A STUDY OF THE NANOSTAR DENDRIMER BY PADMAKAR-IVAN INDEX

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The Padmakar-Ivan index of a graph $G$ is the sum over all edges $uv$ of $G$ of the number of edges which are not equidistant from the vertices $u$ and $v$. In this paper we compute the $PI$ index of extended bridge graphs. This is an efficient method of finding these indices especially when the extended bridge graph has a molecular graph of dendrimers form.

Key words: $PI$ index, Extended bridge graph, Nanostar dendrimer.

INTRODUCTION

The Wiener index is one of the oldest descriptors concerned with the molecular graph. This index was first proposed by H. Wiener¹ and it is concerned with the determination of the boiling points of paraffins. Wieners original definition was different, but equivalent, from that which was written above. The definition of Wiener index in terms of distances between vertices of a graph is due to Hosoya¹⁷. In mathematical research, the Wiener index has been first studied in⁹, and for a long time mathematicians were not aware of the importance of the Wiener index in mathematical chemistry. In theoretical chemistry molecular structure descriptor, also called topological indices, are used to understand the properties of chemical compounds. By now there are many different types of such indices for a general graph $G=(V,E)$. Here, apart from the Wiener index, we are interested in indices such as the Szeged index and the vertex Padmakar-Ivan index, the so called $PI_v$ index of a graph. The Szeged index is a topological index closely related to the Wiener index and is a summation of vertexmultiplicative type and coincides with the Wiener index in the case that the graph $G$ is a tree. Since the Szeged index takes into account how the vertices of the graph $G$ are distributed, it is natural to define an index that takes into account the distribution of the edges of $G$. All the indices mentioned above, when applied to chemical graphs have many chemical applications and it was shown that the $PI_v$ index is related to the Szeged index of a graph, and all of them have connections with the physicochemical properties of many complex compounds. For the topological indices associated to a graph two groups of problems can be distinguished in the theory of topological indices. One is to ask the dependence of the index to the graph and the other is the calculation of these indices efficiently. The greatest progress in solving the above problems was made for trees and hexagonal systems by Gutman et al. in¹⁰. In this paper we will develop a method to calculate Padmakar-Ivan index of the extended bridge graphs with several examples of molecular graphs. Throughout this paper all the graphs are simple and connected.

PRELIMINARIES

Let $G$ be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. We denote the distance between two arbitrary vertices $x$ and $y$ of $G$ by $d_G(x,y)$ ($d(x,y)$ for short). It
is defined as the number of edges in the minimal path connecting the vertices x and y. Given an edge \( e=uv \in E(G) \) of G, we define the distance of e to a vertex \( w \in V(G) \) as the minimum of the distances of its ends to \( w \), i.e. \( d(w,e)=\min\{d(w,u),d(w,v)\} \). Let us denote the number of edges lying closer to the vertex \( u \) than to the vertex \( v \) by \( m_i(e|G) \) and the number of edges lying closer to the vertex \( v \) than to the vertex \( u \) by \( m_i(e|G) \) and similarly for \( m_i(e|G) \). The Padmakar-Ivan (PI) index of a graph G is defined as

\[
\text{PI}(G) = \sum_{e \in E(G)} m_i(e|G)
\]

where \( m_i(G)=m_i(e|G)+m_i(e|G) \) is the number of edges of G that are not equidistant from the two ends of the edge e. Let \( \{G_i\} \) be a set of finite pair-wise disjoint graphs with \( v_i \in V(G_i) \). The bridge graph

\[
B(G_1,G_2, \ldots ,G_n) = B(G_1,G_2, \ldots ,G_n; v_1,v_2, \ldots ,v_n)
\]

of \( \{G_i\} \) with respect to the vertices \( \{v_i\} \) is the graph obtained from the graphs \( G_1,G_2, \ldots ,G_n \) by connecting the vertices \( v_i \) and \( v_{i+1} \) by an edge for all \( i=1, 2, \ldots , n-1 \). Define

\[
G_n(H,v)=B(H,H, \ldots ,H; v, v, \ldots , v),
\]

(n times) which is the special case of bridge graph [12,13].

![Fig. 1. The extended bridge graph.](image)

In this section we derive a formula for the PI index of the extended bridge graph when G is a cycle graph. First we denote the set of all edges uu' such that \( d(u,v)=d(u',v') \) by \( M_i(G) \). The cardinality of \( M_i(G) \) is denoted by \( m_i(G) \).

**Theorem 1.** The PI index of the extended bridge graph \( K=EB(C_n;H_1, \ldots ,H_n; \ v_1, v_2, \ldots , v_n) \) of cycle graph \( C_n \) and \( \{H_i\} \) with respect to \( \{v_i\} \) is given by where \( e_i=v_i^j \) and we have:

\[
\text{PI}(K) = \sum_{i=1}^{n} \text{PI}(H_i) - m(H) \cdot |E(K)| - \lambda_e(H) + \mu_e(H) + \left\{ \begin{array}{ll}
|E(K)| \cdot 2n & \text{if } \lambda_e(H) > 0 \\
|E(K)| \cdot 2n - 1 & \text{if } \lambda_e(H) = 0 \\
|E(K)| + 1 & \text{other}
\end{array} \right.
\]

Where \( m(H)=\sum_{i=1}^{n} m_{v_i}(H_i) \),

\[
\lambda_e(H) = \sum_{i=1}^{n} |E(H_i)|^2, \quad \mu_e(H) = \sum_{i=1}^{n} m_{v_i}(H_i) \cdot |E(H_i)|
\]

**Proof.** Let \( K=EB(C_n;H_1, \ldots ,H_n; \ v_1, v_2, \ldots , v_n) \) of G and \( \{H_i\} \). From the definitions we have that

\[
E(K)=\sum_{i=1}^{n} M_{v_i}(H_i) \cup \left( \bigcup_{i=1}^{n} \left| E(H_i) \right| \setminus M_{v_i}(H_i) \right) \cup \{v_i^j \}_{i=1}^{n}
\]

where \( v_{i+1}=v_i \) then

\[
\text{PI}(K) = \sum_{e \in E(K)} m_e(K) = \sum_{i=1}^{n} \sum_{e \in E(H_i)} m_e(K) + \sum_{i=1}^{n} m_{v_i^j+1}(K)
\]

\[
= \sum_{i=1}^{n} \sum_{e \in E(H_i)} m_e(K) + \sum_{i=1}^{n} \sum_{e \in E(K \setminus H_i)} m_e(K) + \sum_{i=1}^{n} m_{v_i^j+1}(K)
\]

(a) If e is the edge \( v_i^j \) in K, then there exists the following two cases:

Case(i) If G is a even cycle graph then there exists only a edge which is equidistant from the ends of the edge \( e \)

\[
\sum_{i=1}^{n} m_e(K) = \sum_{i=1}^{n} m_{v_i^j+1}(K) = \sum_{i=1}^{n} |E(K)| - 2 = n(|E(K)| - 2)
\]

Case(ii) If G is a odd cycle graph then there exists only a vertex such as \( v_j \) which is equidistant
from the ends of the edge e, thus edges set $E(H_i)$ is equidistant from the ends of the edge e

$$\sum_{i=1}^{n} m_e(K) = \sum_{i=1}^{n} m_e(H_i)$$

(b) If $e \in M_{vi}(H_i)$ then all the edges in $E(K) \setminus E(H_i)$ are equidistant from the ends of the edge e.

$$\sum_{i=1}^{n} m_e(K) = \sum_{i=1}^{n} m_e(H_i)$$

(c) If $e \in E(H_i) \setminus M_{vi}(H_i)$ then each edge in $E(K) \setminus E(H_i)$ is not equidistant from the ends of the edge e.

$$\sum_{i=1}^{n} m_e(K) = \sum_{i=1}^{n} m_e(H_i) - |E(K)| + |E(H_i)|$$

This can be equivalent to

$$PI(K) = \sum_{i=1}^{n} m_e(H_i) + \sum_{i=1}^{n} (|E(K)| - |E(H_i)|) + n(|E(H_i)| - 1) - 2$$

when $C_n$ is an even cycle graph, and when $C_n$ is an odd cycle graph, we can:

$$PI(K) = \sum_{i=1}^{n} m_e(H_i) + \sum_{i=1}^{n} (|E(K)| - |E(H_i)|) + (n-1)|E(K)| + n(|E(H_i)| - 1) - 2$$

We define,

$$EBn(G,H,v) = EB(G;H,H,\ldots,H;v,\ldots,v)$$

(n times and $n \geq 3$) which is the special case of extended bridge graph is built from several copies of the same graph was consider. As a corollary of Theorem 1, we have the following result.

**Corollary 1.** Let H be any graph with fixed vertex v. Then the PI index of the extended bridge graph $EBn(C_n, H, v)$ is given by

$$PI(EB_n(C_n, H, v)) = nPI(H) + (n^2 - n)|E(H)| + (n - n^2)m_e(H) \cdot (H) + \begin{cases} 2n^2 |E(H)| + n^2 - 2n & 2|n| \\ (2n^2 - n)|E(H)| + n^2 - n & \text{other} \end{cases}$$

**Proof.** By use of the definitions and Theorem 1 this proof is straightforward.

![Fig. 2. The extended bridge graph (a) - $\Gamma_{4,6}$, (b) - $\Delta_{6,8}$.](attachment:image.png)

**Example 1.** Let $P_m$ be the path graph on m vertices. Clearly $PI(P_m) = (m-1)(m-2)$, $|V(P_m)| = m-1$ and $m_{vi}(P_m) = 0$, defined $\delta_{n,m,l} = EB_n(C_n, P_m, v_l)$. It is easy to check that $m_{vi}(P_m) = 0$ for any vertex v in $P_m$ the resulting formula is the same for any choice of vertices in the paths. We describe the result more precisely in the following corollary.

**Corollary 2.** For a tree $T_m$ with m vertices, we have

$$PI(\delta_{n,m,l}) = \begin{cases} \frac{n^2m^2 - 2n}{2|n|} & \text{other} \end{cases}$$

We use a path $P_m$ of arbitrary length m and choose a (fixed) vertex $v_1$ with $1 \leq l \leq m$, and define $\delta_{n,m,l} = EB_n(C_n, P_m, v_l)$. It is easy to check that the vertex PI index of the graph $\delta_{n,m,l}$ does not depend on the vertex l which we choose in each path (as long as it is the same in each path). However, checking the formula given in Theorem 1, we see that $m_{vi}(P_m) = 0$ for any vertex v in $P_m$ the resulting formula is the same for all choice of vertices in the paths. We describe the result more precisely in the following corollary.

**Corollary 2.** For a tree $T_m$ with m vertices, we have

$$PI(\delta_{n,m,l}) = \begin{cases} \frac{n^2m^2}{2|n|} & \text{other} \end{cases}$$

**Proof.** By use of the definitions, we have $|V(T_m)| = 1 + m$, $m_{vi}(T_m) = 0$ for $1 \leq i \leq m$ and Clearly $PI(T_m) = (m-1)(m-2)$, then this proof is straightforward.
Corollary 2. The PI index for
\[ \Gamma_{n,m} = \text{EB}_n(C_n, C_m, v) \]
is given by
\[
\text{PI}(\Gamma_{n,m}) = \begin{cases} \left( \frac{nm(nm + 2n - 2) + n(n-2)}{n}, \frac{2n}{2m} \right) & 2|n, 2|m \\
\left( \frac{nm(nm + n - 2n)}{n}, \frac{2n}{2|m} \right) & 2
\end{cases}
\]

Proof. Let \( C_m \) be the cycle graph on \( m \) vertices,
\[
\text{PI}(C_m) = \begin{cases} m(m - 2) & 2|m \\
(m(m - 1)) & \text{other} \end{cases}
\]
and
\[
m_r(C_m) = \begin{cases} 0 & 2|m \\
1 & \text{other} \end{cases}
\]

Example 2. The PI index for \( \Gamma_{n,n} = \text{EB}_n(C_n, C_n, v) \) is given by
\[
\text{PI}(\Gamma_{n,n}) = \begin{cases} (n^3 - n)(n + 2) & 2|n \\
(n^3 - n)(n + 1) & \text{other} \end{cases}
\]

Dendrimers are highly branched macromolecules. They are being investigated for possible uses in nanotechnology, gene therapy, and other fields. Each dendrimer consists of a multifunctional core molecule with a dendritic wedge attached to each functional site. The core molecule without surrounding dendrons is usually referred to as zeros generation. Each successive repeat unit along all branches forms the next generation, 1st generation and 2nd generation and so on until the terminating generation. The topological study of these macromolecules is the aim in investigations mathematical chemistry see [1-4] for details. In this example we will consider a two classes of dendrimer nanostars and find their PI indices.

NS\([r]\) denotes the molecular graph of a nanostar dendrimer with exactly \( r \) generations depicted in Figure 3. In [3] we have:
\[
|V(\text{NS}[r])| = 24 + \sum_{i=1}^{r-1} 18 \cdot 2^i = 18 \cdot 2^r - 12
\]
and
\[
|E(\text{NS}[r])| = 27 + \sum_{i=1}^{r-1} 21 \cdot 2^i = 21 \cdot 2^r - 15.
\]

This dendrimer contains three branches \( B_1\text{NS}[r] \), \( B_2\text{NS}[r] \) and \( B_3\text{NS}[r] \). Hence by use of Theorem 1 one can write:
\[
|V(B_i\text{NS}[r])| = 6 \cdot 2^r - 5
\]
and
\[
|E(B_i\text{NS}[r])| = 7 \cdot 2^r - 7 \text{ for } i = 1, 2, 3.
\]

Also,
\[
m(\text{NS}[r]) = \sum_{i=1}^{3} m_{v_i}(B_i\text{NS}[r]) = 0,
\]
\[
\mu_{v_i}(\text{NS}[r]) = \sum_{i=1}^{3} m_{v_i}(B_i\text{NS}[r])|V(B_i\text{NS}[r])| = 0,
\]
\[
\lambda_{v_i}(\text{NS}[r]) = \sum_{i=1}^{3} |E(B_i\text{NS}[r])|^2 = 3(7 \cdot 2^r - 7)^2.
\]

Therefore,
\[
\text{PI}(\text{NS}[r]) = 441 \cdot 2^{2r} - 630 \cdot 2^r + 213
\]

We now consider PI index for NS4[r] class of nanostar dendrimers with exactly \( r \) generations depicted in Figure 4. In center of Figure 4, the core of dendrimer nanostar NS4[r] is depicted. Thus, we can check that the vertices set and edges set of NS4[n]. In [4],
\[
|V(\text{NS}_4[r])| = 96 \cdot 2^{r-1} - 60 \text{ and }
\]
\[
|E(\text{NS}_4[r])| = 105 \cdot 2^{r-1} - 66
\]
Thus, \[
\lambda_e(BNS_4[r]) = 3(35 \cdot 2^{r-1} - 24)^2
\]
and \[
\mu_e(BNS_4[r]) = 0.
\]
Therefore, \[
PI(NS_4[r]) = 11025 \cdot 2^{2r-2} - 6930 \cdot 2^r + 4344.
\]

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**REFERENCES**