OPTOELECTRONICS AND ADVANCED MATERIALS – RAPID COMMUNICATIONS Vol. 4, No. 9, September 2010, p. 1427 - 1428

The new Zagreb indices of a class of dendrimers

M. GHORBANI
Department of Mathematics, Faculty of Science, Shahid Rajaee, Teacher Training University, Tehran, 16785-136, I. R. Iran

In the present study, we introduce two new versions of Zagreb indices. Let ε(u) be the largest distance between u and any other vertex v of G. These new topological indices are defined as $M_1^*(G) = \sum_{uv \in E(G)} \varepsilon(u) + \varepsilon(v)$ and $M_2^*(G) = \sum_{uv \in E(G)} \varepsilon(u)\varepsilon(v)$. The goal of this paper is computing these new topological indices of a class of dendrimer graphs.

(Received 20 July, 2010; accepted September 15, 2010)

Keywords: Dendrimer, Zagreb indices, Topological index

1. Introduction

The topological index of a molecule is a non-empirical numerical quantity that quantifies the structure and the branching pattern of the molecule. 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. The distance d(u,v) between two vertices u and v of a graph G is defined as the length of a shortest path connecting them. The Wiener index[1] is the first reported distance based topological index and is defined as half sum of the distances between all the pairs of vertices in a molecular graph. For a given vertex u of V(G) its eccentricity, ε(u), is the largest distance between u and any other vertex v of G. The maximum eccentricity over all vertices of G is called the diameter of G and denoted by D(G) and the minimum eccentricity among the vertices of G is called radius of G and denoted by R(G), see [2 - 10] for more details.

The Zagreb indices were introduced 30 years ago by Gutman and Trinajstić as $M_1(G) = \deg(u) + \deg(v)$ and $M_2(G) = \deg(u)\deg(v)$, where deg(u) denotes the degree of vertex u [11 – 13]. Ghorbani et al. [14] defined a new version of Zagreb indices as follows:

$$M_1^*(G) = \sum_{uv \in E(G)} \varepsilon(u) + \varepsilon(v) \text{ and}$$
$$M_1^*(G) = \sum_{uv \in E(G)} \varepsilon(u)\varepsilon(v).$$

This paper addresses the problem of computing the eccentricity and then the new Zagreb indices of a special type of dendrimers. We encourage the readers to consult papers [15 - 20] for computational techniques related to dendrimers, as well as [21 - 23] for background materials. Our notation is standard and taken mainly from the standard books of graph theory.

2. Main result and discussion

In [15-20], Ghorbani computed some topological indices of some nanostructures. In this section the eccentricity of dendrimer T containing r layers is computed. From Fig. 1, it is clear that

$$|V(T)| = 1+2[1 + 2 + 4 + 8 + \ldots + 2^r] = 2^{r+2}-1,$$

$$|E(T)| = 1+2[2 + 4 + 8 + \ldots + 2^r] = 2^{r+2}-2.$$

Lemma 1. $\varepsilon(u) = r$.

Proof. Suppose u is the central vertex of T. Then from Fig. 1, one can see that the shortest path with maximum length is between u and a vertex w of the last layer. ♦

The proof of lemma 1, shows that the eccentricity of vertex v is r + 1. Because distance of every vertex of k^{th} layer and the central vertex of T is k, so for every edge $e = xy$ in k^{th} layer, one can see that $\varepsilon(x) = k$ and $\varepsilon(y) = k+1$. So, it is easy to see that:

Theorem 2. Consider graph of dendrimer T depicted in Fig. 1. Then

$$M_1^*(T) = 2\sum_{i=1}^{r} 2^i [(r+i) + (r+i+1)] = 2^{r+1}(4r-3) - 4r + 6,$$

$$M_2^*(T) = 2\sum_{i=1}^{r} 2^i (r+i)(r+i+1) = 2^{r+1}(4r^2-6r+4) - 2r^2 + 6r - 8$$

Corollary 3. Consider graph of dendrimer G depicted in Fig. 2. Then

$$M_1^*(G) = 3\sum_{i=1}^{r} 2^i [(r+i) + (r+i+1)] = 3\times 2^r(4r-3) - 6r + 9,$$

$$M_2^*(G) = 3\sum_{i=1}^{r} 2^i (r+i)(r+i+1) = 3\times 2^r(4r^2-6r+4) - 3r^2 + 9r - 12$$

.

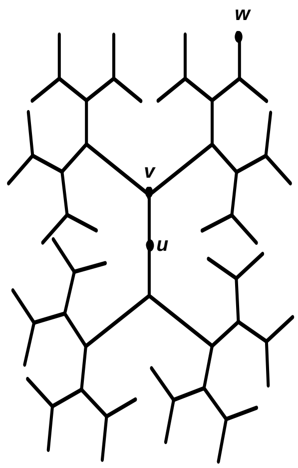

Fig. 1. Dendrimer T with r = 5.

In the following lemma, the eccentricity of central vertex of T is computed.

Corollary 4. Consider graph of dendrimer H depicted in Fig. 3. Then

$$M_1^*(H) = 4\sum_{i=1}^{r} 2^i[(r+i)+(r+i+1)] = 2^{r+2}(4r-3) - 8r + 12,$$

$$M_2^*(H) = 4\sum_{i=1}^{r} 2^i(r+i)(r+i+1) = 2^{r+2}(4r^2-6r+4) - 4r^2 + 12r - 16.$$

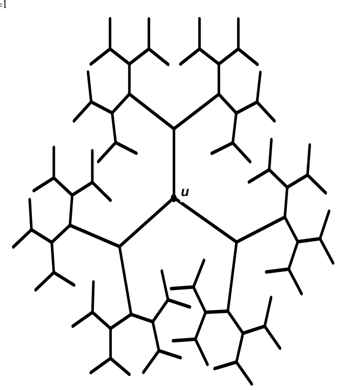

Fig. 2. Dendrimer G with r = 5.

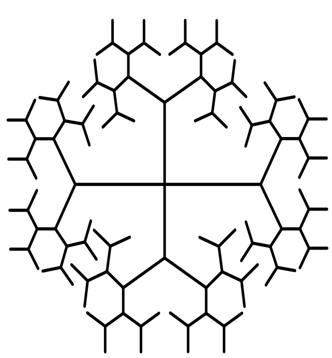

Fig. 3. Dendrimer H with r = 5.

References

[1] H. Wiener, J. Am. Chem. Soc. **69**, 17 (1947).
[2] I. Gutman, K. C. Das, MATCH Commun. Math. Comput. Chem. **50**, 83 (2004).
[3] V. Sharma, R. Goswami, A. K. Madan, J. Chem. Inf. Comput. Sci. **37**, 273 (1997).
[4] H. Dureja, A. K. Madan, Med. Chem. Res. **16**, 331 (2007).
[5] V. Kumar, S. Sardana, A. K. Madan, J Mol Model **10**, 399 (2004).
[6] S. Sardana, A. K. Madan, MATCH Commun. Math. Comput. Chem. **43**, 85 (2001).
[7] A. R. Ashrafi, M. Saheli, M. Ghorbani, J. Comput. Appl. Math., Doi:10.1016/j.cam.2010.03.001.
[8] M. A. Hosseinzadeh, M. Ghorbani, J. Optoelectron. Adv. Mater. **11**, 1671 (2009).
[9] A. R. Ashrafi, M. Ghorbani, M. Jalali, J. Optoelectron. Adv. Mater. **3**, 823 (2009).
[10] A. R. Ashrafi, M. Ghorbani, J. Optoelectron. Adv. Mater. **3**, 596 (2009).
[11] S. Gupta, M. Singh, A. K. Madan, J. Math. Anal. Appl. **266**, 259 (2002).
[12] I. Gutman, N. Trinajstic, Chem. Phys. Lett. **17**, 535 (1972).
[13] J. Braun, A. Kerber, M. Meringer, C. Rucker, MATCH Commun. Math. Comput. Chem. **54**, 163 (2005).
[14] M. Ghorbani, M. A. Hosseinzadeh, Filomat, 2010, accepted.
[15] M. V. Diudea, I. E. Kacso, O. M. Minailiuc, MATCH Commun. Math. Comput. Chem., **28**, 61 (1992).
[16] M. V. Diudea, MATCH Commun. Math. Comput. Chem. **30**, 79 (1994).
[17] M. V. Diudea, MATCH Commun. Math.Comput. Chem. **2**, 71 (1995).
[18] M. V. Diudea, B. Parv, J. Chem. Inf. Comput. Sci. **35**, 1015 (1995).
[19] M. V. Diudea, G. Katona, B. Parv, Croat.Chem. Acta, **70**, 509 (1997).
[20] M. V. Diudea, A. A. Kiss, E. Estrada, N. Guevara, Croat. Chem. Acta, **73**, 367 (2000).
[21] M. Ghorbani, M. Jalali, Iranian Journal of Mathematical Sciences and Informatics, **2**, 61 (2007).
[22] A. R. Ashrafi, M. Ghorbani, M. Jalali and, Indian J. Chem., **47**A, 535 (2008).
[23] H. Yousefi-Azari, B. Manoochehrian, A. R. Ashrafi, Ars Combinatoria, **84**, 255 (2007).

*Corresponding author: mghorbani@srttu.edu