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Balaban Index of Dendrimers

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Abstract

The Balaban index of a graph is the sum of the terms $m/(\mu+1)[d(x)d(y)]^{-0.5}$ over all edges $e = xy$, where μ is the cyclomatic number of G and for every vertex x of G, $d(x)$ denotes the summation of distances between x and all vertices of G. In this article, the Balaban index of a class D_k of dendrimers is computed by a group theoretical method. It shows that the Balaban index of a sequence x_n can be decreased strictly, when n is increased.

1. Introduction

Dendrimers are generally described as a macromolecule, which is built from 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 (a multi connected atom or group of atoms) and growths out to the periphery. In each repeated step, a number of monomers are added to the actual structure, in a radial manner, in resulting 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. These rigorously tailored structures reach rather soon (between the thirds to tenth generation, depending on the number of connections less than three between the branching points, i.e., connections equal or higher than three, along the rays of the molecular star) a spherical shape, which resembles that of a globular protein, after that the

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growth process stops. The stepwise growth of a dendrimer follows a mathematical progression and its size is in the nanometer scale.

Dendrimer chemistry was first introduced in 1978 by Vogtle [1]. He synthesized the first "cascade molecules". In 1985, Tomalia synthesized the first family of dendrimers [2]. The topological study of these macromolecules is the aim of this article.

A topological index for a graph is a number invariant under automorphisms of graph, i.e. is a numeric quantity derived on the structural graph of a molecule. One method to calculate the topological indices efficiently is to use *group theory* and in particular the automorphism group of the graph [3,4]. An automorphism of a graph G is an isomorphism of G with itself and the set of all such mappings is denoted by $Aut(G)$.

The Balaban index is a topological index introduced by Alexandru T. Balaban near to 30 years ago [5, 6]. This graph invariant is one of the widely used topological indices for QSAR and QSPR studies, see [7–12] for details. All over this paper, our notation is standard and taken mainly from the standard books of graph theory as like as [13].

In this paper we continue our earlier works [14–17] on computing topological indices of dendrimers and compute the Balaban index of a class of dendrimers. We encourage the reader to consult papers [18–22] for mathematical properties of the Balaban index, as well as some applications in nanoscience.

2. Results and Discussion

For a molecular structure such as dendrimers consider underlying molecular graph G which is connected and simple, let $V(G)$ be a finite non-empty set of nodes and $E(G)$ is the set of edges. The distance $d(x,y)$ between the nodes x and y, is defined as the length of a minimal path connecting x and y. The summation of all distances between a fixed node x and all other nodes of G, is denoted by $d(x)$.

The definition of some topological indices such as Balaban index is related to $d(x)$. The Balaban index is defined for a graph G on n nodes and m edges by $J(G) = \frac{m}{\mu+1}\sum_{e=xy}[d(x)d(y)]^{-0.5}$, where $\mu = m - n + 1$ is called the cyclomatic number of G.

Define D_k to be the dendrimer molecule depicted in Figures 1 and 2. Notice that in stage k we have 4 step k_1, k_2, k_3 and k_4. Therefore D_k has $4k$ steps and core is in step 0 ($k = 0$) of this molecule.

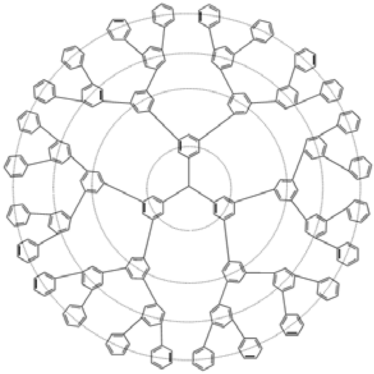

Figure 1. The Dendrimer Molecule D_4.

Suppose Γ and Λ are two groups and Λ acts on set Ω. The *wreath product* of $\Gamma \sim \Lambda$ is defined as the set of all order pairs $(f;\lambda)$ where $\lambda \in \Lambda$ and $f: \Omega \longrightarrow \Gamma$ is a function, such that $(f_1, \lambda_1)(f_2, \lambda_2) = (g, \lambda_1\lambda_2)$ and $g(i) = f_1(i)f_2(i^{\lambda_1})$. Observe that if Ω, Γ and Λ are finite then $|\Gamma \sim \Lambda| = |\Gamma|^{|\Omega|}|\Lambda|$. Begin by making an isomorphic copy Γ_λ of Γ for each $\lambda \in \Lambda$. Suppose Λ act on the right as an automorphism of direct product of all of these $\Gamma_\lambda's$ by defining $(a_\lambda) \cdot g = a_{\lambda g} \in \Gamma_{\lambda g}$ where $g \in \Lambda$ and $a_\lambda \in \Gamma_\lambda$. So $\Gamma \sim \Lambda = \oplus_{\lambda \in \Lambda} \Gamma \rtimes \Lambda$.

Let G be a connected graph and let x be a node of G. The *eccentricity* of x is defined to be the $max\{d(y,x): y \in V\}$ and denote it by $e(x)$.

Proposition. 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 enough to show that if $\alpha \in Aut(G)$ then $d(x) = d(\alpha(x))$, for each node x of G, which is straightforward. ∎

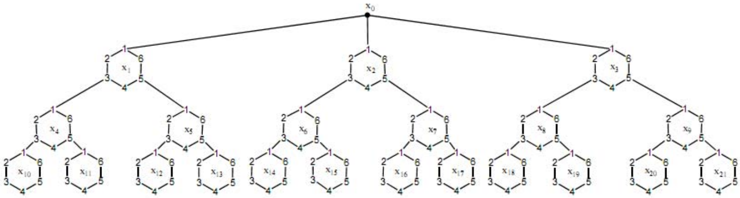

Figure 2. The Dendrimer Molecule D_3 .

Suppose $x_{0,0} = x_0$. Set $V(D_k) = \left\{x_{0,0}, x_{1,1}, \dots, x_{1,6}, \cdots, x_{3(2^k-1),1}, \dots, x_{3(2^k-1),6}\right\}$ and $E(D_k) = \{x_{0,0}x_{1,1}, x_{1,1}x_{1,2}, \dots, x_{1,5}x_{1,6}, \dots\}$. Therefore, $|V(D_k)| = 1 + 18 \times (2^k - 1)$ and $|E(D_k)| = 21 \times (2^k - 1)$.

For computing the Balaban index, we use the automorphism group of dendrimer D_k. In the following theorem the automorphism group of D_k is computed.

Theorem. The automorphism group of D_k is isomorphic to the wreath product $\mathbb{Z}_2 \sim S_3$, where S_3 act on $\Omega = \{1,2, \dots, 3 \times (2^k - 1)\}$.

Proof. Suppose α is an automorphism of D_k. Therefore, for every node x in the step i $(0 \le i \le 4k)$, $\alpha(x)$ is in the same step. The reason is the eccentricity of x and $\alpha(x)$ is the same. For each node $x_{i,1}$, there exists two reflections isomorphic to $\mathbb{Z}_2$. The core has six permutations and so it is isomorphic to S_3, the symmetric group on three symbols. This implies that $Aut(D_k) \cong \bigoplus_{|\Omega|}\mathbb{Z}_2 \rtimes S_3$. So $Aut(D_k) \cong \mathbb{Z}_2 \sim S_3$ where S_3 acts on $\{1,2, \dots, 3 \times (2^k - 1)\}$. ∎

If $Aut(D_k)$ acts on $V(D_k)$ then the orbits of $Aut(D_k)$ on $V(D_k)$ are $V_0 = \left\{x_{0,0}\right\}$, $V_1 = \{x_{1,1}, x_{2,1}, x_{3,1}\}$, …, $V_{4k} = \{x_{3(2^{k-1}-1)+1,4}, \dots, x_{3(2^k-1),4}\}$. Let $v_{0,0} = x_{0,0}$ and $v_{i,r} \in V_m$, where $0 \le m \le 4k$, $i = \left[\frac{m-1}{4}\right] + 1$ and $r = \begin{cases} 1, & m = 4q+1 \\ 2, & m = 4q+2 \\ 3, & m = 4q+3 \\ 4, & m = 4q \end{cases}$. If $v \in V_m$ then obviousely $d(v) = d(v_{i,r})$. Define two quantities $b(t,s) = \sum_{l=1}^{s}(18l + 6t - 3)2^{l-1}$ and $h(z) = 6z + 9$. We have:

$$d(v_{i,r}) = [2b(3(i-1)+r,k)+(3(i-1)+r)] + \sum_{j=0}^{i-2}[b(r+2+3j,k-i+1+j)+h(r+3j)] + b(|3-r|,k-i) + b(3-|r-2|,k-i)+h(0)$$

To simplify above equation, we calculate $d(v_{i,r})$ as follows:

$d(v_{i,r}) = 90 - 15i - 11r + (54k + 54i + 18r - 177)2^k + (102 - 12r + 6|r-3| - 6|r-2|)2^{k-i} - 6|r-3| + 6|r-2|$.

To compute the Balaban index of D_k, we notice that $\mu(D_k) = 3 \times (2^k - 1)$. If $Aut(D_k)$ acts on $E(D_k)$ then the orbits of this action are as follows:

$E_1 = \{x_{0,0}x_{1,1}, x_{0,0}\, x_{2,1}, x_{0,0}\, x_{3,1}\}$,

… ,

$E_{4k} = \{x_{3(2^{k-1}-1)+1,3}x_{3(2^{k-1}-1)+1,4}, x_{3(2^{k-1}-1)+1,4}x_{3(2^{k-1}-1)+1,5}, \dots, x_{3(2^k-1),4}x_{3(2^k-1),5}\}$.

Let $v_{m-1}v_m$ be a representative of E_m. Then

$$J(D_k) = 7 \times \sum_{m=1}^{4k} \frac{3 \times 2^{\left[\frac{m-2}{4}\right]}}{\sqrt{d(v_{m-1})d(v_m)}}\ .$$

This formula can be written as follows:

$$J(D_k) = 7\left[\frac{3}{\sqrt{d(v_{0,0})d(v_{1,1})}} + \sum_{i=2}^{k}\frac{3 \times 2^{i-1}}{\sqrt{d(v_{i-1,3})d(v_{i,1})}} + \sum_{i=1}^{k}\sum_{r=1}^{3}\frac{3 \times 2^{i}}{\sqrt{d(v_{i,r})d(v_{i,r+1})}}\right]$$

In what follows, we simplify this formula.

$d(v_{0,0})d(v_{1,1}) = 4872 + (7668k - 8790)2^k + (2916k^2 - 6804k + 3933)4^k$,

$d(v_{i,3})d(v_{i+1,3}) = [3654 - 13749 \times 2^k + 6534 \times k2^k + 12915 \times 2^{2k} - 12312 \times 88045 \times 2916 \times k^2 2^{2k}] + [-1815 + 9954 \times 2^k - 1620 \times k2^k - 13312 \times 2^{2k} + 5832 \times k2^{2k}]i + [225 - 1620 \times 2^k + 2916 \times 2^{2k}]i^2 + [6504 \times 2^k - 12204 \times 2^{2k} + 5832 \times k2^{2k}]2^{-i} + [-1620 \times 2^k + 5832 \times 2^{2k}]i2^{-i} + [2880 \times 2^{2k}]2^{-2i}$,

$d(v_{i,1})d(v_{i,2}) = [4526 - 20151 \times 2^k + 7290 \times k2^k + 22419 \times 2^{2k} - 16200 \times k2^{2k} + 2916 \times k^2 2^{2k}] + [-2025 + 11790 \times 2^k - 1620 \times k2^k - 16200 \times 2^{2k} + 5832 \times k2^{2k}]i + [225 - 1620 \times 2^k + 2916 \times 2^{2k}]i^2 + [12084 \times 2^k - 26892 \times 2^{2k} + 9720 \times k2^{2k}]2^{-i} + [-2700 \times 2^k + 9720 \times 2^{2k}]i2^{-i} + [8064 \times 2^{2k}]2^{-2i}$,

$d(v_{i,2})d(v_{i,3}) = [3906 - 16509 \times 2^k + 6750 \times k2^k + 17343 \times 2^{2k} - 14256 \times k2^{2k} + 2916 \times k^2 2^{2k}] + [-1875 + 10710 \times 2^k - 1620 \times k2^k - 14256 \times 2^{2k} + 5832 \times k2^{2k}]i + [225 - 1620 \times 2^k + 2916 \times 2^{2k}]i^2 + [9012 \times 2^k - 18792 \times 2^{2k} + 7776 \times k2^{2k}]2^{-i} + [-2160 \times 2^k + 7776 \times 2^{2k}]i2^{-i} + [5040 \times 2^{2k}]2^{-2i}$,

$d(v_{i,3})d(v_{i,4}) = [3276 - 13011 \times 2^k + 6210 \times k2^k + 12915 \times 2^{2k} - 12312 \times k2^{2k} + 2916 \times k^2 2^{2k}] + [-1725 + 9630 \times 2^k - 1620 \times k2^k - 12312 \times 2^{2k} + 5832 \times k2^{2k}]i + [225 - 1620 \times 2^k + 2916 \times 2^{2k}]i^2 + [6144 \times 2^k - 12204 \times 2^{2k} + 5832 \times k2^{2k}]2^{-i} + [-2160 \times 2^k + 5832 \times 2^{2k}]i2^{-i} + [2880 \times 2^{2k}]2^{-2i}$.

Therefore,

$$
\begin{aligned}
J(D_k) &= 21\Bigg(\frac{1}{\sqrt{4872 - 8790.2^k + 7668.k2^k + 3933.4^k - 6804.k4^k + 2916.k^2 4^k}} \\
&+ \frac{2}{\sqrt{2726 - 5289.2^k + 5670.k2^k + 2565.4^k - 5508.k4^k + 2916.k^2 4^k}} \\
&+ \frac{2}{\sqrt{2256 - 3993.2^k + 5130.k2^k + 1755.4^k - 4536.k4^k + 2916.k^2 4^k}} \\
&+ \frac{2}{\sqrt{1776 - 2739.2^k + 4590.k2^k + 1053.4^k - 3564.k4^k + 2916.k^2 4^k}} + \cdots \\
&+ \frac{2^{k-1}}{\sqrt{33462 - 5505k + 225k^2 - 61395.2^k + 44676k2^k - 3240k^2 2^k + 28143.4^k - 36288k4^k + 11664k^2 4^k}} \\
&+ \frac{2^k}{\sqrt{24674 - 4725k + 225k^2 - 47043.2^k + 38520k2^k - 3240k^2 2^k + 22419.4^k - 32400k4^k + 11664k^2 4^k}} \\
&+ \frac{2^k}{\sqrt{17958 - 4035k + 225k^2 - 35301.2^k + 33012k2^k - 3240k^2 2^k + 17343.4^k - 28512k4^k + 11664k^2 4^k}} \\
&+ \frac{2^k}{\sqrt{12300 - 3345k + 225k^2 - 25215.2^k + 27504k2^k - 3240k^2 2^k + 12915.4^k - 24624k4^k + 11664k^2 4^k}}\Bigg).
\end{aligned}
$$

In Table 1, the Balaban index $J(D_k)$, $1 \le k \le 10$, are computed.

Table 1. The Balaban index $J(D_k)$, $1 \le k \le 10$.

k	$J(D_k)$
1	0.4825253209
2	0.2524778703
3	0.1542313952
4	0.1058526496
5	0.07838438075
10	0.03139831699
100	0.002550680375
1000	0.0002504964864
10000	0.00002500495478

From these calculations, one can see that by increasing k, the Balaban index of D_k is decreased strictly.

3. Conclusions

The article presented exact formulae for the Balaban index of a class of dendrimers. Even the number of generations of such a (hypothetical) dendrimer is rather limited, the established formulae have a valuable diagnostic value, as composition rules of a global (topological) property by local contributions of the structural repeat units.

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