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WIENER INDEX OF MICELLE-LIKE CHIRAL DENDRIMERS

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ABSTRACT. A map taking graphs as arguments is called a graph invariant or topological index if it assigns equal values to isomorphic graphs. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this paper, the Wiener index of the micelle-like chiral dendrimers is computed.

Keywords: *Micelle-like chiral dendrimer, molecular graph, Wiener index.*

INTRODUCTION

The basic assumption for all molecules based hypothesis is that similar molecules have similar activities. This principle is also called Structure-Activity Relationship (SAR). Quantitative Structure Activity Relationship, QSAR, is the process by which a chemical structure is quantitatively correlated with a well defined process, such as biological activity or chemical reactivity.

In mathematical chemistry, molecules are often modeled by graphs named "molecular graphs". A molecular graph is a simple graph in which vertices are the atoms and edge are bonds between them. A topological index for a molecular graph G is a numerical value for correlation of chemical structure with various physical properties, chemical reactivity or biological activity [1]. The Wiener index [2] is the first topological index introduced by Harold Wiener. This index is defined as the sum of all topological distances between the pair vertices. In an exact phrase, if G is a graph and d(x,y) denotes the length of a minimal path connecting vertices x and y of G then $W(G) = \sum_{\{x,y\}\subseteq V(G)} d(x,y)$ will be the Wiener index of G.

Nano-biotechnology is a rapidly advancing area of scientific and technological opportunity that applies the tools and processes of nanofabrication to build devices for studying biosystems. Dendrimers are among the main objects of this new area of science. Here a dendrimer is a synthetic 3-dimensional

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macromolecule, prepared in a step-wise fashion from simple branched monomer units, the nature and functionality of which can be easily controlled and varied. The aim of this article is a mathematical study of this class of nano-materials. Cyclopropane and its derivatives are among the most intensely structurally studied molecules. Triangulanes are hydrocarbons consisting of spirofused cyclopropane rings. They are one of the most exotic groups of cyclopropane derivatives. Many of them show fascinating chemical, physical and sometimes biological properties [3].

Diudea and his co-workers [4-12] was the first scientist which considered the topological properties of nanostructures. After leading works of Diudea, some researchers from China, Croatia, Germany, India, Iran, Italy and UK continued these programs to compute distance-based topological indices of nanostructures [13-24].

MAIN RESULTS AND DISCUSSION

Consider the molecular graph of micelle-like chiral dendrimer G[2] depicted in Figure 1(c). We extend this molecular graph to the case that there exists a maximal chain of length n from the core to the end hexagon and denote its molecular graph by G[n]. The aim of this section is to compute the Wiener index of this class of dendrimers.

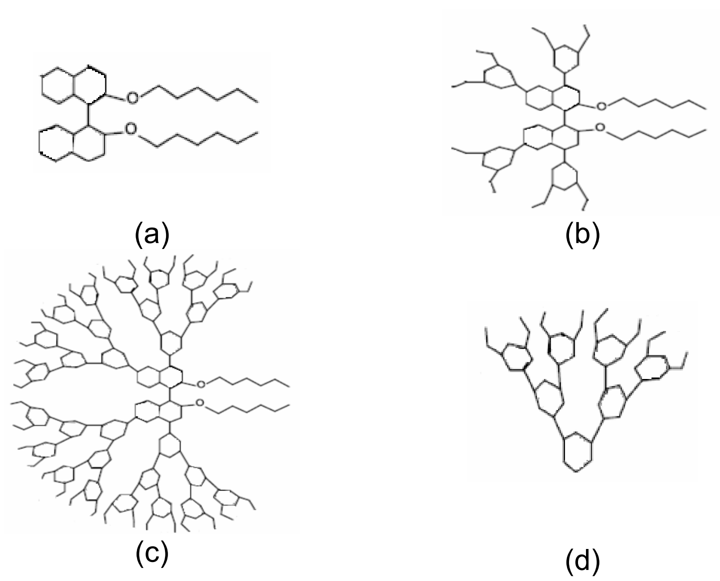


Figure 1. a) The Core of Micelle-Like Chiral Dendrimer G[n]; b) The Molecular Graph of G[0]; c) The Molecular Graph of G[2]; d) A Branch of G[2].

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by V(G) and E(G), respectively. A path of length n in G is a sequence of n + 1 vertices such that from each of its vertices there is an edge to the next vertex in the sequence. For two vertices x and y of G, d(x,y) denotes the length of a minimal path connecting x and y. A graph G is called connected, if there is a path connecting vertices x and y of G, for every x, y $\in$ V(G).

Suppose X is a set, X_i, $1 \le i \le m$, are subsets of X and F = $\{X_i\}_{1\le i\le m}$ is a family of subsets of X. If X_i's are non-empty, $X = \bigcup_{i=1}^{m} X_i$ and $X_i \cap X_j = \varnothing$, $i \ne j$, then F is called a partition of X. If G is not connected then G can be partitioned into some connected subgraphs, which is called component of G. Here a subgraph H of a graph G is a graph such that V(H) $\subseteq$ V(G) and E(H) $\subseteq$ E(G). A subgraph H of G is called *convex* if x, y $\in$ V(H) and P(x,y) is a shortest path connecting x and y in G then P is a subgraph of H.

Let's start by computing the number of vertices and edges of G[n]. From Figure 1(c), one can easily seen that this graph can be partitioned into four similar branches Figure 1(d) and a core depicted in Figure 1(a). Suppose a_n and b_n denote the number of edges and vertices in each branch of G[n], respectively. Then $a_n = 9 \times 2^{n+1} - 8$ and $b_n = 2^{n+4} - 6$. By Figure 1, one can see that $|V(G[n])| = 4b_n + 34 = 2^{n+6} + 10$ and $|E(G[n])| = 9 \times 2^{n+3} + 9$.

A graph G is called to satisfy the condition (*) if G is connected and there exists a partition $\{F_i\}_{1\le i\le k}$ for E(G) such that for each i, $G - F_i$ has exactly two components, say $G_{i,1}$ and $G_{i,2}$, where they are convex subgraphs of G. The following theorem[25] is crucial in our calculations.

Theorem 1. If G satisfy the condition (*) then $W(G) = \sum_{i=1}^{k} |V(G_{i,1})| \times |V(G_{i,2})|$.

We are now ready to prove our main result. To do this, we first define the notion of parallelism in a graph. The edge e_1 = xy said to be parallel with edge e_2 = ab, write $e_1 \parallel e_2$, if and only if D(x,ab) = D(y,ab), where D(x,ab) = *min*{d(x,a),d(x,b)} and D(y,ab) is defined similarly. In general this relation is not an equivalence relation; even it is not symmetric or transitive. But it is an equivalence relation in the edges of graph G[n] (by a few mathematical background one can see that this equivalence relation defines a partition on E(G[n]) each part being an equivalence class). The equivalence class of G[n] containing the edge e is denoted by [e]. So G[n] satisfies condition (*).

Theorem 2. The Wiener index of G[n] is computed as follows:

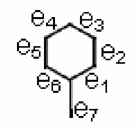
$$W(G[n]) = \left(\frac{33}{2}n + 61\right)2^{n+8} + 3\left(n + \frac{5}{8}\right)4^{n+6} + 1189.$$

Proof. Consider the parallelism relation “||” on the edges of G[n]. Since “||” is an equivalence relation on E(G), E(G) can be partitioned into equivalence classes. From Figure 1(c), there are two equivalence classes of size 3 and other classes have sizes 1 or 2. It is also clear that for each edge $e \in E(G[n])$, G[n] – [e] has exactly two components where each of them is convex, thus we can use the Theorem 1. The hexagons nearest to the endpoints of G[n] are called the end hexagons of G[n].

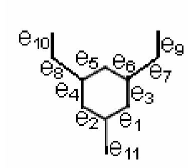
Consider the subgraph A of G[n] depicted in Figure 2(a) is not an end hexagon. It is easy to see that $F_1 = \{e_7\}$, $F_2 = \{e_1,e_4\}$, $F_3 = \{e_3,e_6\}$ and $F_4 = \{e_2,e_5\}$ are the equivalence classes of A. The components of G[n] – F_1 have b_r and $b_r^c = |V(G[n])| - b_r$ vertices; the components of G[n] – F_4 have $b_r - 3$ and $(b_r - 3)^c$ vertices and the components of G[n] – F_2, G[n] – F_3 have exactly $b_{r-1} - 3$ and $(b_{r-1} - 3)^c$ vertices, where $1 \le r \le n$. One can see that for an arbitrary r, the number of hexagons in the (n – r)-th generation of G[n] is $4 \times 2^{n-r}$.

Next we consider an end hexagon, the subgraph B depicted in Figure 2(b). Then $H_1 = \{e_{11}\}$, $H_2 = \{e_7\}$, $H_3 = \{e_9\}$, $H_4 = \{e_8\}$, $H_5 = \{e_{10}\}$, $H_6 = \{e_2,e_6\}$, $H_7 = \{e_1,e_5\}$ and $H_8 = \{e_3,e_4\}$ are the equivalence classes of B. On the other hand, one of the component G[n] – H_1, G[n] – H_2, …, G[n] – H_8 have exactly 10, 2, 1, 2, 1, 5, 5 and 7 vertices, respectively. Also, one can see the number of end hexagons is 4×2^n.

The Subgraph A



(b) The Subgraph B



(c) The Core of G[n]

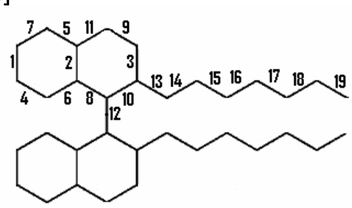


Figure 2. Fragments of the dendrimer G[n]

Finally, we consider the core of G[n], Figure 2(c). The equivalence classes of the core are $X_1 = \{1,2,3\}$, $X_2 = \{4,5\}$, $X_3 = \{6,7\}$, $X_4 = \{8,9\}$, $X_5 = \{10,11\}$, $X_6 = \{13\}$, $X_7 = \{14\}$, $X_8 = \{15\}$, $X_9 = \{16\}$, $X_{10} = \{17\}$, $X_{11} = \{18\}$, $X_{12} = \{19\}$ and

X_{13} = {12}. Again G[n] – X_i, 1 ≤ i ≤ 13, are two component graphs, say $H_{i,1}$ and $H_{i,2}$. Define a* = a × a^c , a is integer, and $X_i^* = |V(X_{i,1})| \times |V(X_{i,2})|, 1 \le i \le 13.$ Then we have the following equalities:

$$X_1^* = (2b_n + 5)^*,\ X_2^* = X_3^* = (b_n + 3)^*,\ X_4^* = (2b_n + 7)^*,\ X_5^* = (b_n + 10)^*,$$

$$X_{13}^* = \frac{|V(G[n])|^2}{4},\ X_i^* = (13 - i)^*,\ 6 \le i \le 12.$$

Now, applying Theorem 1, we have:

$$\begin{aligned} W(G[n]) &= \sum_{i=1}^{n-1} 4 \times 2^i \left(b_{n-i}^* + (b_{n-i} - 3)^* + 2(b_{n-i-1} + 3)^*\right) \\ &+ 4 \times 2^n \left(2 \times (1^* + 2^* + 5^*) + 7^* + 10^*\right) + \left(\frac{|V(G[n])|}{2}\right)^* \\ &+ 2\left[\sum_{i=1}^{7} i^* + (2b_n + 5)^* + (2b_n + 7)^* + 2(b_n + 3)^* + (b_n + 10)^*\right] \end{aligned}.$$

The proof is now complete by substituting the variables with those given above.

CONCLUSIONS

In this paper a simple method enabling to compute the Wiener index of dendrimers was presented. We apply this method on the molecular graph of a micelle-like chiral dendrimer to obtain an exact formula for the Wiener index of this class of dendrimers. Our method is efficient and can be applied on other classes of dendrimers.

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