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A New Method for Computation Infinite Family Nanostar Dendrimer by Vertex Padmakar-Ivan Index

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ABSTRACT

The vertex Padmakar-Ivan(PI_v) index of a graph G is defined as the sum of $n_u(e|G)$ and $n_v(e|G)$ over all edges $e = uv$ of G, where $n_u(e|G)$ is the number of vertices whose distance to vertex u is smaller than the distance to vertex v. In this paper the vertex PI index of NS[n] and NS_4[n] dendrimer are determined by numerical method. In this method we ferst calculation PI_v for the extended bridge graph, then this result will communicate to molecular graph of dendrimers.

KEYWORDS: Vertex PI index, Extended bridge graph, Nanostar dendrimer.

1 INTRODUCTION

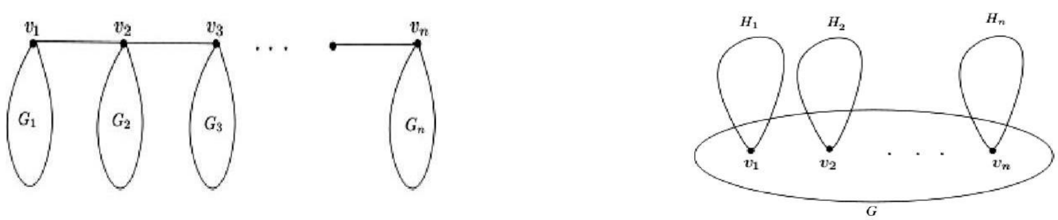
A topological index is a real number related to a molecular graph, which is a graph invariant. Topological indices have been used extensively for the prediction of physical properties of specific classes of molecules. The Wiener index is one of the oldest descriptors concerned with the molecular graph. This index first was proposed by H. Wiener [12] and it is concerned with the determination of the boiling points of paraffins. There exist many different types of such indices for a general molecular graph. Here, apart from the Wiener index, we are interested in index such as the vertex Padmakar–Ivan index, the so called PI_v index of a graph [1,4,10].

Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. As usual, 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 vertices lying closer to the vertex u than to the vertex v by $n_u(e|G)$ and the number of vertices lying closer to the vertex v than to the vertex u by $n_v(e|G)$, thus $n_u(e|G) = |\{a \in V(G) \mid d(u,a) < d(v,a)\}|$, and similarly for $n_v(e|G)$. The vertex Padmakar-Ivan index of a graph G is defined as $PI_v(G) = \sum_{e=vu\in E(G)} n_e(G)$ where $n_e(G) = n_v(e|G) + n_u(e|G)$,[10].

Let $\{G_i\}_{i=1}^n$ be a set of finite pairwise 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 $\{G_i\}_{i=1}^n$ with respect to the vertices $\{v_i\}_{i=1}^n$ 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 [9,10,11]. Clearly, $G_1(H,v) = H$ for any vertex v of H (Fig.1(a)).

Let G be a graph with vertex set $V(G) = \{v_1, v_2, \cdots, v_n\}$ and $\{H_i\}_{i=1}^n$ a sequence of finite connected pairwise disjoint graphs such that $V(G) \bigcap V(H_i) = \{v_i\}$.

The extended bridge graph $EB(G; H_1, \cdots, H_n; v_1, \cdots v_n)$ of G and $\{H_i\}_{i=1}^n$ with respect to $\{v_i\}_{i=1}^n$ is constructed by identifying the vertex v_i in G and H_i, by connecting the vertices v_i and v_{i+1} by an edge for all $i \in N$ and (i mod n). An example is shown in Fig.1(b). In special case of extended bridge graph, if G a path graph then $EB(G; H_1, \cdots, H_n; v_1, \cdots v_n) = B(H_1, H_2, \ldots, H_n; v_1, v_2, \ldots, v_n)$.



(a) The bridge graph *(b) The extended bridge graph*

Figure 1

2 MAINE RESULTS

Theorem 1. The vertex Padmakar-Ivan index of the extended bridge graph $K = EB(C_n; H_1, ..., H_n; v_1, v_2, \cdots, v_n)$ of cycle graph C_n and $\{H_i\}_{i=1}^n$ with respect to $\{v_i\}_{i=1}^n$ is given by

$$PI_v(K) = \sum_{i=1}^n PI_v(H_i) + \mu_v(H) - \lambda_v(H) + \begin{cases} (|E(K)| - m(H))|V(K)| & 2 \mid n \\ (|E(K)| - m(H) - 1)|V(K)| & 2 \nmid n \end{cases}$$

Where $m(H)=\sum_{i=1}^{n} m_{v_i}(H_i)$, $\lambda_v(H)=\sum_{i=1}^{n}|E(H_i)||V(H_i)|$, $\mu_v(H)=\sum_{i=1}^{n} m_{v_i}(H_i)|V(H_i)|$.

Proof. Let $K=EB(C_n,H_1,...,H_n;v_1,v_2,\cdots,v_n)$. From the definitions we have that

$$PI_v(K)=\sum_{e\in E(K)} n_e(K)=\sum_{i=1}^{n}\sum_{e\in E(H_i)} n_e(K)+\sum_{i=1}^{n} n_{v_i v_{i+1}}(K)$$

$$=\sum_{i=1}^{n}\sum_{e\in M_{v_i}(H_i)} n_e(K)+\sum_{i=1}^{n}\sum_{e\in E(H_i)\backslash M_{v_i}(H_i)} n_e(K)+\sum_{i=1}^{n} n_{v_i v_{i+1}}(K)$$

The edges set of extended bridge graph K following three form :

(a) If e is the edge $\{v_i v_{i+1}\}_{i=1}^{n}$ of $E(K)$ then there exist the following two cases:

Case(i). For even cycle graph C_n there exist no vertex which is equidistant from the ends of the edge e, thus $n_e(K)=n_{v_i v_{i+1}}(K)=|V(K)|$, and $\sum_{i=1}^{n} n_{v_i v_{i+1}}(K)=n|V(K)|$.

Case(ii). For odd cycle graph C_n there exist $v_j\in V(c_n)$ such that $d(v_i,v_j)=d(v_{i+1},v_j)$, where $i,i+1\neq j$. So $n_e(K)=n_{v_i v_{i+1}}(K)=|V(K)|-|V(H_j)|$ and

$\sum_{i=1}^{n} n_{v_i v_{i+1}}(K)=n|V(K)|-\sum_{j=1}^{n}|V(H_j)|=(n-1)|V(K)|$.

(b) If $e\in M_{v_i}(H_i)$ then all the vertices in $V(K)\backslash V(H_i)$ are equidistant from the ends of the edge e, thus $n_e(K)=n_e(H_i)$ and $\sum_{i=1}^{n}\sum_{e\in M_{v_i}(H_i)} n_e(K)=\sum_{i=1}^{n}\sum_{e\in M_{v_i}(H_i)} n_e(H_i)$.

(c) If $e\in E(H_i)\backslash M_{v_i}(H_i)$ then each vertex in $V(K)\backslash V(H_i)$ is not equidistant from the ends of the edge e, thus $n_e(K)=n_e(H_i)+|V(K)|-|V(H_i)|$ and

$\sum_{i=1}^{n}\sum_{e\in E(H_i)\backslash M_{v_i}(H_i)} n_e(K)=\sum_{i=1}^{n}\sum_{e\in E(H_i)\backslash M_{v_i}(H_i)}(n_e(H_i)+|V(K)|-|V(H_i)|)$.

This is equivalent to

$$PI_v(K)=\sum_{i=1}^{n}\sum_{e\in E(H_i)} n_e(H_i)+\sum_{i=1}^{n}\sum_{e\in E(H_i)\backslash M_{v_i}(H_i)}(|V(K)|-|V(H_i)|)+n|V(K)|$$

$$=\sum_{i=1}^{n} PI_v(H_i)+\sum_{i=1}^{n}(|E(H_i)|-m_{v_i}(H_i))(|V(K)|-|V(H_i)|)+n|V(K)|$$

$$=\sum_{i=1}^{n} PI_v(H_i)+(|E(K)|-m(H))|V(K)|-\sum_{i=1}^{n}|E(H_i)||V(H_i)|+\sum_{i=1}^{n} m_{v_i}(H_i)|V(H_i)|$$

when C_n is a even cycle, and if C_n is a odd cycle, we have:

$$PI_v(K)=\sum_{i=1}^{n}\sum_{e\in E(H_i)} n_e(H_i)+\sum_{i=1}^{n}\sum_{e\in E(H_i)\backslash M_{v_i}(H_i)}(|V(K)|-|V(H_i)|)+(n-1)|V(K)|$$

$$=\sum_{i=1}^{n} PI_v(H_i)+(|E(K)|-m(H)-1)|V(K)|-\sum_{i=1}^{n}|E(H_i)||V(H_i)|+\sum_{i=1}^{n} m_{v_i}(H_i)|V(H_i)|.$$

then this proof is complete.

Corollary 2. Let H be any graph with fixed vertex v. Then the vertex Padmakar-Ivan index of the extended bridge graph $EB_n(C_n, H, v)$ is given by

$$PI_v(EB_n(C_n,H,v)) = nPI_v(H) + (n^2 - n)|V(H)||E(H)| + (n - n^2)m_v(H)|V(H)|$$
$$+\begin{cases} n^2|V(H)| & 2 \mid n \\ (n^2-n)|V(H)| & 2 \nmid n \end{cases}$$

Proof. By use of the definitions we have $|E(K)| = n|E(H)| + n$ and $|V(K)| = n|V(H)|$ then this proof is straightforward.

Example 3. Let P_m be the path graph on m vertices, Clearly $PI_v(P_m) = m(m-1)$, $|V(P_m)| = m$ and $|E(P_m)| = m-1$. For vertex(first and fixed) v_1 in P_m define $\delta_{n,m,1} = EB_n(C_n, P_m, v_1)$. It is not very difficult to check $m_{v_1}(P_m) = 0$. Then the PI_v index for $\delta_{n,m,1}$ is given

$$PI_v(\delta_{n,m,1}) = \begin{cases} n^2m^2 & 2 \mid n \\ nm(mn-1) & 2 \nmid n \end{cases}$$

We use a path P_m of arbitrary length m and choose a (fixed) vertex v_l with $1 \le l \le m$, and we have $\delta_{n,m,l} = EB_n(C_n, P_m, v_l)$. 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 $m_{v_l}(P_m) = 0$ for any vertex v_l in P_m the resulting formula is the same for any choice of vertices in the paths. So we define $\Delta_{n,m} = EB_n(C_n, T_m, v_l)$ where v_l independent of choose vertex of $V(T_m)$ see Fig.2-(b). We describe the result more precisely in the following corollary [3,8].

(a) a dendrimer graph $\Gamma_{4,6}$ *(b) a* dendrimer *graph* $\Delta_{6,8}$

Figure 2:

Corollary 4. The PI_v index for $\Delta_{n,m} = EB_n(C_n, T_m, v_l)$, where l independent of choose of set $l \in \{i \mid 1 \le i \le mi \in N\}$, then

$$PI_v(\Delta_{n,m}) = \begin{cases} n^2m^2 & 2 \mid n \\ n^2m^2 - mn & 2 \nmid n \end{cases}$$

Corollary 5. The PI_v index for $\Gamma_{n,m} = EB_n(C_n, C_m, v)$ is given by

$$PI_v(\Gamma_{n,m}) = \begin{cases} n^2m^2 + n^2m & 2 \mid n, \quad 2 \mid m \\ n^2m^2 & 2 \mid n, \quad 2 \nmid m \\ n^2m^2 + n^2m - nm & 2 \nmid n, \quad 2 \mid m \\ n^2m^2 - nm & 2 \nmid n, \quad 2 \nmid m \end{cases}$$

and when $m = n$ implies that

$$PI_v(\Gamma_{n,n}) = \begin{cases} n^3(n-1) & 2 \mid n \\ n^2(n^2-1) & 2 \nmid n \end{cases}$$

Proof. Clearly $PI_v(C_m) = \begin{cases} m^2 & 2 \mid m \\ m(m-1) & 2 \nmid m \end{cases}$ and one can see

$$m_v(C_m) = \begin{cases} 0 & 2 \mid m \\ 1 & 2 \nmid m \end{cases}$$

Thus by use Corollary 2 this proof is completed.

3 CONCLUSIONS

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 [5,6,7] for details. In this example we will consider a two classes of dendrimer[2,5,6] nanostars and find their PI_v indices.

$NS[n]$ denotes the molecular graph of a nanostar dendrimer with exactly n generations depicted in Figure 3. Obviously [6], $|V(NS[n])| = 24 + \sum_{i=1}^{n-1} 18 \cdot 2^i = 18 \cdot 2^n - 12$ and $|E(NS[n])| = 27 + \sum_{i=1}^{n-1} 21 \cdot 2^i = 21 \cdot 2^n - 15$.

This dendrimer contain three branch $B_1NS[n]$, $B_2NS[n]$ and $B_3NS[n]$. Hence by use of Theorem 1 one can see $m(NS[n]) = \sum_{i=1}^{3} m_{v_i}(B_iNS[n]) = 0$,

$\mu_v(BNS[n]) = \sum_{i=1}^{3} m_{v_i}(B_iNS[n]) |V(B_iNS[n])| = 0$, $|V(B_iNS[n])| = 6 \cdot 2^n - 5$ and $|E(B_iNS[n])| = 7 \cdot 2^n - 7$ for $i = 1,2,3$.

Then $PI_v(NS[n]) = 378 \cdot 2^{2n} - 522 \cdot 2^n + 180$

We now consider vertex PI index for $NS_4[n]$ class of nanostar dendrimers with exactly n generations depicted in Figure 4. In center of Figure 4, the core of dendrimer nanostar $NS_4[n]$ is depicted. It is easy to check that the vertices set and edges set of $NS_4[n]$. Obviously [6], $|V(NS_4[n])| = 96 \cdot 2^{n-1} - 60$

$|E(NS_4[n])| = 105 \cdot 2^{n-1} - 66$, $|V(B_i NS_4[n])| = 32 \cdot 2^{n-1} - 21$,
$|E(B_i NS_4[n])| = 35 \cdot 2^{n-1} - 24$ for $i = 1,2,3$.

It is clear

$\lambda_v(BNS_4[n]) = 3(32 \cdot 2^{n-1} - 21)(35 \cdot 2^{n-1} - 24)$, $\mu_v(BNS_4[n]) = 0$.

Therefore $PI_v(NS_4[n]) = 2520 \cdot 2^{2n} - 6318 \cdot 2^n + 3960$

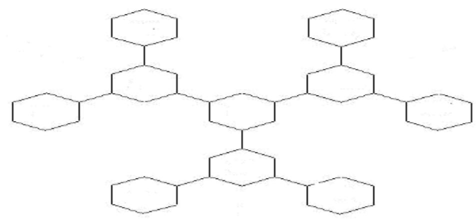


Figure 3: The nanostar dendrimer $NS[n]$

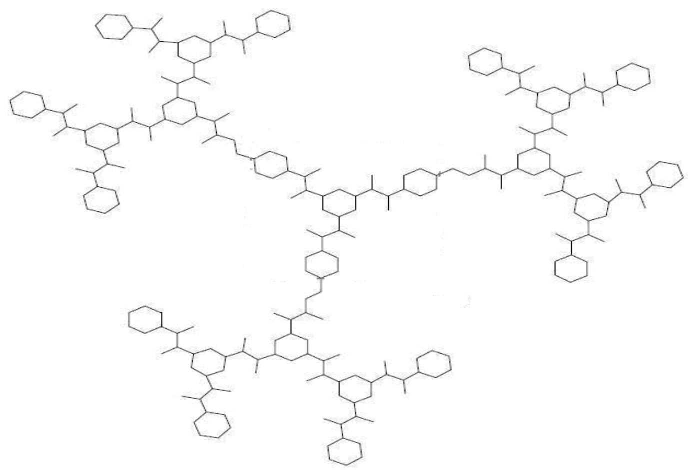


Figure 4: The nanostar dendrimer of $NS_4[n]$

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