 2[\tfrac{r+2}{2}]) - (2r - 2) > 0 \end{aligned}$$

when r is even; and

$$\begin{aligned} d_1(x_{11}, x_{rt}) - d_2(x_{11}, x_{rt'}) &= (t - 1 + 2[\tfrac{t-1}{2}]) - (r + t' - 2) \\ &\geq (r + 1 + 2[\tfrac{r+1}{2}]) - (2r - 2) > 0 \end{aligned}$$

when r is odd.

Now by Lemma 4, we can directly give a formula of calculating the distances from x_{11} in $G = TUVC_6[2p, q]$.

Theorem 1. (i) $d(x_{11}, x_{rt}) = d_1(x_{11}, x_{rt})$ if $1 \leq t \leq p + 1$;
(ii) $d(x_{11}, x_{rt}) = d_2(x_{11}, x_{rt})$ if $p + 2 \leq t \leq 2p$.

Next, we consider the distances from x_{21}. Using the same methods as above, we can calculate the distances from x_{21} in G_1 as showing in Figure 4 and list the values of $d_1(x_{21}, x_{rt}) - t$ in Table 3.

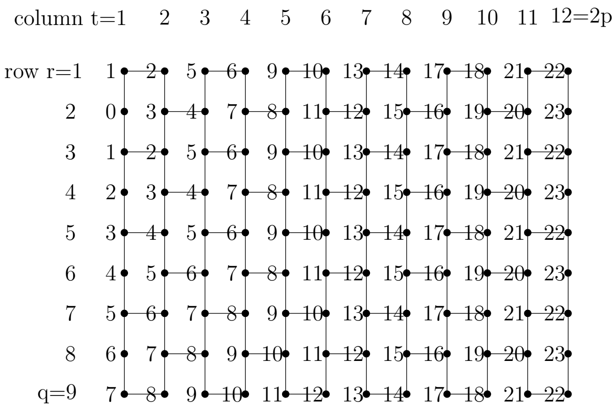

Figure 4. G_1 and the distances from the vertex x_{21} in G_1.

Table 3. The values of $d_1(x_{21}, x_{rt}) - t$.

	1	2	3	4	5	6	7	8	9	10	11	12
1	0	0	2	2	4	4	6	6	8	8	10	10
2	-1	1	1	3	3	5	5	7	7	9	9	11
3	0	0	2	2	4	4	6	6	8	8	10	10
4	1	1	1	3	3	5	5	7	7	9	9	11
5	2	2	2	2	4	4	6	6	8	8	10	10
6	3	3	3	3	3	5	5	7	7	9	9	11
7	4	4	4	4	4	4	6	6	8	8	10	10
8	5	5	5	5	5	5	5	7	7	9	9	11
9	6	6	6	6	6	6	6	6	8	8	10	10

If $r \geq 2$, we can see that from Table 3

$$d_1(x_{21}, x_{rt}) - t = \begin{cases} r-3, & 1 \leq t \leq r-1; \\ 2[\frac{t}{2}] - 1, & t \geq r \text{ and r is even}; \\ 2[\frac{t-1}{2}], & t \geq r \text{ and r is odd}. \end{cases}$$

So, we have

Lemma 5. If $r \geq 2$, then

$$d_1(x_{21}, x_{rt}) = \begin{cases} t+r-3, & 1 \leq t \leq r-1; \\ t-1+2[\frac{t}{2}], & t \geq r \text{ and r is even}; \\ t+2[\frac{t-1}{2}], & t \geq r \text{ and r is odd}. \end{cases}$$

and $d_1(x_{21}, x_{1t}) = d_1(x_{21}, x_{3t})$ if $r = 1$.

Also, we can calculate the distances from x_{21} in G_2 as showing in Figure 5 and list the values of $d_2(x_{21}, x_{rt'}) - t'$ in Table 4.

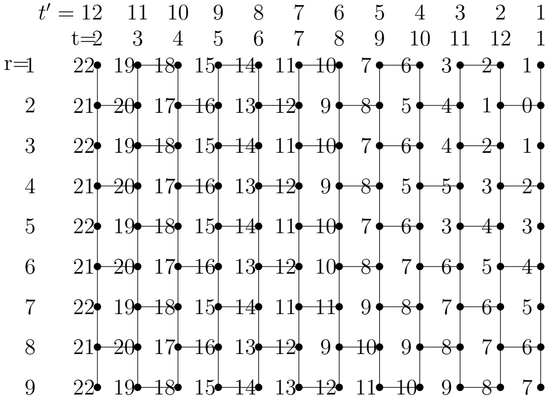

Figure 5. G_2 and the distances from the vertex x_{21} in G_2.

Table 4. The values of $d_2(x_{21}, x_{rt'}) - t'$.

	1	2	3	4	5	6	7	8	9	10	11	12
1	0	0	0	2	2	4	4	6	6	8	8	10
2	-1	-1	1	1	3	3	5	5	7	7	9	9
3	0	0	0	2	2	4	4	6	6	8	8	10
4	1	1	1	1	3	3	5	5	7	7	9	9
5	2	2	2	2	2	4	4	6	6	8	8	10
6	3	3	3	3	3	3	5	5	7	7	9	9
7	4	4	4	4	4	4	4	6	6	8	8	10
8	5	5	5	5	5	5	5	5	7	7	9	9
9	6	6	6	6	6	6	6	6	6	8	8	10

If $r \geq 2$, we can see that from Table 4

$$d_2(x_{21}, x_{rt'}) - t' = \begin{cases} r-3, & 1 \leq t' \leq r; \\ 2[\frac{t'-1}{2}] - 1, & t' \geq r+1 \text{ and r is even}; \\ 2[\frac{t'}{2}] - 2, & t' \geq r+1 \text{ and r is odd}. \end{cases}$$

So, we have

Lemma 6. If $r \geq 2$, then

$$d_2(x_{21}, x_{rt'}) = \begin{cases} t' + r - 3, & 1 \le t' \le r; \\ t' - 1 + 2[\frac{t'-1}{2}], & t' \ge r + 1 \text{ and r is even}; \\ t' - 2 + 2[\frac{t'}{2}], & t' \ge r + 1 \text{ and r is odd}. \end{cases}$$

and $d_2(x_{21}, x_{1t'}) = d_1(x_{21}, x_{3t'})$ if $r = 1$.

As in Lemma 4, we can prove the following result by using Lemmas 5 and 6.

Lemma 7. (i)If $t = 1$, then $d_1(x_{21}, x_{rt}) = d_2(x_{21}, x_{rt'})$;
(ii) If $2 \le t \le p$, then $d_1(x_{21}, x_{rt}) < d_2(x_{21}, x_{rt'})$;
(iii) If $p + 1 \le t \le 2p$, then $d_1(x_{21}, x_{rt}) \ge d_2(x_{21}, x_{rt'})$.

And now, we can give a formula of calculating the distances from x_{21} in $G = TUVC_6[2p, q]$ by Lemma 4.

Theorem 2. (i) $d(x_{21}, x_{rt}) = d_1(x_{21}, x_{rt})$ if $1 \le t \le p$;
(ii) $d(x_{21}, x_{rt}) = d_2(x_{21}, x_{rt})$ if $p + 1 \le t \le 2p$.

4 A formula for calculating PI index of $TUVC_6[2p, q]$

In this section, we first find the subset X of vertices of $V(G)$ which are closer to x_{11} than x_{21} and the subset Y of vertices which are closer to x_{21} than x_{11} in G, and give the formula of calculating $n(e)$ for all vertical edges e. And then we calculate the PI index of $TUVC_6[2p, q]$.

Let $X = \{x_{rt} | x_{rt} \in G, d(x_{11}, x_{rt}) < d(x_{21}, x_{rt})\}$, and $Y = \{x_{rt} | x_{rt} \in G, d(x_{11}, x_{rt}) > d(x_{21}, x_{rt})\}$. Since G is a bipartite graph, $Y = V(G) - X$.

A example for $p = 6$ and $q = 9$ is showed in Figure 6, where X is the set of large dots and Y is the set of small dots.

Lemma 8. (i) If p is even, then

$$X = \{x_{rt} | 1 \le r \le t \le p \text{ and } r \le q\} \bigcup \{x_{r,p+1} | r = 2, 4, \cdots, p \text{ and } r \le q\};$$

(ii) If p is odd, then

$$X = \{x_{rt} | 1 \le r \le t \le p \text{ and } r \le q\} \bigcup \{x_{r,p+1} | r = 1, 3, \cdots, p \text{ and } r \le q\};$$

(iii) $n(e) = \begin{cases} 2p, & q \ge p + 1 \\ 2(q - 1), & q \le p. \end{cases}$

where $e = x_{11}x_{21}$.

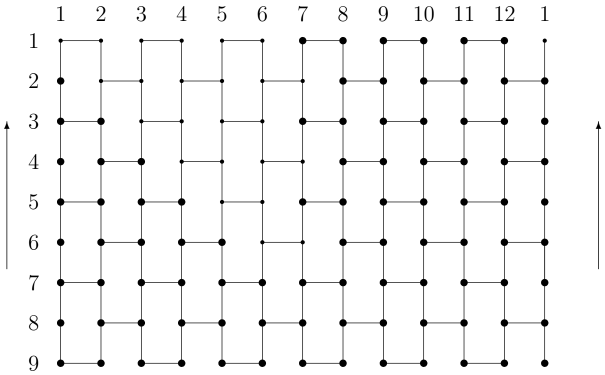

Figure 6.

Proof. Let $\Delta = d(x_{11}, x_{rt}) - d(x_{21}, x_{rt})$.

Case 1. $t \le p$. Then by Theorems 1 and 2, $\Delta = d_1(x_{11}, x_{rt}) - d_1(x_{21}, x_{rt})$.

Case 1.1. If $r \le t-2$, then $r \le p-2$, $t' = 2p+2-t \ge p+2 \ge r+4$. From Lemmas 2 and 5,

$$\Delta = \begin{cases} (t-2+2[\frac{t}{2}]) - (t-1+2[\frac{t}{2}]), & \text{r is even;} \\ (t-1+2[\frac{t-1}{2}]) - (t+2[\frac{t-1}{2}]), & \text{r is odd} \end{cases}$$
$$= -1 < 0.$$

So, $d(x_{11}, x_{rt}) < d(x_{21}, x_{rt})$, and $x_{rt} \in X$.

Case 1.2. If $t-1 \le r \le t$, then $t' = 2p+2-t \ge p+2 \ge r+2$. From Lemmas 2 and 5,

$$\Delta = \begin{cases} (r+t-2) - (t-1+2[\frac{t}{2}]) = r-1-2[\frac{t}{2}], & \text{r is even;} \\ (r+t-2) - (t+2[\frac{t-1}{2}]) = r-2-2[\frac{t-1}{2}], & \text{r is odd} \end{cases}$$
$$< 0.$$

So, $d(x_{11}, x_{rt}) < d(x_{21}, x_{rt})$, and $x_{rt} \in X$.

Case 1.3. If $r \ge t+1$, then by Lemmas 2 and 5,

$$\Delta = (t+r-2) - (t+r-3) = 1 > 0.$$

So, $d(x_{11}, x_{rt}) > d(x_{21}, x_{rt})$, and $x_{rt} \notin X$.

Case 2. $t = p+1$. Then by Theorems 1 and 2, $\Delta = d_1(x_{11}, x_{rt}) - d_2(x_{21}, x_{rt})$.

Case 2.1. If $r \le t-2$, then $t' \ge r+4$. From Lemmas 2 and 6,

$$\Delta = (t-2+2[\frac{t}{2}]) - (t'-1+2[\frac{t'-1}{2}]) = -1 + 2([\frac{t}{2}] - [\frac{t-1}{2}])$$
$$= \begin{cases} -1, & \text{p is even (i.e., t is odd);} \\ 1, & \text{p is odd (i.e., t is even)} \end{cases}$$

when r is even; and

$\Delta = (t-1+2[\frac{t-1}{2}]) - (t'-2+2[\frac{t'}{2}]) = 1+2([\frac{t-1}{2}]-[\frac{t}{2}])$
$= \begin{cases} 1, & \text{p is even (i.e., t is odd);} \\ -1, & \text{p is odd (i.e., t is even)} \end{cases}$
when r is odd.

So, $x_{r,p+1} \in X$ if and only if the pairity of r and p are the same.

Case 2.2. If $r = t-1$, then $t' = r+1$. From Lemmas 2 and 6,
$\Delta = (r+t-2) - (t'-1+2[\frac{t'-1}{2}]) = r-1-2[\frac{t-1}{2}]$
$= \begin{cases} -1, & t = r+1 \text{ (i.e., } p = t-1 = r \text{ is even);} \\ 1, & t = r \text{ (i.e., } p = t-1 = r-1 \text{ is odd)} \end{cases}$
when r is even; and
$\Delta = (r+t-2) - (t'-2+2[\frac{t'}{2}]) = r-2[\frac{t}{2}]$
$= \begin{cases} -1, & t = r+1 \text{ (i.e., } p = t-1 = r \text{ is odd);} \\ 1, & t = r \text{ (i.e., } p = t-1 = r-1 \text{ is even)} \end{cases}$
when r is odd.

So, $x_{p,p+1} \in X$, $x_{p+1,p+1} \notin X$. (Thus, $x_{r,p+1} \in X$ if and only if the pairity of r and p are the same.)

Case 2.3. If $r \geq t$, then $t' \leq r$, by Lemmas 2 and 6,

$$\Delta = (t+r-2) - (t'+r-3) = 1 > 0.$$

So, $x_{r,p+1} \notin X$, $r \geq p+1$.

Case 3. $t \geq p+2$. Then by Theorems 1 and 2, $\Delta = d_2(x_{11}, x_{rt}) - d_2(x_{21}, x_{rt})$. From Lemmas 3 and 6, we have

$$\Delta = 1 > 0.$$

So, $x_{r,t} \notin X$ when $t \geq p+2$.

Summarizing above-mentioned, (i) and (ii) hold.

Since $n(e) = |[X, Y]|$ and $Y = V(G) - X$, (iii) holds from (i) and (ii).

In the following, we calculate $n(e)$ for vertical edges $e_r = x_{r1}x_{r+1,1}$ and $2 \leq r \leq q-2$. Let $TUVC_6[2p, r+1]$ be the polyhex nanotube consisting of the first $r+1$ rows of $TUVC_6[2p, q]$ and $TUVC_6[2p, q-r+1]$ the one consisting of the last $q-r+1$ rows of $TUVC_6[2p, q]$. Then the edge $e_r = x_{r1}x_{r+1,1}$ in $TUVC_6[2p, q]$ can be viewed as the vertical edge at row 1 and column 1 in $TUVC_6[2p, r+1]$ and also in $TUVC_6[2p, q-r+1]$. By Lemma 8 (iii), we have
$n_1(e_r) = \begin{cases} 2p, & r \geq p \\ 2r, & r \leq p-1. \end{cases}$
in $TUVC_6[2p, r+1]$. And
$n_2(e_r) = \begin{cases} 2p, & q-r \geq p \\ 2(q-r), & q-r \leq p-1. \end{cases}$
in $TUVC_6[2p, q-r+1]$. Since $n(e_r) = n_1(e_r) + n_2(e_r) - 2$, $2 \leq r \leq q-2$,

and using Lemma 8 for $r = 1$, we have the following result.

Lemma 9. Let $e = x_{r1}x_{r+1,1}$ be a vertical edge between row r and row $r+1$ in $TUVC_6[2p,q]$, $1 \le r \le q-1$.
(i) If $q \le p$, then $n(e) = 2q - 2$.
(ii) If $p+1 \le q < 2p$, then
$$n(e) = \begin{cases} 2p + 2r - 2, & 1 \le r \le q-p; \\ 2q - 2, & q-p+1 \le r \le p-1; \\ 2p + 2(q-r) - 2, & p \le r \le q-1. \end{cases}$$
(iii) If $q \ge 2p$, then
$$n(e) = \begin{cases} 2p + 2r - 2, & 1 \le r \le p-1; \\ 4p - 2, & p \le r \le q-p; \\ 2p + 2(q-r) - 2, & r \ge q-p+1. \end{cases}$$

Using Lemma 1 and 9, we can give a formula for calculating PI index of $TUVC_6[2p,q]$.

Theorem 3. The PI index of $G = TUVC_6[2p,q]$ is as follows:
If q is even, then

$$PI(G) = \begin{cases} 9p^2q^2 - 12p^2q + 4p^2 - 5pq^2 + 8pq - 4p, & q \le p; \\ 9p^2q^2 - 20p^2q + 4p^3 - pq^2 + 8p^2 + 4pq - 4p, & q \ge p+1. \end{cases}$$

If q is odd, then

$$PI(G) = \begin{cases} 9p^2q^2 - 12p^2q + 4p^2 - 5pq^2 + 8pq - 4p, & q \le p \text{ and p is odd;} \\ 9p^2q^2 - 20p^2q + 4p^3 - pq^2 + 8p^2 + 4pq - 4p, & q \ge p+1 \text{ and p is odd;} \\ 9p^2q^2 - 12p^2q + 4p^2 - 5pq^2 + 8pq - 3p, & q \le p \text{ and p is even;} \\ 9p^2q^2 - 20p^2q + 4p^3 - pq^2 + 8p^2 + 6pq - 5p, & q \ge p+1 \text{ and p is even;} \end{cases}$$

Proof. Let $N_1 = \sum_{r=1}^{q-1} n(e_r)$ be the sum of $n(e_r)$ over all vertical edges e_r of column 1 in $TUVC_6[2p,q]$. By Lemma 9,
(i) If $q \le p$, then $N_1 = 2(q-1)^2$;
(ii) If $p+1 \le q < 2p$, then
$$\begin{aligned} N_1 &= \sum_{r=1}^{q-p}(2p+2r-2) + \sum_{r=q-p+1}^{p-1}(2q-2) + \sum_{r=p}^{q-1}(2p+2(q-r)-2) \\ &= 4(q-p)(p-1) + 2(q-p)(q-p+1) + 2(q-1)(2p-q-1) \\ &= 4pq - 2p^2 - 2p - 2q + 2 \end{aligned}$$
(iii) If $q \ge 2p$, then
$$\begin{aligned} N_1 &= \sum_{r=1}^{p-1}(2p+2r-2) + \sum_{r=p}^{q-p}(4p-2) + \sum_{r=q-p+1}^{q-1}(2p+2(q-r)-2) \\ &= 4(p-1)^2 + 2(p-1)p + 2(2p-1)(q-2p+1) \\ &= 4pq - 2p^2 - 2p - 2q + 2 \end{aligned}$$

If N is the sum of $n(e_r)$ over all vertical edges e_r in $TUVC_6[2p,q]$, then

$$N = 2pN_1 = \begin{cases} 4p(q-1)^2, & q \le p; \\ 4p(2pq - p^2 - p - q + 1), & q \ge p+1. \end{cases}$$

And $PI(G) = |E(G)|^2 - \sum_{e \in E(G)} n(e) = (3pq - 2p)^2 - (H + N)$. From Lemma 1, if q is even, then

$$PI(G) = \begin{cases} 9p^2q^2 - 12p^2q + 4p^2 - 5pq^2 + 8pq - 4p, & q \le p; \\ 9p^2q^2 - 20p^2q + 4p^3 - pq^2 + 8p^2 + 4pq - 4p, & q \ge p+1. \end{cases}$$

and if q is odd, then

$$PI(G) = \begin{cases} 9p^2q^2 - 12p^2q + 4p^2 - 5pq^2 + 8pq - 4p, & q \le p \text{ and p is odd;} \\ 9p^2q^2 - 20p^2q + 4p^3 - pq^2 + 8p^2 + 4pq - 4p, & q \ge p+1 \text{ and p is odd;} \\ 9p^2q^2 - 12p^2q + 4p^2 - 5pq^2 + 8pq - 5p, & q \le p \text{ and p is even;} \\ 9p^2q^2 - 20p^2q + 4p^3 - pq^2 + 8p^2 + 4pq - 5p, & q \ge p+1 \text{ and p is even.} \end{cases}$$

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