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Note

Balaban Index of an Infinite Class of Dendrimers

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Abstract. The Balaban index of a graph G is the first simple index of very low degeneracy. It is defined as the sum of topological distances from a given atom to any other atoms in a molecule. In this paper the Balaban index of an infinite family of dendrimers is computed. The result can be of interest in molecular data mining, particularly in searching the uniqueness of tested (hyper-branched) molecular graphs.

Keywords: Balaban index, dendrimer

INTRODUCTION

Dendrimers are highly branched macromolecules. 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 (*i.e.*, repeat units) are added to the core (or 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 of degree 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 growth process stops. The stepwise growth of a dendrimer follows a mathematical progression.[1]

The size of dendrimers is in the nanometer scale. The endgroups (*i.e.*, the groups reaching the outer periphery) can be functionalized, thus modifying their physico-chemical or biological properties. Dendrimers are investigated for possible uses in nanotechnology, gene therapy, and other fields. The topological study of these macromolecules is the aim of this article.

A graph G is defined as a pair $G = (V, E)$ where V is defined to be a finite non-empty set of vertices and E is the set of edges. 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 $d(x)$.

A topological index is a numeric quantity derived on the structural graph of a molecule. Being a structural invariant it does not depend on the labeling or the pictorial representation of the graph. Despite the considerable loss of information by *compressing* in a single number of a whole structure, such descriptors found broad applications in prediction of several molecular properties and biological activities. These studies called QSPR/QSAR (*i.e.*, quantitative structure-property/activity relationships) have both diagnostic and prognostic abilities and aimed to elucidate the relation between the structure of a molecule and its properties or biological activities (if any). It is of particular usefulness to predict values of some molecular properties, namely those which are difficult to measure or show health risk or for unavailable substances.[2] In the side of biological activities, is noteworthy the economy registered in synthesis and biological screening of bioactive molecules, in time, money and environment protection as well. A nice example, in this respect, is the article of Grassy et al. on peptides having immunosuppressive activity.[3] The authors used 27 structure descriptors, of which 12 topological indices. From a library of 280 000 compounds they selected 26 peptides, with predicted high activity. Five of them were next synthesized and tested in clinics. The most potent of these structures was 100 times more active than the lead compound.

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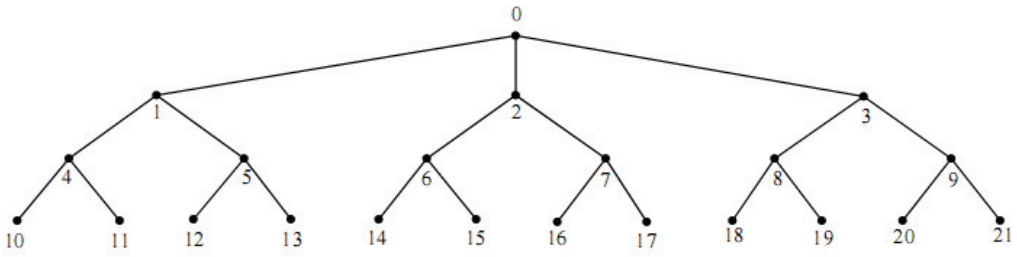

Figure 1. The Dendrimer Molecule whit 22 vertices.

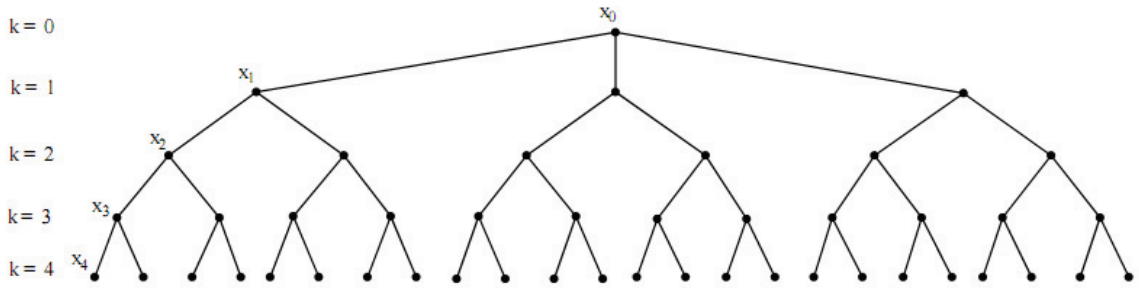

Figure 2. The Dendrimer Molecule D_4.

The Balaban index is a topological index introduced by Balaban near to 30 years ago.[4,5] It is defined as

$$J(G) = \frac{m}{\mu + 1} \sum_{e=uv} \left[d(u) d(v) \right]^{-0.5},$$

where m is the number of edges of G, n is the number of vertices and $\mu = m - n + 1$ is called the cyclomatic number of G The Balaban index is one of the widely used topological indices for QSAR and QSPR studies, see Refs. 6–12 for details.

Throughout this paper, our notation is standard and taken mainly from the standard books of graph theory (like Ref. 13). In this paper we continue our earlier works[14–17] on computing topological indices of dendrimers and compute the Balaban index of an infinite class of dendrimers. We encourage the reader to consult papers[18–21] for mathematical properties of the Balaban index, as well as basic computational techniques. Finally, the Wiener index of a graph G is defined as the summation of all distances between vertices of G. This was the first distance based topological index introduced by Harold Wiener.[22]

RESULTS AND DISCUSSION

In recent years, 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 these techniques to obtain formula for computing the Balaban index of an infinite class of dendrimers, Figure 1. Define D_k to be the dendrimer molecule depicted in Figures 1 and 2.

It is easy to see that the number of vertices and the number of edges in D_k are $|V(D_k)| = 1 + 3(1 + 2 + 2^2 + \ldots + 2^k = 1 + 3 \times (2^{k+1}1)$ and $|E(D_k)| = 3 \times (2^{k+1}1)$ respectively.

In this paper we compute the Balaban index by using the group of automorphism of Dendrimer D_k At first, it is proved that $Aut(D_k)$ is isomorphic to the $\mathbb{Z}_2 \sim S_3$, when S_3 act on $\{1, 2, \ldots, 3 \times (2^k - 1)\}$ and the symbol $\sim$ denotes the wreath product of group $\mathbb{Z}_2$ by the symmetric group S_3. If $Aut(D_k)$ acts on $V(D_k)$ then the orbits of $Aut(D_k)$ on $V(D_k)$ are $V_0 = \{0\}$, $V_1 = \{1, 2, 3\}, \ldots, V_k = \{1 + 3 \times (2^{k-1} - 1), \ldots, 3 \times (2^k - 1)\}$ In each orbit of the action the quantity $d(v)$ is fixed. If u an v are in the same orbit then $d(u) = d(\sigma(v))$, for every $\sigma \in Aut(D_k)$. Let $x_i \in V_i$ for $0 \le i \le k$.

Define $\alpha(t, s) = (1 + t).2^0 + (2 + t).2^1 + (3 + t).2^2 + \ldots + (s + t)2^{s-1}$. Then obviously $\alpha(t, s) = 1 - t + (s + t - 1)2^s$. Therefore,

$$d(x_i) = \alpha(i, k) + \alpha(0, k - i) + \sum_{j=0}^{n} \left[i - j + \alpha(i - j, k - j) \right] = 3 + 2^{k1+2} + (3k + 3i - 7)2^k.$$

We now compute the Wiener and Balaban indices of D_k. Since the action of $Aut(G)$ on $V(G)$ has the orbits

$$V_0, V_1, \ldots, V_k, \; W(G) = \frac{1}{2} \sum_{i=0}^{k} |V_i| d(x_i).$$

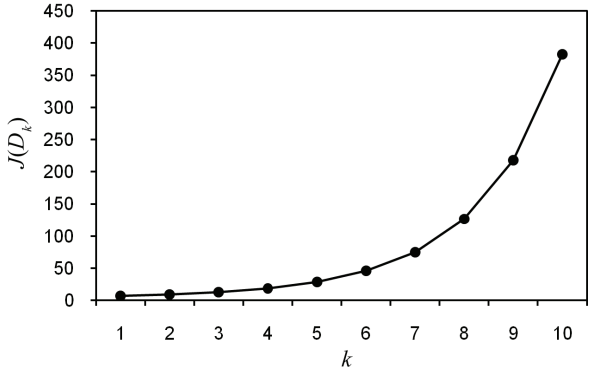

Figure 3. Diagram of the Balaban Index $J(D_k)$ when $1 \le k \le 10$.

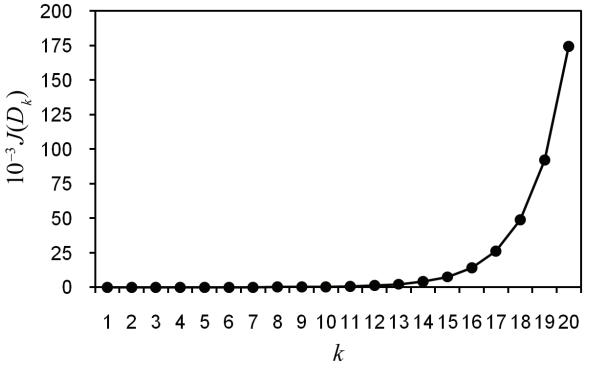

Figure 4. Diagram of the Balaban Index $J(D_k)$ when $1 \le k \le 20$.

So, the Wiener index of D_k is computed as

$$W(D_k) = \frac{1}{2}\left(3 + 2^{k+2} + (3k-7)2^k\right) + \sum_{i=1}^{k}\left[3.2^{i-1}(3 + 2^{k-i+2} + (3k+3i-7)2^k))\right]$$

Suppose E_1, E_2, ... , E_k are the orbits of the action of $Aut(D_k)$ on E_k. Thus,

$$J(D_k) = \frac{m}{\mu+1}\sum_{e=uv}\frac{1}{\sqrt{d(u)d(v)}} = \frac{m}{\mu+1}\sum_{i=1}^{k}\frac{|E_i|}{\sqrt{d(x_{i-1})d(x_i)}}.$$

On the other hand, since D_k is a tree, $\mu(D_k) = 0$ and for all vertices in step i, $d(x_i)$'s are equal. Therefore, the Balaban index is written as:

$$J(D_k) = 3.(2^m - 1)\sum_{i=1}^{m}\frac{3.2^{i-1}}{\sqrt{d(x_{i-1})d(x_i)}}.$$

On the other hand,

$$d(x_{i-1})d(x_i) = \left(9 + 9.2^{2k}k^2 - 51.2^k + 18.k2^k + 70.2^{2k} - 51.k2^{2k}\right) + \left(18.2^k + 18.k2^{2k} - 51.2^{2k}\right)i + \left(9.2^{2k}\right)i^2 + \left(36.2^k + 36.k2^{2k} - 96.2^{2k}\right)2^{-i} + \left(36.2^{2k}\right)i2^{-i} + \left(32.2^{2k}\right)2^{-2i}.$$

Define $f(i,k) = d(x_{i-1})d(x_i) = \alpha + \beta i + \lambda i^2 + \gamma 2^{-i} + \delta i 2^{-i} + \mu 2^{-2i}$, where $\alpha = \alpha(k) = 9 + 9.2^{2k}k^2 - 51.2^k + 18.k2^k + 70.2^{2k} - 51.k2^{2k}$, $\beta = \beta(k) = 18.2^k + 18.k2^{2k} - 51.2^{2k}$, $\lambda = \lambda(k) = 9.2^{2k}$, $\gamma = \gamma(k) = 36.2^k + 36.k2^{2k} - 96.2^{2k}$, $\delta = \delta(k) = 36.2^{2k}$ and $\mu = \mu(k) = 32.2^{2k}$. Therefore,

$$J(D_k) = 3\left(2^{k+1} - 1\right)\sum_{i=1}^{k}\frac{3.2^{i-1}}{\sqrt{f(i,k)}} = 3^2\left(2^{k+1} - 1\right).$$

Table 1. The Balaban Index $J(D_k)$ for some k

k	$J(D_k)$
1	6.971370023
2	9.294833832
3	12.91731911
4	18.86237367
5	28.81483133
10	382.4309633
100	$0.3877483364 \times 10^{29}$
1000	$0.3220700546 \times 10^{299}$

$$\left(\frac{1}{\sqrt{9 - 15.2^k + 18k2^k + 6.2^{2k} - 15k2^{2k} + 9k^2 2^{2k}}} + \frac{2}{\sqrt{9 - 6.2^k + 18.k.2^k - 6.k.2^{2k} + 9.k^2.2^{2k}}} + \ldots + \frac{2^{k-1}}{\sqrt{77 - 147.2^k + 108.k.2^k + 70.2^{2k} - 102.k.2^{2k} + 36.k^2.2^{2k}}}\right)$$

In the Table 1 The Balaban index $J(D_k)$ are computed, for some k.

CONCLUSION

The article presented exact formulae for the Wiener and Balaban indices of a class of dendrimers. Even the number of generations of such dendrimers is rather limited, the established formulae have a valuable diagnostic value, particularly in establishing composition rules of a global (topological) property by local contributions of the structural repeat units/monomers. In this respect, the Balaban index can be used both as a classifier of data downloaded from molecular structure databases and molecular descriptor in quantitative structure-property relationships.

REFERENCES

1. M. V. Diudea and G. Katona: Molecular Topology of Dendrimers, in: G. A. Newkome (Ed.), *Advan. Dendritic Macromol*. **4** (1999) 135–201.
2. M. V. Diudea, (Ed.): *QSPR/QSAR Studies by Molecular Descriptors*, NOVA, New York, 2001.
3. G. Grassy, B. Calas, A. Yasri, R. Lahana, J. Woo, S. Iyer, M. Kaczorek, R. Floćh, and R. Buelow, *Nat. Biotechnol.* **16** (1998) 748–752.
4. A. T. Balaban, *Chem. Phys. Lett.* **89** (1982) 399–404.
5. A. T. Balaban, *Pure Appl. Chem.* 55 (1983) 199–206.
6. A. T. Balaban, *MATCH Commun. Math. Comput. Chem*. **21** (1986) 115–131.
7. A. T. Balaban and P. Filip, *MATCH Commun. Math. Comput. Chem*. **16** (1984) 163–190.
8. A. T. Balaban, N. Ionescu-Pallas, and T. S. Balaban, *MATCH Commun. Math. Comput. Chem*. **17** (1985) 121–146.
9. A. T. Balaban, P. V. Khadikar, C. T. Supuran, A. Thakur, and M. Thakur, *Bioorg. Med. Chem.* **15** (2005) 3966–3973.
10. T. S. Balaban, A. T. Balaban, and D. Bonchev, *J. Mol. Struct.* (*Theochem*) **535** (2001) 81–92.
11. J. Devillers and A. T. Balaban (Eds.): "Topological Indicesand Related Descriptors in QSAR and QSPR", Gordon & Breach, Amsterdam, 1999.
12. O. Ivanciuc, T. Ivanciuc, and A. T. Balaban: "Design of Topological Indices. Part 10. Parameters Based on Electronegativity and Covalent Radius for the Computation of Molecular Graph Descriptors for Heteroatom-Containing Molecules", *J. Chem. Inf. Comput. Sci.* **38** (1998) 395–401.
13. F. Buckley and F. Harary: "Distance in Graphs", Addison-Wesley, Reading, MA, 1990.
14. A. R. Ashrafi and M. Mirzargar, *Util. Math*. **77** (2008) 249–255.
15. A. Karbasioun and A. R. Ashrafi, *Macedonian J. Chem. Chem. Eng.* **28** (2009) 49–54.
16. A. Karbasioun, A. R. Ashrafi, and M. V. Diudea, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 239–246.
17. A. Iranmanesh and A. R. Ashrafi, *J. Comput. Theoret. Nanosci.* **4** (2007) 514–517.
18. H. Dong and X. Guo, *MATCH Commun. Math. Comput. Chem.* **63** (2010), in press.
19. M. Eliasi and B. Taeri, *J. Comput. Theor. Nanosci.* **4** (2007) 1174–1178.
20. B. Zhou and N. Trinajstić, *Croat. Chem. Acta* **81** (2008) 319–323.
21. B. Zhou and N. Trinajstić, *Croat. Chem. Acta* **82** (2009) 537–541.
22. H. Wiener, *J. Am. Chem. Soc*. **69** (1947) 17–20.

SAŽETAK

Balabanov index beskonačne klase dendrimera

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Balabanov indeks grafa *G* prvi je jednostavni indeks vrlo niske degeneracije. Definiran je kao zbroj topoloških udaljenosti od danog atoma do svih preostalih atoma u molekuli. U radu je izračunan Balabanov indeks beskonačne obitelji dendrimera. Rezultat može biti zanimljiv u obradi podataka koji opisuju molekule, posebice u traženju jednoznačnosti jako razgranatih molekularnih grafova.