Computing the PI index of some chemical graphs related to nanostructures

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Abstract. The Padmakar–Ivan (PI) index of a graph G is defined as $\text{PI}(G) = \sum_{e \in G} [n_+(e|G) + n_-(e|G)]$, where $n_+(e|G)$ is the number of edges of G lying closer to u than to v, $n_-(e|G)$ 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 we report on new results about computing PI index of nanotubes.

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 from the structural graph of a molecule.

The Wiener index (W) is the oldest topological indices. Numerous of its chemical applications were reported and its mathematical properties are well understood [1-5]. We encourage the reader to consult [6], for a good survey on the topic.

In Refs. [7,8], 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 [9-11].

In a series of papers, Diudea and coauthors [12-18] computed the Wiener index of some nanotubes. In this letter, a problem in mathematical chemistry related to topological index of molecules has been considered. We report on new results about PI index of nanotubes. Our notation is standard and mainly taken from [12-14] and [19,20]. We encourage reader to consult [5] and [21-24] for discussion and background material about the symmetry properties of molecules.

2. Main Results
In this section we describe some notations which will be kept throughout. 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 v of G is denoted by $d(u,w)$. We define for $e=uv$ two quantities $n_+(e|G)$ and $n_-(e|G)$. $n_+(e|G)$ is the number of edges lying closer to the vertex u than the vertex v, and $n_-(e|G)$ is the number of edges lying closer to
the vertex v than the vertex u. Then the Padmakar–Ivan (PI) index of a graph G is defined as \( \text{PI}(G) = \sum [n_{v}(e|G) + n_{u}(e|G)] \). We notice that the edges equidistant from both ends of the edge uv are not counted in calculating the PI index of a graph. In fact, if \( G_{u,e} = \{ x \mid d_{G}(u,x) < d_{G}(v,x) \} \) and \( G_{v,e} = \{ x \mid d_{G}(u,x) > d_{G}(v,x) \} \) then \( n_{u}(e|G) = |E(G_{u,e})| \), \( n_{v}(e|G) = |E(G_{v,e})| \) 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. It is easy to see that \( |E(G)| = N(e) + n_{u}(e|G) + n_{v}(e|G) \).

The first serious work for computing the PI index of chemical graphs was done by Khadikar, Kale, Deshpande, Karmarkar and Agrawal [9]. They introduced a method for the calculating the PI index of hexagonal chains. In [21], Deng introduced another method for calculating the PI indices of catacondensed hexagonal systems according to the lengths of their segments, and to determine the catacondensed hexagonal systems with minimum and maximum PI index. Here a catacondensed hexagonal system G consists of a sequence of segments \( S_1, S_2, \ldots, S_n \), \( n \geq 1 \), with lengths \( l(S_i) = l_i \), \( i = 1, 2, \ldots, n \), where \( l_1 + l_2 + \ldots + l_n = h + n - 1 \) and two neighboring segments have always one hexagon in common, see Figure 1. Then the PI index of G may be calculated from these structural parameters.

![Figure 1: A Catacondensed Hexagonal System.](image)

**Theorem 1** (Han-Yuan Deng [21]). Let G be a catacondensed hexagonal system with h hexagons and consisting of n segments of lengths \( l_1, l_2, \ldots, l_n \), \( n \geq 1 \). Then

\[
\text{PI}(G) = 25h^2 + n - 1 - \sum_{i=1}^{n} l_i^2.
\]

Carbon nanotubes, the one-dimensional carbon allotropes, are intensively studied, with respect to their promise to exhibit unique physical properties: mechanical, optical, electronic, etc. In [22] the authors presented a method for computing PI index of zig-zag polyhex nanotubes. We proved that:

**Theorem 2** (Ashrafi-Loghman [22]). The PI index of the zig-zag polyhex nanotube in the terms of their circumference \( 2p \) and their length \( q \), Figure 2, is as follows:

\[
\text{PI}(TUHC_{6}[2p,q]) = \begin{cases} 
 p^2(9q^2 - 7q + 2) - 4pq^2 & \text{if } q \leq p \\
 p^2(9q^2 - 15q + 4p - 2) + 4pq & \text{if } q \geq p 
\end{cases}
\]

Using a similar arguments in [23,24] Ashrafi and Loghman computed the PI index of some other nanotubes. They proved that:

**Theorem 3** (Ashrafi-Loghman [24]). The PI index of armchair polyhex nanotube in the terms of their circumference \( 2p \) and their length \( q \), Figure 4, is as follows:
\[ \text{PI} (\text{TUVC}_d[2p,q]) = \begin{cases} 
X - p & q \leq p + 1 \\
Y - p & q \geq p + 1 \\
X & q \leq p + 1 \\
Y & q \geq p + 1 
\end{cases}, \]

where \( X = 9p^2q^2 - 12p^2q - 5pq^2 + 8pq + 4p^2 - 4p \) and \( Y = 9p^2q^2 - 20p^2q - pq^2 + 4pq + 4p^2 + 8p^2 - 4p \).

**Theorem 4** (Ashrafi-Loghman [23]). The PI index of \( \text{TUC}_d[4p,q] \) nanotube in the terms of their circumference (2p) and their length (q), Figure 3, is as follows:

\[ \text{PI}(\text{TUC}_d[4p,q]) = \begin{cases} 
X & q \leq p \\
Y & q \geq p 
\end{cases}, \]

where \( X = 36p^2q^2 - 28p^2q + 8p^2 - 8pq^2 \) and \( Y = 36p^2q^2 - 36p^2q - 4pq^2 + 4pq + 4p^2 + 4p \).

**Figure 2.** Zig-zag TUHC_d[20,q] (The figure is taken from [17])

**Figure 3:** An Armchair TUVC_d[20,n] (The figure is taken from [18])

**Figure 4:** A TUC_d[S] Nanotubes (The figure is taken from [19])
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