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COMPUTING WIENER AND BALABAN INDICES OF DENDRIMERS BY AN ALGEBRAIC APPROACH

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ABSTRACT. The Balaban index J is one of the oldest topological indices introduced by the Romanian chemist, A. T. Balaban. The chemical meaning of this topological index was investigated in several research papers. The aim of this paper is to introduce a new algebraic method for computing Wiener and Balaban indices of dendrimers.

Keywords: *Dendrimer, Balaban index.*

INTRODUCTION

A topological index for a graph G is a number invariant under the automorphism group of G. These numbers have been proposed for the characterization of chemical structures. The Wiener index, one of the oldest descriptors, was proposed by H. Wiener [1]. This topological index is defined as the sum of all distances in the hydrogen-depleted graph representing the skeleton of a molecule [2].

For a connected and simple (molecular) graph G, let $V(G)$ be a finite non-empty set of vertices/atoms and $E(G)$ the set of edges/bonds. The distance between the vertices x and y, $d(x,y)$, is defined as the length of a minimal path connecting x and y. The summation of all distances between a fixed vertex x and all other vertices of G, is denoted by $d(x)$.

The Balaban index is a topological index introduced by Balaban about 30 years ago [3,4]. It is defined as $J(G) = \frac{m}{\mu + 1} \sum_{e=uv} [d(u)d(v)]^{-0.5}$, where $\mu = m - n + 1$ is called the cyclomatic number of G, with m being the number of edges and n the number of vertices of G. The Balaban index is one of the widely used topological indices for QSAR and QSPR studies, see [5–10] for details.

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Two groups of problems for the topological indices associated to a graph can be distinguished. One is to ask the dependence of the index to the graph and the other is the calculation of these indices efficiently. For the Wiener index, the greatest progress in solving the above problems was reported for trees and hexagonal systems in [11-13]. Another method is to use the *Group Theory*, in particular the automorphism group of the graph under consideration [14].

Throughout this paper, our notations are standard and taken mainly from the standard books of graph theory as like as [15]. In this paper we continue our earlier works [16–22] on computing topological indices of dendrimers and derive a formula for the Balaban index of an infinite class of dendrimers. We encourage the reader to consult papers [23–27] for mathematical properties of the Balaban index, as well as basic computational techniques.

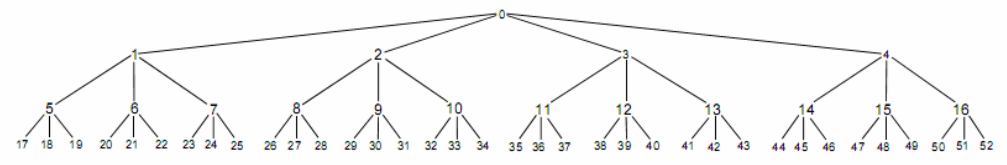

Figure 1. The molecular graph of a dendrimer with 52 vertices.

RESULTS AND DISCUSSION

In the recent years, some topological indices such as the Balaban index has attracted the interest of many chemists, mathematicians and computer scientists and has motivated a large number of research papers involving extremal properties and applications. In this section, we apply an algebraic procedure to obtain formula for computing the Balaban index of an infinite class of dendrimers, Figure 1. For this purpose we need some concepts.

Let G be a connected graph and let v be a vertex of G. The *eccentricity* $e(G)$ of v is the distance to a vertex farthest from v. So, $e(v) = \max\{d(u,v) : u \in V\}$. The *centre* of G we call all vertices with the minimum eccentricity.

Suppose H and K are two groups and K acts on the set Ω. The *wreath product* of $H \sim K$ is defined as the set of all ordered pairs (f,k) where $k \in K$ and $f : \Omega \to H$ is a function, such that $(f_1,k_1)(f_2,k_2) = (g,k_1k_2)$ and $g(i) = f_1(i)f_2(i^{k_1})$. Observe if Ω, H and K are finite then $|H \sim K| = |H|^{|\Omega|}|K|$. Let's begin by making an isomorphic copy H_k of H for each $k \in K$. Now we can let K act on the right as an automorphism of direct product of all of

these H_k by defining $(a_k).g = a_{kg} \in H_{kg}$ where $g \in K$ and $a_k \in H_k$. So $H \sim K = \oplus_{k \in K} K \propto H$.

Proposition. In the graph G, if $Aut(G)$ acts on $V(G)$ and the orbits of this action are V_0, V_1, … , V_k then $W(G) = \frac{1}{2}\sum_{i=1}^{k} |V_i| d(x_i)$ where $x_i \in V_i$. If $Aut(G)$ acts on $E(G)$ and the orbits of this action are E_1, E_2, … , E_k then $J(G) = \frac{m}{\mu + 1}\sum_{i=1}^{k} \frac{|E_i|}{\sqrt{d(x_{i-1})d(x_i)}}$ where $x_{i-1}x_i \in E_i$.

Proof. It is sufficient to show that if $\alpha \in Aut(G)$ then $d(u) = d(\alpha(u))$ that is evident.

Define D[k] as the dendrimer molecule depicted in Figure 2. We label the vertices of D[k] by 0, 1, ..., 2 × (3^k – 1). If an edge ij ($i < j$) is shown by j then the edges of D[k] can be labelled by 1, 2, ..., 2 × (3^k – 1). So, the number of vertices and edges of D[k] are 1 + 2 × (3^k – 1) and 2×(3^k – 1), respectively.

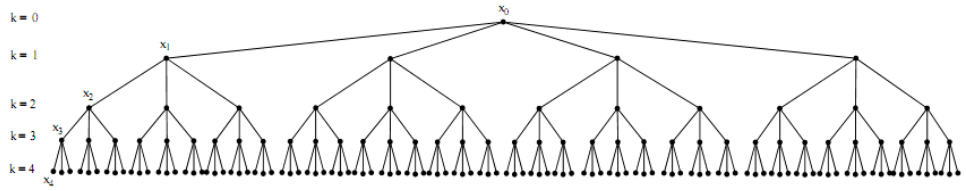

Figure 2. The Dendrimer Molecule D[4].

Theorem. The automorphism group of D[k] is isomorphic to the wreath product $S_3 \sim S_4$ where S_4 act on $\Omega = \{1,2,...,2 \times (3^k - 1)\}$.

Proof. Fix a vertex x_0 as root and assume that $\alpha \in Aut(D[k])$. Then for vertex v in level i, Figure 2, $\alpha(v)$ is also in level i, since v and $\alpha(v)$ have the same eccentricity. Consider the action of S_4 on $\{1,2,...,2 \times (3^k - 1)\}$. Therefore $Aut(D[k])$ is isomorphic to the wreath product of group S_3 via the permutation group S_4. ∎

Corollary 1. The orbits of $Aut(D[k])$ under its natural action on $V(D[k])$ are $V_0 = \{0\}$, $V_1 = \{1,2,3,4\}$, … , $V_k = \{1 + 2 \times (3^{k-1} - 1),...,2 \times (3^k - 1)\}$.

Let $x_i \in V_i$, $0 \le i \le k$. In each orbit $d(v) = d(x_i)$ when v is a fixed element of V_i. Define:

$$\alpha(t,s) = (1+t).3^0 + (2+t).3^1 + (3+t).3^2 + \cdots + (s+t)3^{s-1}.$$

Then obviously $\alpha(t,s) = 1/4[1-2t+(2s+2t-1).3^s]$. Therefore,

$$d(x_i) = \alpha(i,k) + \alpha(0,k-i) + \sum_{j=0}^{i}[i-j+2\alpha(i-j,k-j)]$$

To simplify above equation, we compute $d(x_i)$. We claim that $d(x_i) = 1 + (2k - \frac{5}{2}).3^k + (2\times 3^k).i + (\frac{3^{k+1}}{2}).3^{-i}$.

We now compute the Wiener and Balaban indices of D[k]. The Wiener index of a graph G is half of the summation of all $d(v)$ over all vertices of G. From the orbits of the action of $Aut(D[k])$ on $V(D[k])$, one can see that $W(G) = \frac{1}{2}\left(\sum_{i=1}^{k}[4\times 3^{i-1}d(x_i)] + d(x_0)\right)$. So the Wiener index of D[k] is given by the following formula:

$$W(D[k]) = \frac{1}{4}.\frac{1}{(32k^2-12k+1)3^{2k}+(24k-4)3^k+4}.(4+16k+(144k^2+16k)3^k$$
$$+(416k^3-16k^2-40k+5)3^{2k}+(384k^4-80k^3-44k^2+14k-1)3^{3k})$$

Corollary 2. The orbits of the action of $Aut(D[k])$ on $E(D[k])$ are $E_1 = \{1,2,3,4\}$, … , $E_k = \{1+2\times(3^{k-1}-1),\ldots,2\times(3^k-1)\}$.

Since D[k] is a tree, $\mu(D[k]) = 0$ and next,

$$J(D[k]) = 2\times(3^k-1)\sum_{i=1}^{k}\frac{4\times 3^{i-1}}{\sqrt{d(x_{i-1})d(x_i)}}$$

To simplify above equation, we first compute $d(x_{i-1})d(x_i)$. We have:

$$d(x_{i-1})d(x_i) = (1-7.3^k+4k3^k+\frac{45}{4}.3^{2k}-14k3^{2k}+4k^2 3^{2k})+$$
$$(4.3^k-14.3^{2k}+8k3^{2k})i+(4.3^{2k})i^2+(6.3^k-18.3^{2k}+12k3^{2k})3^{-i}$$
$$+(12.3^{2k})i3^{-i}+(\frac{27}{4}.3^{2k})3^{-2i}$$

Define: $f(i,k) = d(x_{i-1})d(x_i) = \alpha+\beta i+\lambda i^2+\gamma 3^{-i}+\delta i3^{-i}+\mu 3^{-2i}$, where,

$$\alpha = \alpha(k) = 1 - 7.3^k + 4k3^k + \frac{45}{4}.3^{2k} - 14k3^{2k} + 4k^2 3^{2k}$$

$$\beta = \beta(k) = 4.3^k - 14.3^{2k} + 8k3^{2k}$$

$$\lambda = \lambda(k) = 4.3^{2k}$$

$$\gamma = \gamma(k) = 6.3^k - 18.3^{2k} + 12k3^{2k}$$

$$\delta = \delta(k) = 12.3^{2k}$$

$$\mu = \mu(k) = \frac{27}{4}.3^{2k}$$

Therefore,

$$J(D[k]) = 8.(3^k - 1)\sum_{i=1}^{k} \frac{3^{i-1}}{\sqrt{f(i,k)}}$$

In the following table, the Balaban index $J(D[k])$ is computed, for some k.

Table 1. The Balaban index of D[k], k ≤ 20.

k	$J(D[k])$	k	$J(D[k])$	k	$J(D[k])$	k	$J(D[k])$
1	3.023715783	6	150.3527448	11	17983.21943	16	2.896950741×10^6
2	6.365606476	7	374.3679197	12	48967.03417	17	8.142315294×10^6
3	12.85128466	8	958.8910307	13	1.344850778×10^5	18	2.297691366×10^7
4	27.51789936	9	2509.007693	14	3.720218719×10^5	19	6.506856261×10^7
5	62.72145108	10	6673.758448	15	1.035416212×10^6	20	1.848495377×10^8

CONCLUSIONS

In this paper an algebraic method for computing Balaban index of dendrimers is presented. By this method the Wiener and Balaban indices of an infinite class of dendrimers are calculated. It is possible to extend our method for a general tree. These indices can be used in QSAR/QSPR studies.

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