# PI Index of Armchair Polyhex Nanotubes

**Ali Reza Ashrafi*** **and Amir Loghman**

Department of Mathematics, Faculty of Science, University of Kashan,
Kashan 87317-51167, Iran

## Abstract

The Padmakar–Ivan (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. The PI Index is a Szeged-like topological index developed very recently. In this paper an exact expression for PI index of the armchair polyhex nanotubes is given.

**Keywords:** PI index, armchair nanotube.

## 1. Introduction

Graph theory was successfully provided the chemist with a variety of very useful tools, namely, the topological index. A topological index is a numeric quantity of the structural graph of a molecule. With hundreds of topological indices one would expect that most molecules could be well characterized and their physicochemical properties correlated with the available descriptors.

The oldest topological indices is the Wiener index. Numerous of its chemical applications were reported and its mathematical properties are well understood [17,19]. We encourage the reader to consult [10,11], for a good survey on the topic.

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* Author to whom correspondence should be addressed. (E-mail: Ashrafi@kashanu.ac.ir)

In Refs. [12,13], the authors defined a new topological index and named it Padmakar-Ivan index. They abbreviated this new topological index as PI. This newly proposed topological index, PI, does not coincide with the Wiener index (W) for acyclic (trees) molecules. The derived PI index is very simple to calculate and has a discriminating power similar to that of the W index, for details see [14-16].

We now recall some algebraic definitions that will be used in the paper. Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-shapes of which are represented by V(G) and E(G), respectively. If e is an edge of G, connecting the vertices u and v then we write e=uv. The number of vertices of G is denoted by n. The distance between a pair of vertices u and w of G is denoted by d(u,w). We define for e=uv two quantities $n_{eu}(e|G)$ and $n_{ev}(e|G)$. $n_{eu}(e|G)$ is the number of edges lying closer to the vertex u than the vertex v, and $n_{ev}(e|G)$ is the number of edges lying closer to the vertex v than the vertex u. Edges equidistant from both ends of the edge uv are not counted. In fact, if $G_{u,e} = \{x \mid d(u,x) < d(v,x)\}$, $G_{v,e} = \{ x \mid d(u,x) > d(v,x)\}$ and $G_e = \{x \mid d(u,x) - d(v,x) = \pm 1\}$ then $n_{eu}(e|G) = |E(G_{u,e})|$, $n_{ev}(e|G) = |E(G_{v,e})|$ 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, Diudea and coauthors [4-9] computed the Wiener index of some nanotubes. In this paper an exact expression for PI index of zig-zag polyhex nanotubes is given. The present authors in Ref. [1] computed the PI index of the zig zag polyhex nanotube. In this paper we continue our study to compute the PI index of the armchair polyhex nanotube.

Our notation is standard and mainly taken from [2-18]. Throughout this paper T = $TUVC_6[2p,q]$ denotes an arbitrary armchair polyhex nanotube, see Figure 1.

## 2. PI Index of $TUHC_6[2p,q]$

In this section, the PI index of the graph T = $TUVC_6[2p,q]$ were computed. We assume that E = E(T) is the set of all edges and $N(e) = |E| - (n_{eu}(e|G) + n_{ev}(e|G))$. Then $PI(T) = |E|^2 - \sum_{e\in E} N(e)$. But $|E(T)| = p(3q-2)$ and so $PI(T) = p^2(3q-2)^2 - \sum_{e\in E} N(e)$. Therefore, for computing the PI index of T, it is enough to calculate N(e), for every $e \in E$. To calculate N(e), we consider two cases that e is horizontal or non-horizontal.

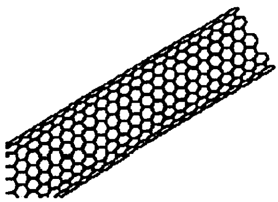

**Figure 1:** An Armchair $TUVC_6[20,n]$(The figure is taken from [4])

**Lemma 1.** *If e is an horizontal edge then* $N(e) = \begin{cases} \begin{cases} q-1 & e \in T_{2k} \\ q+1 & e \in T_{2k-1} \end{cases} & 2|p \& 2|q-1 \\ q & \text{otherwise} \end{cases}$ *, where $T_i$ denotes the set of all horizontal edges of the $i^{th}$ row of the armchair polyhex lattice, Figure 2.*

**Proof.** We first assume that p is even, q is odd and $e = UV \in T_{2k}$. It is enough to consider the case that u is in the second column of the armchair polyhex lattice, Figure 2. Suppose $E_k = U_{(2k)2}U_{(2k)3}$ and $F_k = U_{(2k)(p+2)}U_{(2k)(p+3)}$, $1 \le k \le [q/2]$, are arbitrary horizontal edges of the second and $(p+2)^{th}$ column, respectively. Since $d(U, U_{(2k)2}) = d(V, U_{(2k)3})$ and $d(U, U_{(2k)(p+2)}) = d(V, U_{(2k)(p+3)})$, $E_k, F_k \in E(T_e)$. and so $X = \{ E_k, F_k \mid 1 \le k \le [q/2] \} \subseteq E(T_e)$. We claim that $X = E(T_e)$. To prove, we assume that $f = U_{sl}U_{(s+1)l}$ is a non-horizontal edge of the armchair polyhex lattice of T. If $l \le 2$ or $l \ge p+3$ then $d(U_{sl},U) < d(U_{sl},V)$ and $d(U_{(s+1)l},U) < d(U_{(s+1)l},V)$. Thus $U_{sl}U_{(s+1)l} \notin E(T_e)$. In the case that $3 \le l \le p+2$ we have $d(U_{sl},U) > d(U_{sl},V)$ and $d(U_{(s+1)l},U) > d(U_{(s+1)l},V)$ and so $U_{sl}U_{(s+1)l} \notin E(T_e)$. Therefore, $X = E(T_e)$ and $N(e) = |X| = [q/2] + [q/2] = q-1$, in which [x] denotes the greatest integer less than or equal to x. If p is even, q is odd and $e = UV \in T_{2k-1}$ then a similar argument as above shows that $N(e) = 2[(q+1)/2] = q+1$.

Next we assume that p and q are even and $e = UV \in T_{2k}$. Then using a similar argument $N(e) = 2[q/2] = q$ and if $e = UV \in T_{2k}$, $N(e) = 2[(q+1)/2] = q$. Finally, if p is odd then $N(e) = [q/2] + [(q+1)/2] = q$. ■

**Lemma 2.** *If e is a non-horizontal edge in the $k^{th}$ row, $1 \le k \le p$, of the* armchair polyhex lattice of T = $TUVC_6[2p,q]$, *then* $N(e) = \begin{cases} 2p+2(k-1) & q \ge p+k \\ 2q-2 & q \le p+k \end{cases}$.

**Proof.** Let $E_{ij}$ denote the non-horizontal edge of T in the $i^{th}$ row and $j^{th}$ column. We first notice that for every i, $1 \le i \le q-1$, $N(E_{i1}) = N(E_{i2}) = \cdots = N(E_{i(2p)})$. So it is enough to calculate $N(E_{11})$, $N(E_{21})$, $\cdots$, $N(E_{(q-1)1})$. Compute the value of $N(E_{11})$. Suppose $q \ge p$. We consider the edges $E_{1(p+1)}$, $E_{2(p+1)}$, $\cdots$, $E_{p(p+1)}$. If $1 \le t \le p$ then $E_{t(p+1)} = U_{t(p+1)}U_{(t+1)(p+1)}$ and we have $d(U_{t(p+1)},U_{11}) = d(U_{(t+1)(p+1)},U_{21})$. So $E_{t(p+1)} \in E(T_{E_{11}})$, $1 \le t \le p$. Similarly, for $1 \le i \le p$, $E_{ii} \in T_{E_{11}}$ and $E(T_{E_{11}}) = \{E_{1(p+1)}, E_{2(p+1)}, \cdots, E_{p(p+1)}, E_{11}, E_{22}, \cdots, E_{pp}\}$. Thus $N(E_{11}) = |E(T_{E_{11}})| = 2p$. If $q \le p$ by above calculations $E(T_{E_{11}}) = \{E_{1(p+1)}, E_{2(p+1)}, \cdots, E_{(q-1)(p+1)}, E_{11}, E_{22}, \cdots, E_{(q-1)(q-1)}\}$. This shows that $N(E_{11}) = |E(T_{E_{11}})| = 2q-2$. We continue our argument by considering the edge $E_{21}$. To prove this case, we delete the first row of the armchair polyhex lattice of T and obtain a $TUVC_6[2p,q-1]$. Since $E_{21}$ is the (1,1) entry of this lattice, we have

$$N(E_{21}) = R + \begin{cases} 2p & q-1 \ge p \\ 2q-4 & q-1 \le p \end{cases},$$

where R is the number of edges $E(T_{E_{21}})$ in the first row of $TUVC_6[2p,q]$. On the other hand, $E_{1(p+1)}$ and $E_{12}$ are only edges of $TUVC_6[2p,q]$ in the first row. Therefore,

$$N(E_{21}) = \begin{cases} 2p+2 & q \ge p+1 \\ 2q-2 & q \le p+1 \end{cases}.$$

We can continue this method for computing $N(E_{31})$, $\cdots$, $N(E_{p1})$ to complete the proof. ■

**Lemma 3.** *If $q \le 2p$ then* $N(E_{11}) = N(E_{q1})$, $N(E_{21}) = N(E_{(q-1)1})$, $\cdots$, $N(E_{s1}) = N(E_{(s+1+b)1})$, where $s = [q/2]$ is the greatest integer less than or equal to q/2, and $b = [(q+1)/2] - [q/2]$.

**Proof.** Since the armchair polyhex lattice is symmetric, the proof is straightforward. ■

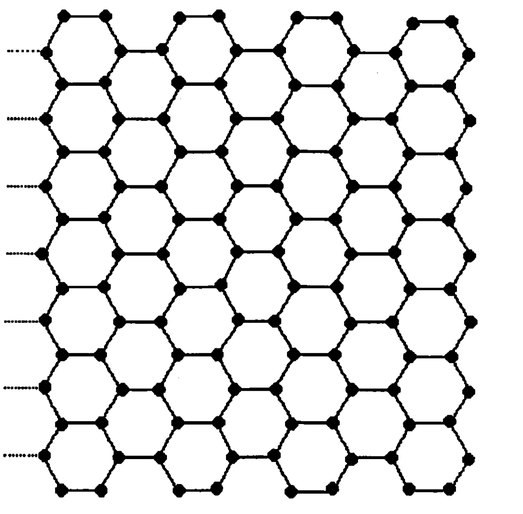

**Figure 2:** A Zig-Zag Polyhex Lattice with p = 4 and q = 15

**Lemma 4.** *If $q > 2p$ then $N(E_{11}) = N(E_{q1})$, $N(E_{21}) = N(E_{(q-1)1})$, $\cdots$, $N(E_{p1}) = N(E_{(q-p+1)1})$, and $N(E_{(p+1)1}) = N(E_{(p+2)1}) = \cdots = N(E_{(q-p)1}) = N(E_{p1})$.*

**Proof.** The first part of the lemma is a conclusion of this fact that the armchair polyhex lattice is symmetric. To prove the second part, we notice that for a fixed row j there are exactly p-1 row with two edges belongs to $E(T_{E_{j1}})$. The other rows don't intersect $E(T_{E_{j1}})$. Thus $N(E_{(p+1)1}) = N(E_{(p+2)1}) = \cdots = N(E_{(q-p)1}) = N(E_{p1})$. ■

We now ready to state the main result of the paper. We have:

**Theorem.** The PI index of armchair polyhex nanotube is as follows:

$$PI(TUVC_6[2p,q]) = \begin{cases} \begin{cases} X-p & q \le p+1 \\ Y-p & q \ge p+1 \end{cases} & 2|p \,\&\, 2\nmid q-1 \\ \begin{cases} X & q \le p+1 \\ Y & q \ge p+1 \end{cases} & \text{Otherwise} \end{cases},$$

where $X = 9p^2q^2 - 12p^2q - 5pq^2 + 8pq + 4p^2 - 4p$ and $Y = 9p^2q^2 - 20p^2q - pq^2 + 4pq + 4p^3 + 8p^2 - 4p$.

**Proof.** Since $PI(T) = |E|^2 - \sum_{e\in E} N(e)$, it is enough to compute $\sum_{e\in E} N(e)$. Suppose A and B are the set of all horizontal and non-horizontal edges of T. Then

$$PI(T) = |E|^2 - \sum_{e\in A} N(e) - \sum_{e\in B} N(e)$$

$$= p^2(3q-2)^2 - \begin{cases} pq^2+p & 2|p \& 2|q-1 \\ pq^2 & \text{Otherwise} \end{cases} - \sum_{e\in B} N(e)$$

$$= -\sum_{e\in B} N(e) + \begin{cases} 9p^2q^2-12p^2q+4p^2-pq^2-p & 2|p \& 2|q-1 \\ 9p^2q^2-12p^2q+4p^2-pq^2 & \text{Otherwise} \end{cases}$$

By Lemma 2, $N(E_{i1}) = N(E_{11}) + 2(i-1)$ and so we have

$$PI(T) = \begin{cases} -2p(q-1)N(E_{11}) & q\le p+1 \\ -2p(q-1)N(E_{11})-4p(p-1)(q-p-1) & q\ge p+1 \end{cases}$$

$$+ \begin{cases} 9p^2q^2-12p^2q+4p^2-pq^2-p & 2|p \& 2|q-1 \\ 9p^2q^2-12p^2q+4p^2-pq^2 & \text{Otherwise} \end{cases}$$

But $N(E_{11}) = \begin{cases} 2p & q\ge p+1 \\ 2q-2 & q\le p+1 \end{cases}$, so we have

$$PI(T) = \begin{cases} \begin{cases} X-p & q\le p+1 \\ Y-p & q\ge p+1 \end{cases} & 2|p \& 2|q-1 \\ \begin{cases} X & q\le p+1 \\ Y & q\ge p+1 \end{cases} & \text{Otherwise} \end{cases}$$

, which completes the proof. ■

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## REFERENCES

1. A.R. Ashrafi and A. Loghman, PI Index of Zig-Zag Polyhex Nanotubes, *MATCH Commun. Math. Comput. Chem.*, 55(2)(2006), 447-452.

2. P.J. Cameron, Combinatorics: Topics, Techniques, Algorithms, Cambridge University Press, Cambridge, 1994.

3. H. Deng, Extremal Catacondensed Hexagonal Systems with Respect to the PI Index, *MATCH Commun. Math. Comput. Chem.*, 55(2)(2006), 453-460.

4. M. V. Diudea, M. Stefu, B. Pârv and P. E. John, Wiener Index of Armchair Polyhex Nanotubes, *Croat. Chem. Acta*, 77(1-2)(2004) 111-115.

5. M.V. Diudea, Graphenes from 4-valent tori, *Bull. Chem. Soc. Japan*, 75 (2002), 487-492.

6. M.V. Diudea, Hosoya Polynomial in Tori, *MATCH Commun. Math. Comput. Chem.*, 45 (2002), 109-122.

7. M.V. Diudea and A. Graovac, *MATCH Commun. Math. Comput. Chem.* 44 (2001) 93.

8. M.V. Diudea, I. Silaghi-Dumitrescu and B. Parv, *MATCH Commun. Math. Comput. Chem.* 44 (2001) 117.

9. M.V. Diudea and P.E. John, *MATCH Commun. Math. Comput. Chem.* 44 (2001) 103.

10. A. A. Dobrynin, R. Entringer and I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.*, 66(2001), 211-249.

11. A.A. Dobrynin, I. Gutman, S. Klavzar and P. Zigert., Wiener index of hexagonal systems, *Acta Appl. Math.*, 72(2002), 247-294.

12. P.V. Khadikar, On a Novel Structural Descriptor PI, *Nat. Acad. Sci. Lett.*, 23(2000), 113-118.

13. P.V. Khadikar, S. Karmarkar and V.K. Agrawal, Relationships and Relative Correlation Potential of the Wiener, Szeged and PI Indices, *Nat. Acad. Sci. Lett.*, 23(2000), 165-170.

14. P.V. Khadikar, S. Karmarkar and V.K. Agrawal, A Novel PI Index and its Applications to QSPR/QSAR Studies, *J. Chem. Inf. Comput. Sci.*, 41(2001), 934-949.

15. P.V. Khadikar, P.P. Kale, N.V. Deshpande, S. Karmarkar and V.K. Agrawal, Novel PI Indices of Hexagonal Chains, *J. Math. Chem.*, 29(2001), 143-150.

16. P.V. Khadikar, S. Karmarkar and R.G. Varma, The Estimation of PI Index of Polyacenes, *Acta Chim. Slov.*, 49(2002), 755-771.

17. R. Todeschini and V. Consonni, Handbook of Molecular Descriptors, Wiley, Weinheim, 2000.

18. N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton, FL. 1992.

19. H. Wiener, Structural determination of the paraffin boiling points, *J. Am. Chem. Soc.*, 69(1947), 17-20.