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COMPUTING SOME TOPOLOGICAL INDICES OF TRIANGULAR BENZENOID

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One of the best known and widely used is the connectivity index, χ introduced in 1975 by Milan Randić. In this paper we compute Randić, Zagreb, *GA* and *ABC* indices of some nanostructures.

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1. Introduction

All of the graphs in this paper are simple. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted [1].

Let $\sum$ be the class of finite graphs. A topological index is a function Top from $\sum$ into real numbers with this property that *Top*(*G*) = *Top*(*H*), if *G* and *H* are isomorphic. Obviously, the number of vertices and the number of edges are topological index. The Wiener [7] index 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. If $x, y \in V(G)$ then the distance $d_G(x, y)$ between *x* and *y* is defined as the length of any shortest path in *G* connecting *x* and *y*.

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstić [2]. They are defined as:

$$M_1(G) = \sum_{v \in V(G)} (\mathrm{d}_v)^2 \text{ and } M_2(G) = \sum_{uv \in E(G)} \mathrm{d}_u \, \mathrm{d}_v \, , \tag{1}$$

where d_u and d_v are the degrees of *u* and *v*.

The connectivity index introduced in 1975 by Milan Randić [3, 4, 5, 8], who has shown this index to reflect molecular branching. Randić index (Randić molecular connectivity index) was defined as follows:

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \, . \tag{2}$$

Another topological index namely, geometric – arithmetic index (GA) defined by Vukicević and Furtula [6] as follows:

$$GA(G) = \sum_{uv \in E} \frac{2\sqrt{\mathrm{d}_u \, \mathrm{d}_v}}{\mathrm{d}_u + \mathrm{d}_v} \, . \tag{3}$$

Recently Furtula et al. [1] introduced atom-bond connectivity (*ABC*) index, which it has been applied up until now to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows:

$$ABC(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \, d_u}} . \quad (4)$$

In this paper we compute these topological indices for two infinite classes of graphs, *e. g.* Triangular Benzenoid and *k*-polyomino system. Throughout this paper our notations are standard and mainly taken from [5]. Many papers, including those of our group of research have been dedicated to the topological indices [8-34].

2. Polyomino Chains of *k* – Cycles

A *k*-polyomino system is a finite 2-connected plane graph such that each interior face (also called cell) is surrounded by a regular 4*k*-cycle of length one. In other words, it is an edge-connected union of cells, see Klarner [3]. In Fig. 1, one can see the polyomino chains of 8 – cycles.

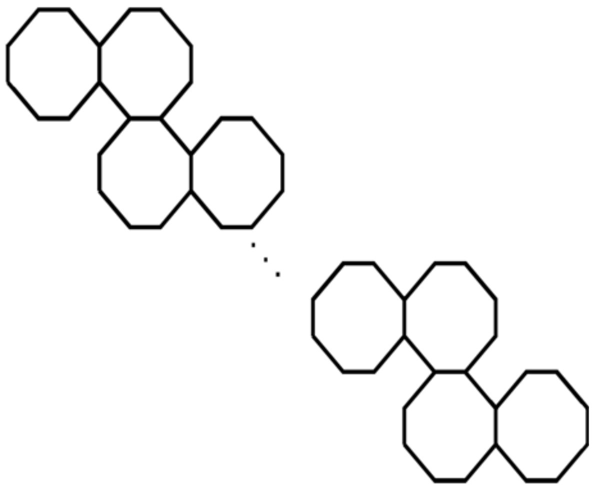

Fig. 1 The zig-zag chain of 8-cycles.

This graph has $n^2 + 4n + 1$ vertices and $\frac{3(n^2+3n)}{2}$ edges.

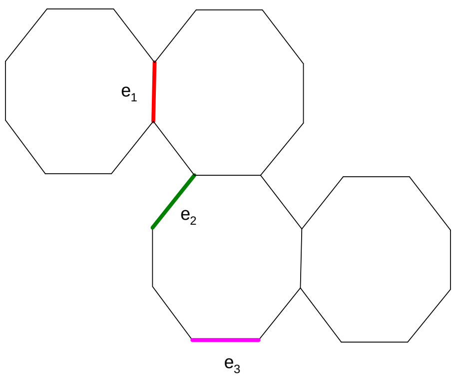

Fig. 2 The zig-zag chain of 8-cycles, n = 1.

For $n = 1$ (Fig. 2) there exist 3 type of edges, namely $e_1 = uv$, $e_2 = xy$ and $e_3 = ab$. On the other hand $d_u = d_v = 3$, $d_a = d_b = 2$ and $d_x = 2$, $d_y = 3$. This implies $M_1(G) = 134$, $M_2(G) = 157$, ABC(G) =

$12\sqrt{2}+5\sqrt{\frac{2}{3}}$, $GA(G) = 21+16\sqrt{\frac{6}{5}}$ and $\chi(G)=(29+4\sqrt{6})/3$. In generally, this graph has $24n + 12$ vertices, $28n + 1$ edges and the edge set of graph can be dividing to three partitions, *e. g.* $[e_1]$, $[e_2]$ and $[e_3]$. For every $e = uv$ belong to $[e_1]$, $d_u = d_v = 2$. Similarly, for every $e = uv$ belong to $[e_2]$, $d_u = d_v = 3$. Finally, if $e = uv$ be an edge of $[e_3]$, then $d_u = 2$ and $d_v = 3$. On the other hand, there are $8n - 3$, $12n + 4$ and $8n$ edges of type e_1, e_2 and e_3, respectively. Thus, we proved the following Theorem:

Theorem 1. Consider the graph G of zig-zag chain of 8-cycles. Then

$$M_1(G) = \sum_{uv\in[e_1]} 2+2 + \sum_{uv\in[e_2]} 3+3 + \sum_{uv\in[e_3]} 2+3 = (12n+4)4 + (8n-3)6 + 8n\times 5$$
$$= 136n - 2$$

$$M_2(G) = \sum_{uv\in[e_1]} 2\times 2 + \sum_{uv\in[e_2]} 3\times 3 + \sum_{uv\in[e_3]} 2\times 3 = (12n+4)4 + (8n-3)9 + 8n\times 6$$
$$= 168n - 11$$

$$GA(G) = \sum_{uv\in[e_1]} 1 + \sum_{uv\in[e_2]} 1 + \sum_{uv\in[e_3]} \frac{2\sqrt{2\times 3}}{5} = (\frac{16}{5}\sqrt{6}+20)n+1,$$

$$ABC(G) = \sum_{uv\in[e_1]}\sqrt{\frac{1}{2}} + \sum_{uv\in[e_2]}\frac{2}{3} + \sum_{uv\in[e_3]}\sqrt{\frac{1}{2}} = (\frac{30\sqrt{2}+8\sqrt{6}}{3})n + 2\sqrt{2}-\sqrt{6},$$

$$\chi(G) = \sum_{uv\in[e_1]}\frac{1}{2} + \sum_{uv\in[e_2]}\frac{1}{3} + \sum_{uv\in[e_3]}\frac{1}{\sqrt{6}} = (\frac{26+4\sqrt{6}}{3})n+1.$$

3. Triangular Benzenoid

In this section we compute four topological indices of triangular benzenoid graph depicted in Fig. 3. This graph has $n^2 + 4n + 1$ vertices and $\frac{3(n^2+3n)}{2}$ edges.

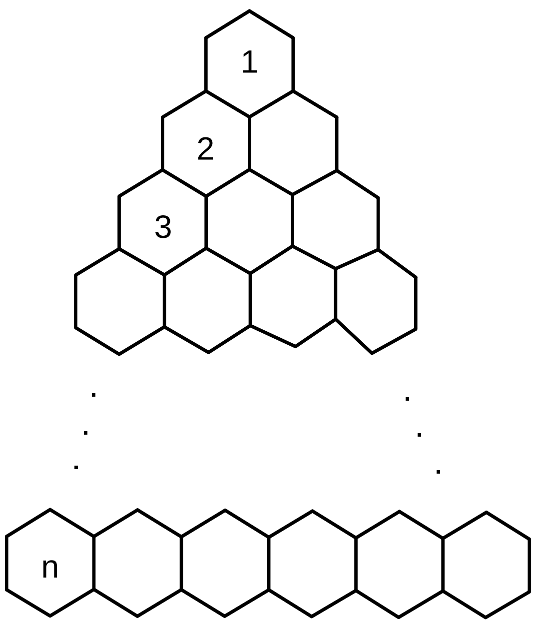

Fig. 3 Graph of triangular benzenoid G[n].

For n = 1 all of vertices are of degree 2. This implies $M_1(G) = M_2(G) = 24$, $ABC(G) = 3\sqrt{2}$, $GA(G) = 6$ and $\chi(G) = 3$. For n = 2, there are three type of edges, *e. g.* edges with endpoints 2 (e_1), edges with endpoints 3 (e_2) and edges with endpoints 2, 3 (e_3). By enumerating these edges there are 6, 3 and 6 edges of types 1, 2 and 3, respectively. In other words, $M_1(G) = 72$, $M_2(G) = 87$, $ABC(G) = 6\sqrt{2} + 2$, $GA(G) = \frac{12\sqrt{6}}{5} + 9$ and $\chi(G) = 4 + \sqrt{6}$. By continuing this method and using Fig. 4, the edge set of graph can be dividing to three partitions, e. g. $[e_1]$, $[e_2]$ and $[e_3]$.
The degree of end points of e_1 is 3, the degree of end points of e_2 is 3 and the degrees of end points of e_3 are 2, 3. On the other hand $|[e_1]| = 3n(n-1)/2$, $|[e_2]| = 6$ and $|[e_3]| = 6(n-1)$. Hence we have:

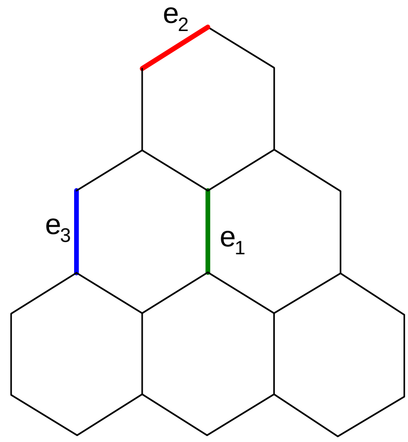

Fig. 4 Partition of edges of graph G[n], n = 3.

Theorem 2. Consider the triangular benzenoid graph $G[n]$. Then

$$M_1(G) = \sum_{uv\in[e_1]} 2+2 + \sum_{uv\in[e_2]} 3+3 + \sum_{uv\in[e_3]} 2+3 = 30(n-1) + 24 + 9n(n-1)$$

$$= 9n^2 + 21n - 6,$$

$$M_2(G) = \sum_{uv\in[e_1]} 2\times 2 + \sum_{uv\in[e_2]} 3\times 3 + \sum_{uv\in[e_3]} 2\times 3 = 36(n-1) + 24 + 27n(n-1)/2$$

$$= (27n^2 - 45n - 24)/2,$$

$$GA(G) = \sum_{uv\in[e_1]\cup[e_3]} 1 + \sum_{uv\in[e_2]} \frac{2\sqrt{6}}{5} = \frac{12\sqrt{6}}{5}(n-1) + \frac{(3n^2 - 3n + 12)}{2},$$

$$ABC(G) = \sum_{uv\in[e_1]\cup[e_3]} \frac{1}{\sqrt{2}} + \sum_{uv\in[e_2]} \sqrt{\frac{2}{3}} = 3\sqrt{2}n + n^2 - n,$$

$$\chi(G) = \sum_{uv\in[e_1]} \frac{1}{2} + \sum_{uv\in[e_2]} \frac{1}{3} + \sum_{uv\in[e_3]} \frac{1}{\sqrt{6}} = \sqrt{6}(n-1) + 3 + \frac{n(n-1)}{2}.$$

References

[1] E. Estrada, L. Torres, L. Rodriguez, I. Gutman, Indian J. Chem. 37A, 849 (1998).

[2] I. Gutman, N. Trinajstić, Chem. Phys. Lett. **17**, 535 (1972).
[3] D. A. Klarner, Polyominoes, In: J. E. Goodman, J. O'Rourke, (eds.) Handbook of Discrete and Computational Geometry, pp. 225–242. CRC Press, Boca Raton (1997) Chapter 12.
[4] M. Randić, J. Amer. Chem. Soc. **97**, 6609 (1975).
[5] N. Trinajstić, Chemical Graph Theory, CRC Press, Boca Raton, FL (1992).
[6] D. Vukičević and B. Furtula, J. Math. Chem. **46**, 1369 (2009).
[7] H. Wiener, J. Am. Chem. Soc. **69**, 17 (1947).
[8] P. Yu, J. Math. Study (Chinese) **31**, 225 (1998).
[9] M. Ghorbani, Optoelectronics and Advanced Materials-(RC), **4**(2), 261, 2010.
[10] A. R. Ashrafi, M. Saheli and M. Ghorbani, Journal of Computational and Applied Mathematics, http://dx.doi.org/10.1016/j.cam.2010.03.001.
[11] A. R. Ashrafi, H. Saati and M. Ghorbani, Digest Journal of Nanomaterials and Biostructures, **3**(4), 227 (2008).
[12] A. R. Ashrafi, M. Ghorbani and M. Jalali, Digest Journal of Nanomaterials and Biostructures, **3**(4), 245 (2008).
[13] M. Ghorbani and M. Jalali, Digest Journal of Nanomaterials and Biostructures, **3**(4), 269 (2008).
[14] A. R. Ashrafi and M. Ghorbani, Digest Journal of Nanomaterials and Biostructures, **4**(2), 313 (2009).
[15] A. R. Ashrafi, M. Ghorbani and M. Hemmasi, Digest Journal of Nanomaterials and Biostructures, **4**(3), 483 (2009).
[16] A. R. Ashrafi and M. Ghorbani, Digest Journal of Nanomaterials and Biostructures, **4**(2), 389 (2009).
[17] M. Ghorbani, M. B. Ahmadi and M. Hemmasi, Digest Journal of Nanomaterials and Biostructures, **3**(4), 269 (2009).
[18] M. Ghorbani and M. Jalali, Digest Journal of Nanomaterials and Biostructures, **4**(1), 177 (2009).
[19] M. Ghorbani and M. Jalali, Digest Journal of Nanomaterials and Biostructures, **4**(3), 403 (2009).
[20] A. R. Ashrafi, M. Ghorbani and M. Jalali, Optoelectron. Adv. Mater. – Rapid Comm., **3**(8), 823 (2009).
[21] A. R. Ashrafi and M. Ghorbani, Optoelectron. Adv. Mater. – Rapid Comm., **3**(6), 596 (2009).
[22] M. A. Hosseinzadeh and M. Ghorbani, J. Optoelectron. Adv. Mater., **11**(11), 1671 (2009).
[23] M. Ghorbani, A. R. Ashrafi and M. Hemmasi, Optoelectron. Adv. Mater. – Rapid Comm., **3**(12), 1306 (2009).
[24] M. Ghorbani and M. Jalali, Digest Journal of Nanomaterials and Biostructures, **4**(4), 681 (2009).
[25] M. Ghorbani, Optoelectron. Adv. Mater. – Rapid Comm., **4**(2), 261 (2010).
[26] M. A. Hosseinzadeh and M. Ghorbani, Optoelectron. Adv. Mater. – Rapid Comm., **4**(3), 378 (2010).
[27] M. Ghorbani and M. Jaddi, Optoelectron. Adv. Mater. – Rapid Comm., **4**(4), 540 (2010).
[28] H. Maktabi, J. Davoudi and M. Ghorbani, Optoelectron. Adv. Mater. – Rapid Comm., **4**(4), 550 (2010).
[29] M. Ghorbani and H. Hosseinzadeh, Optoelectron. Adv. Mater. – Rapid Comm., **4**(4), 538 (2010).
[30] M. Ghorbani, M. Ghazi and S. Shakeraneh, Optoelectron. Adv. Mater. – Rapid Comm., **4**(4), 538 (2010).
[31] M. Ghorbani, M. Ghazi and S. Shakeraneh, Optoelectron. Adv. Mater. – Rapid Comm., **4**(6), 893 (2010).
[32] A. Azad and M. Ghorbani, Optoelectron. Adv. Mater. – Rapid Comm., **4**(7), 1261 (2010).
[33] H. Mesgarani and M. Ghorbani, Optoelectron. Adv. Mater. – Rapid Comm., **4**(7), 1264 (2010).
[34] M. Ghorbani, A. Azad and M. Ghasemi, Optoelectron. Adv. Mater. – Rapid Comm., **4**(7), 1268 (2010).