

COMPUTING GEOMETRIC ARITHMETIC INDEX OF SOME GRAPHS

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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.

Let Σ be the class of finite graphs. A topological index is a function *Top* from Σ 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:

$$M_1(G) = \sum_{v \in V(G)} (d_v)^2 \text{ and } M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

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

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

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

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

$$GA(G) = \sum_{uv \in E} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

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:

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

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].

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 *4k*-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.

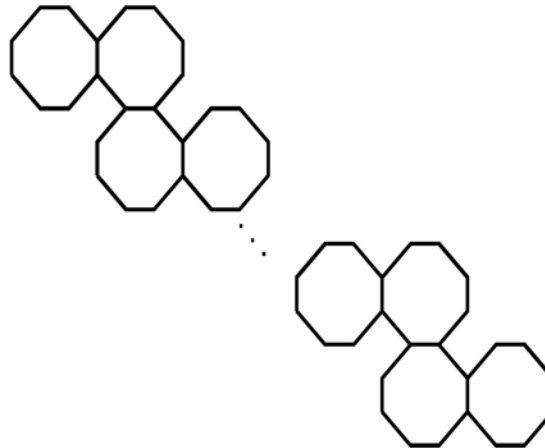


Fig. 1 The zig-zag chain of 8-cycles.

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

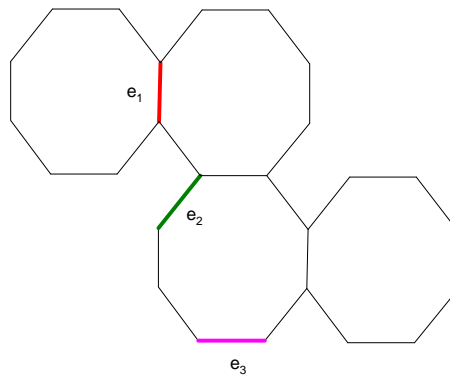


Fig. 2 The zig-zag chain of 8-cycles, $n = 1$.

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

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

$$= 136n - 2$$

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

$$= 168n - 11$$

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

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

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

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.

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 $[e_3]$.

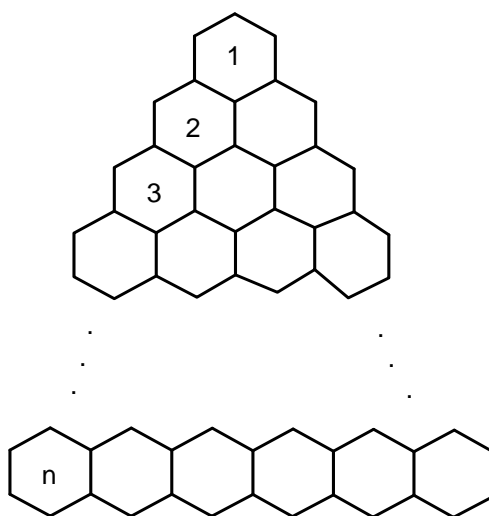


Fig. 3 Graph of triangular benzenoid $G[n]$.

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:

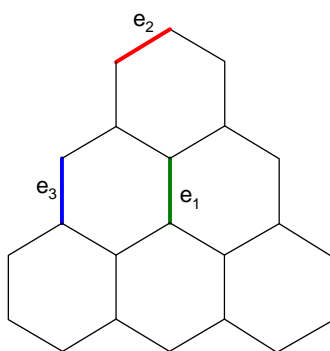


Fig. 4 Partition of edges of graph $G[n]$, $n = 3$.

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

$$\begin{aligned} M_1(G) &= \sum_{uv \in [e_1]} 2+2 + \sum_{uv \in [e_2]} 3+3 + \sum_{uv \in [e_3]} 2+3 = 30(n-1) + 24 + 9n(n-1) \\ &= 9n^2 + 21n - 6, \end{aligned}$$

$$\begin{aligned} M_2(G) &= \sum_{uv \in [e_1]} 2 \times 2 + \sum_{uv \in [e_2]} 3 \times 3 + \sum_{uv \in [e_3]} 2 \times 3 = 36(n-1) + 24 + 27n(n-1) / 2 \\ &= (27n^2 - 45n - 24) / 2, \end{aligned}$$

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

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

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

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