On the PI index of some nanotubes

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Abstract. The PI index is a graph invariant defined as the summation of the sums of edges of $n_{uv}$ and $n_{vu}$ over all the edges of connected graph $G$, where $n_{uv}$ is the number of edges of $G$ lying closer to $u$ than to $v$ and $n_{vu}$ is the number of edges of $G$ lying closer to $v$ than to $u$. The index is very simple to calculate and has disseminating power similar to that of the Wiener and the Szeged indices. The comprehensive studies show that the PI index correlates highly with W and Sz as well as with physicochemical properties and biological activities of a large number of diversified and complex compounds. In this paper we prove an algorithm which is very simple for computing PI index of nanotubes. Using this algorithm the PI index of a polyhex zig-zag nanotube is computed.

1. Introduction

Usage of topological indices in physics, biology and chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of types of alkanes known as paraffins [1]. In general, topological indices are one of the oldest and most widely used descriptors in quantitative structure activity relationships (QSAR).

Amongst the topological indices used as descriptors in QSAR, the Wiener index is by far the most popular index, as it has been shown that the Wiener index has a strong correlation with the chemical properties of the compound [2-5]. Therefore, to construct a compound with a certain property correlated to some Wiener index, the objective becomes to build substructures in the target chemical compound giving the compound that Wiener index. This in turn leads to the following important problem: given a Wiener index, find a compound with that Wiener index. An overwhelming majority of the chemical applications of the Wiener index deal with chemical compounds that have acyclic organic molecules. The molecular graphs of these compounds are trees. Therefore most of the prior work on Wiener indices deals with trees, relating the structure of various trees to their Wiener indices.

We now define a newly introduced topological index which is very simple to calculate and has disseminating power similar to that of the Wiener index. In order to propose the methods for the calculation of PI-index, we first need to specify our notations and terminology, in particular, to define PI. Let $G$ be the usual, graph representation of the molecule under consideration. Hence, $G$ is a connected graph without directed and multiple edges and without loops. By $V(G)$ and $E(G)$ we denote the vertex and edge sets, respectively, of $G$. 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 $|G|$. Let $U$ be the subset of vertices of $V(G)$ which are closer to $u$ than $v$ and $V$ be the subset of vertices of $V(G)$ which are closer to $v$ than $u$. Then
we have $U = \{x \mid x \in V(G), d(u,x) < d(x,v)\}$ and $V = \{y \mid y \in V(G), d(v,y) < d(y,v)\}$. Let $\langle U \rangle = (U,E_1)$, $\langle V \rangle = (V,E_2)$, $n_1(e) = |E_1|$ and $n_2(e) = |E_2|$. Here, $n_1(e) = |E_1|$ is the number of edges nearer to $u$ than $v$ and $n_2(e) = |E_2|$ is the number of edges nearer to $v$ than $u$. In all cases of cyclic graphs there are edges equidistant to both ends of the edges. Such edges are not taken into account. Then, the $PI$ index is defined as:

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

In this paper, formulas for calculating the $PI$ index of zig-zag nanotubes are given. The same method was applied in the case of armchair and TUC$_4$C$_8$(S) tubes. The motivation for this study is outlined in Refs. [6-10] by Khadikar and his co-authors. We encourage the reader to consult these papers for background material as well as basic computational techniques.

2. Results and Discussion

In this section we describe some results which is useful in studying $PI$ index. We begin with two elementary results.

**Lemma 1.** If $G$ is an acyclic graph containing $n$ vertices then $PI(G) = n^2 - 3n - 2 = (n-1)(n-2)$.

By the previous lemma, $PI = 0$, for acyclic graphs when $n = 1$ and $2$. On the other hand, computing Wiener index of acyclic graphs is an unsolved problem in graph theory, but by Lemma 1, there is an exact expression for calculating $PI$ index of acyclic graphs.

Linear polyacenes (Figure 1) are the most thoroughly investigated homologous series of conjugated molecules (benzenoid systems). Khadikar, Karmarkar and Varma computed in [10] the $PI$ index of linear polyacenes. They proved that:

**Lemma 2.** $PI$ index of the hexagonal chain $L_h$ (Figure 1) whose $h$ hexagons are arranged in a linear manner, is equal to $24h^2$.

![Figure 1: Polyacene Molecule $L_h$.](image)

Recently, Moghani, Ashrafi and Loghman [11] extended this result to a pericondensed benzenoid graph, Figure 2. They proved that:

**Lemma 3.** $PI$ index of a pericondensed benzenoid graph containing two rows, Figure 2, is equal to $8a^2 + 24b^2 + 30ab + 10b + 2$.

![Figure 2: A Pericondensed Benzenoid Graph with Two Rows](image)

We now consider an arbitrary zig-zag nanotube to compute its $PI$ index, see Figure 3. M.V. Diudea and co-authors [13-20] investigated the topological index of this and some other nanotubes.
Ashrafi and Loghman [21-23] computed the PI index of some nanotubes. Here we explain an algorithm for computing PI index of zig-zag nanotubes. We use [24,25] for standard notation of graph theory. To compute the PI index of zig-zag nanotube, we first consider a horizontal edge. In this case it is straightforward to prove that \( N(e) = p \), in which \( N(e) = |E| - |E_1| - |E_2| \). So it is enough to consider non-horizontal case. Suppose \( e \) is a non-horizontal edge in the \( k^{th} \) column of the graphene lattice of zig-zag nanotube, \( 1 \leq k \leq p \), then \( N(e) = \frac{2p + 2(k - 1) - q \geq p + k - 1}{2q} \) \( q \leq p + k - 1 \).

Since zig-zag nanotube is symmetric, it is enough to choose a reference vertex \( v \), in every column from which the topological distances to all other vertices are evaluated. Let \( E_{ij} \) denote the non-horizontal edge of \( T \) in the \( i^{th} \) row and \( j^{th} \) column. Suppose \( q \leq 2p \) then \( N(E_{11}) = N(E_{1q}), N(E_{12}) = N(E_{1(q-1)}), \ldots, N(E_{1s}) = N(E_{1(s+1-b)}), \) where \( s = \lceil q/2 \rceil \), the greatest integer less than or equal to \( q/2 \), and \( b = \lceil (q+1)/2 \rceil - \lceil q/2 \rceil \). If \( q > 2p \) then \( N(E_{11}) = N(E_{1q}), N(E_{12}) = N(E_{1(q-1)}), \ldots, N(E_{1p}) = N(E_{1(q-p+1)}), \) and \( N(E_{1(p+1)}) = N(E_{1(p+2)}) = \ldots = N(E_{1(q-p)}) = N(E_{1p}). \) Using these facts we can prove the PI index of the zig-zag polyhex nanotube \( T \) is as follows:

\[
\text{PI}(T) = \begin{cases} 
  p^2 (9q^2 - 7q + 2) - 4pq & \text{if } q \leq p \\
  p^2 (9q^2 - 15q + 4p - 2) + 4pq & \text{if } q \geq p 
\end{cases}
\]

\[\text{Figure 3: A Zig-Zag Nanotube}\]

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