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Computing Padmakar-Ivan index of four classes of dendrimers

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Suppose G is a connected graph, $e = uv$ is an edge of G, $n_u(e)$ is the number of edges lying closer to u than v *and* $n_v(e)$ is defined analogously. The Padmakar–Ivan index of G is a graph invariant defined as the summation of $[n_u + n_v]$ over all edges of G. General formulas are given for the Padmakar–Ivan index of dendrimers.

Key words: Dendrimer, PI index.

1. INTRODUCTION

A topological index or graph invariant for a molecular graph G is a number reflecting certain structural features of molecules that are obtained from the molecular graph. Here, a molecular graph is a labeled graph whose vertices correspond to the atoms and the edges correspond to chemical bonds**.** Suppose x and y are vertices of G. Then $d(x,y)$ denotes the length of the shortest path connecting x and y. A topological index defined by the distance function $d(-,-)$ is called a distance–based topological index. One of the oldest topological index is the Wiener index, introduced by Harold Wiener [1]. It is defined as the summation of distances between all pairs of vertices in G.

Another molecular graph invariant, referred to as the PI index, and denoted by PI is put forward by Padmakar V. Khadikar based on distances on edges of the molecular graph under consideration. The PI index is the first topological index considering the distance between edges as those of vertices. It is defined as $PI(G) = \Sigma[n_u(e) + n_v(e)]$, where $n_u(e)$ is the number of edges of G lying closer to u than v, $n_v(e)$ is the number of edges of G lying closer to v than u and summation goes over all edges of G[2].

Many topological indices have been defined and several of them have found applications as means to model physical, chemical, pharmaceutical and other properties of molecules. Khadikar and his team [3–9] investigated the behavior of some physico–chemical quantities under PI index. Diudea and his co–workers [10–17] considered the problem of computing distance–based topological indices of nanostructured materials. After proposing the PI index, one of us (ARA) [18–28] computed the PI index of some classes of nanotubes, nanotori, nanocones and also of dendrimers. The motivation of this study is taken from the leading works of Diudea and his team on the problem of computing Wiener index of nanostructured materials. For the mathematical properties of the PI index we encourage the interested readers to consult papers [29–39] and references therein for background material as well as basic computational techniques.

3. MAIN RESULTS AND DISCUSSION

The dendrimer is part of a new group of macromolecules that appear to be photon funnels just like artificial antennas. This is built by a starting atom, such as nitrogen, to which carbon and other elements are added by a repeating series of chemical reactions that produce a spherical branching structure. In a divergent synthesis of a dendrimer, one starts from the core and grows out to the periphery. In each repeated step, a number of monomers are added to the core or actual structure in a radial manner, resulting in quasi concentric shells, called generations. In a convergent synthesis, the periphery is first built up and next the branches (called dendrons) are connected to the core. The stepwise growth of a dendrimer follows a mathematical progression and its size is in the nanometer scale.

In this section, we consider four classes of dendrimers are shown in Figures 1–4. These dendrimers are denoted by $D_1[k]$, $D_2[k]$, $D_3[k]$ and $D_4[k]$, where $k \geq 1$ is a positive integer denoting the stepwise growth of the dendrimers. The set of edges of these dendrimers is denoted by $E(D_i[k])$, where i = 1, 2, 3, 4. To compute the PI index of these dendrimers we apply the following theorem.

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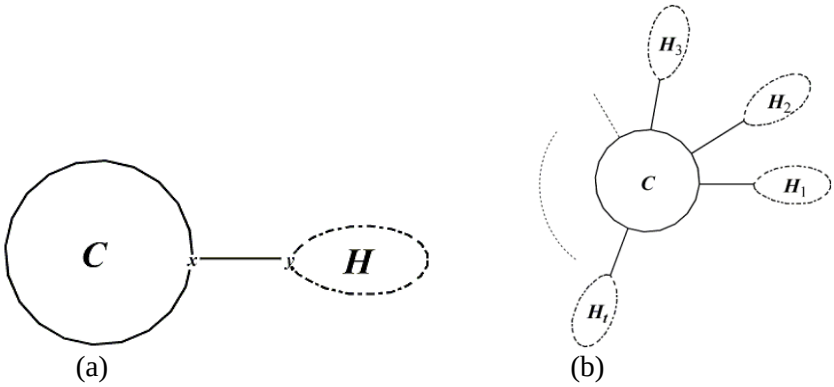

(a) (b)

Fig. 1. a) The Graph F; b) The Graph J.

Theorem. Let G be a graph constructed from cycles of even lengths C_1, C_2, … ,C_k joined by paths P_1, P_2, … ,P_s such that for every $i \neq j$, C_i and C_j do not have a common vertex. Then the PI index of G is computed as follows:

$$PI(G) = \left(\sum_{i=1}^{s}|V(P_i)| - s\right)\left(\sum_{i=1}^{k}|V(C_i)| + \sum_{i=1}^{s}|V(P_i)| - s - 1\right) + \left(\sum_{i=1}^{k}|V(C_i)|\right)\left(\sum_{i=1}^{k}|V(C_i)| + \sum_{i=1}^{s}|V(P_i)| - s - 2\right)$$

Proof. Suppose G is a graph with exactly m edges. If $e = uv$ is a cut edge of G, then $n_u(e) + n_v(e) = m - 1$. On the other hand, suppose H is an arbitrary graph, C is an even cycle, $x \in V(H)$, $y \in V(C)$ and F is a graph constructed from H and C joined by an edge xy, Figure 1(a). Then for each edge $f = uv \in E(C)$, $n_u(e) + n_v(e) = |V(C)| + |E(H)| - 1$. Similarly, if H_1, H_2, …, H_t are arbitrary graphs, C is an even cycle, x_1, x_2, …, x_t are different vertices of C, $y_i \in H_i$, $1 \leq i \leq t$, and J is the graph such that $V(J) = V(C) \cup V(H_1) \cup V(H_2) \cup \ldots \cup V(H_t)$ and $E(J) = E(C) \cup E(H_1) \cup E(H_2) \cup \ldots \cup E(H_t) \cup \{x_1y_1, x_2y_2, \ldots, x_ty_t\}$ then $n_u(e) + n_v(e) = |V(C)| + |E(H_1)| + |E(H_2)| + \ldots + |E(H_t)| - 1$, Figure 1(b). Therefore,

$$PI(G) = \left(\sum_{i=1}^{s}|V(P_i)| - s\right)\left(\sum_{i=1}^{k}|V(C_i)| + \sum_{i=1}^{s}|V(P_i)| - s - 1\right) + \left(\sum_{i=1}^{k}|V(C_i)|\right)\left(\sum_{i=1}^{k}|V(C_i)| + \sum_{i=1}^{s}|V(P_i)| - s - 2\right)$$

Corollary. Suppose G is a connected graph constructed from h hexagons such that hexagons do not have a common edge. Then $PI(G) = |E(G)|^2 - |E(G)| - 6h$.

In what follows, four classes of nanostars with above conditions are presented. In each case the PI index of the dendrimer molecule is computed by our main theorem.

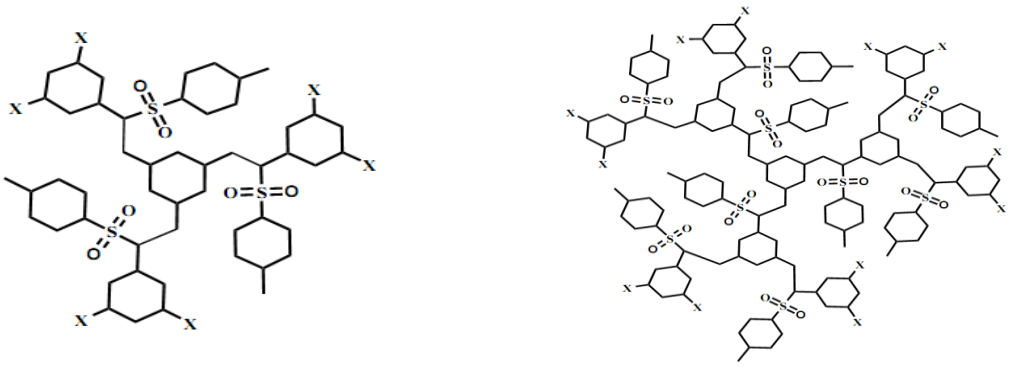

Fig. 2. The bulky dendrimers $D_1[1]$ and $D_1[2]$.

$|E(D_1[k])| = 63 \times 2^k - 54$; $h(D_1[k]) = 6 \times 2^k - 5$; $PI(D_1[k]) = 3969 \times 4^k - 6903 \times 2^k + 3000$.

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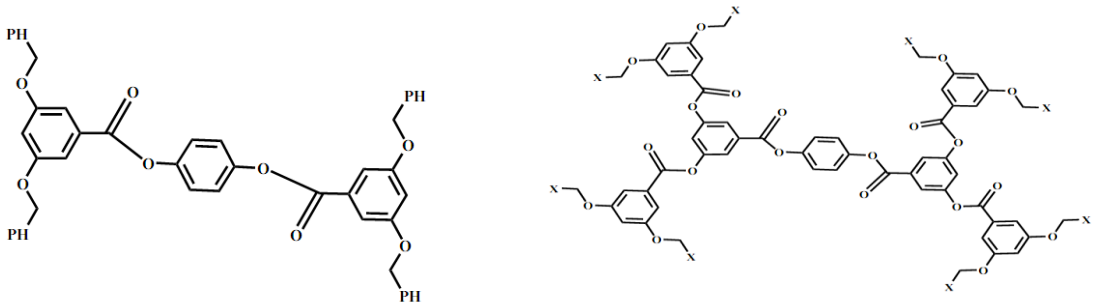

Fig. 3. The Dendrimers $D_2[1]$ and $D_2[2]$.

$|E(DNS_2[k])| = 26 \times 2^k - 14$, $h(DNS_2[k]) = 2^{k+1} - 1$; $\mathrm{PI}(DNS_2[k]) = 676 \times 4^k - 766 \times 2^k + 216$.

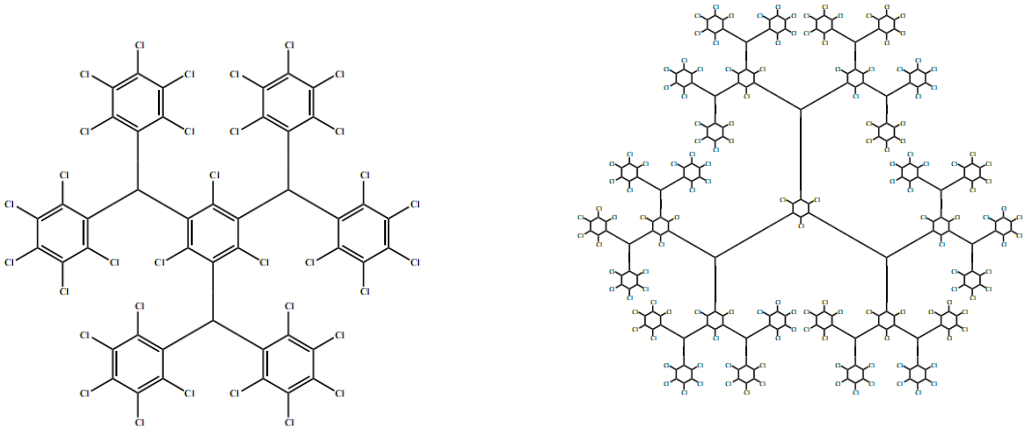

Fig. 4. The dendrimers $D_3[1]$ and $D_3[2]$.

$|E(DNS_3[k])| = 72 \times 2^k - 60$, $h(DNS_3[k]) = 6 \times 2^k - 5$, $\mathrm{PI}(DNS_3[k]) = 5184 \times 4^k - 8748 \times 2^k + 3690$.

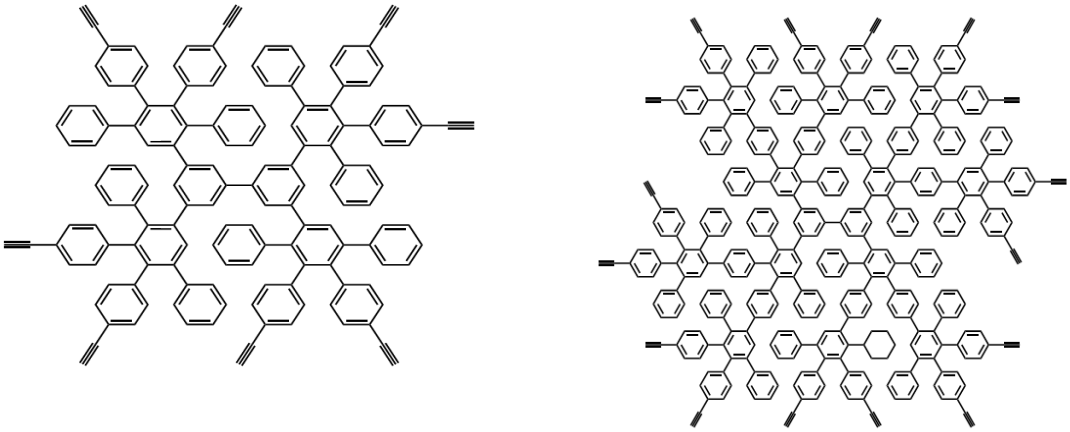

Fig. 5. The dendrimers $D_4[1]$ and $D_4[2]$.

$|E(DNS_4[k])| = 144 \times 2^k - 127$, $h(DNS_4[k]) = 20 \times 2^k - 18$, $\mathrm{PI}(DNS_4[k]) = 20736 \times 4^k - 36840 \times 2^k + 16364$

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ПРЕСМЯТАНЕ НА ИНДЕКСА PADMAKAR-IVAN ЗА ЧЕТИРИ КЛАСА ДЕНДРИМЕРИ

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(Резюме)

Приема се, че G е свързан граф, $e = uv$ е ръба на G, $n_u(e)$ е броя на ръбовете, разположени по-близо до u отколкото v, а $n_v(e)$ се дефинира аналогично. Индексът Padmakar–Ivan на G е инвариант на графа, дефиниран като сумиране на $[n_u + n_v]$ по всички ръбове на G. Получении са общи формули на индевксите Padmakar–Ivan за дендримери.