International Journal of Engineering and Technology Research
Vol. 3, No. 2, March 2015, pp. 1 - 4, ISSN: 2327 - 0349 (Online)
Available online at www.ijeatr.org

Short Communication

On Atom Bond Connectivity and Geometric-Arithmetic indices of a Benzenoid System

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Abstract:

The *GA* index is a topological index was defined as $GA(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d_u d_v}}{d_u+d_v}$ in which degree of a vertex u denoted by d_u. Atom bond connectivity index is another topological index was defined as $ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_u d_v}}$. In this paper we compute these topological indices for a type of Benzenoid Systems "*jagged-rectangle*".

Keywords: Molecular graph, Atom Bond Connectivity index, Geometric-Arithmetic index, Benzenoid Systems, jagged-rectangle.

INTRODUCTION

Throughout this paper graph means simple connected graph. Let $G=(V,E)$ be a simple connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. In chemical graph theory, the vertices of G correspond to the atoms and the edges of G correspond to the chemical bonds.

There exits many topological indices in Mathematical chemistry and Theoretical Chemistry [1-3]. The Wiener index [3] is the first reported distance based topological index by chemist *Harold Wiener* in 1947 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 $d(x,y)$ between x and y is defined as the length of any shortest path in G connecting x and y. The *Wiener index* [3] is equal to

$$W(G)=½\sum_{u\in V(G)}\sum_{v\in V(G)}d(u,v)$$

One of the important topological index is the *Geometric-Arithmetic index (GA)* considered by *D. Vukičević* and *B. Furtula* [4] as

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

where d_u and d_v are the degrees of the vertices u and v, respectively.

Recently *B. Furtula et al.* [5] introduced *Atom Bond Connectivity index (ABC)* is defined as follows

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

in which degree of vertex v, denoted by d_v.

In this paper, we compute these connectivity topological indices for a type of Benzenoid Systems "*jagged-rectangle*". Throughout this paper our notation is standard and mainly taken from standard book of graph theory [1-3, 6, 7].

MAIN RESULTS AND DISCUSSSION

Let $G(V, E)$, be a molecular graph with the vertex set $V(G)$ and edge set $E(G)$. The aim of this section is to compute the Atom Bond Connectivity and Geometric-Arithmetic indices for a type of Benzenoid Systems and called *jagged-rectangle* $B_{a,b}$ $(\forall a,b\in\mathbb{N})$.
This family of hexagonal systems was defined *Shui Ling-Ling et al.* A hexagonal jagged-rectangle $B_{a,b}$ whose shape forms a rectangle and the number of hexagonal cells in each chain alternate a and $a-1$. For $a\geq2$. Reader can see general representation of this benzenoid system in Figure 1 and references [8-12].

The vertex set of the jagged-rectangle $B_{a,b}$ defined as

$$V(B_{a,b})=\{(x,y)|0\leq x\leq 2a,\ 0\leq y\leq 2b-1\}\cup\{(x,-1)|\ 0\leq x\leq 2a-1\}\cup\{(x,2b)|1\leq x\leq 2b-1\}$$

The number of vertices in this benzenoid system is

$$|V(B_{a,b})|=2b(2a+1)+(2a-1)+(2a-1)=4ab+4a+2b-2$$

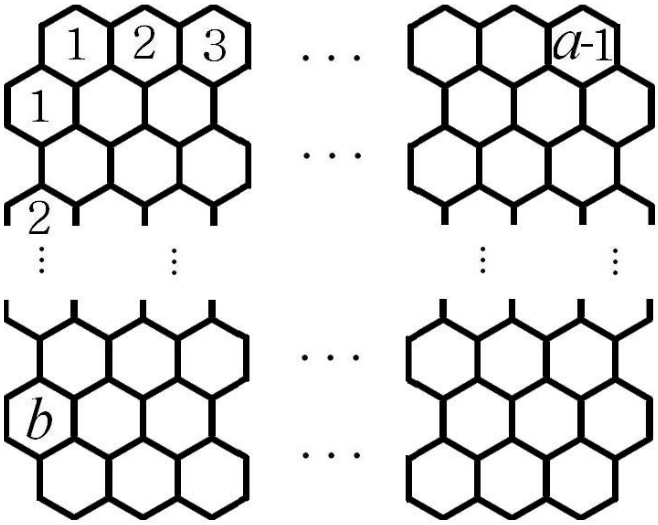

Fig. 1: A general representation of the Benzenoid system jagged-rectangle $B_{a,b}$ $(\forall a,b\geq2)$.

Theorem 1. $\forall a,b\in\mathbb{N}-\{1\}$, consider the Benzenoid system jagged-rectangle $B_{a,b}$. Then its Atom Bond Connectivity and Geometric-Arithmetic indices are equal to

$$ABC(B_{a,b})=4ab+(2/3+2\sqrt{2})a+(4\sqrt{2}-10/3)b-8/3$$

$$\text{And } GA(B_{a,b})=6ab+(4\sqrt{6}/5+1)a+(4\sqrt{6}/5-1)b-4\sqrt{6}/5$$

Before computing a extended formula for atom bond connectivity and geometric-arithmetic indices, we present this following definition:

Definition 1. Let G be the molecular graph and d_v is degree of vertex $v\in V(G)$ $(1\leq\delta\leq d_v\leq\Delta\leq n-1$, δ and Δ are the minimum and maximum degree of $d_v)$. We divide edge set $E(G)$ and vertex set $V(G)$ of graph G to several partitions, as follow:

$\forall k$: $\delta\leq k\leq\Delta$, $V_k=\{v\in V(G)|\ d_v=k\}$
$\forall i$: $2\delta\leq i\leq 2\Delta$, $E_i=\{e=uv\in E(G)|d_u+d_v=i\}$
$\forall j$: $\delta^2\leq j\leq\Delta^2$, $E_j^*=\{uv\in E(G)|d_u\times d_v=j\}$.

Proof. $\forall\ a,b\geq 2$, Let $G=B_{a,b}$ be the hexagonal system jagged-rectangle. From the structure of the jagged-rectangle $B_{a,b}$, one can see that there are two partitions V_2 and V_3 with their size as follow:

$V_2=\{v\in V(B_{a,b})|\ d_v=2\}\rightarrow|V_2|=2a+4b+2$
$V_3=\{v\in V(B_{a,b})|\ d_v=3\}\rightarrow|V_3|=|V(B_{a,b})|-|V_2|=4ab+2a-2b-4$

Thus, $|E(B_{a,b})|=½[2(2a+4b+2)+3(4ab+2a-2b-4)]=6ab+5a+b-4$.

By according to Definition 1, one can see that

$E_4=\{e=uv\in E(B_{a,b})|\ d_u=d_v=2\}\rightarrow|E_4|=|E_4^*|=b+4+b$
$E_5=\{e=uv\in E(B_{a,b})|\ d_u=3\ \&d_v=2\}\rightarrow|E_5|=|E_6^*|=2|E_4|+2(2(a-1-2))=4a+4b-4$
$E_6=\{e=uv\in E(B_{a,b})|\ d_u=d_v=3\}\rightarrow|E_6|=|E_9^*|=|E(B_{a,b})|-|E_4|-|E_5|=6ab+a-5b-4$

Hence $ABC(B_{a,b})=\sum_{uv\in E(B_{a,b})}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$

$$=\sum_{uv\in E_9^*}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}+\sum_{uv\in E_6^*}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}+\sum_{uv\in E_4^*}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$$
$$=|E_9^*|\sqrt{\frac{6-2}{9}}+|E_6^*|\sqrt{\frac{5-2}{6}}+|E_4^*|\sqrt{\frac{4-2}{4}}$$
$$=⅔\times(6ab+a-5b-4)+½\sqrt{2}\times(|E_4|+|E_5|)$$
$$=⅔(6ab+a-5b-4)+(2a+4b)\sqrt{2}$$
$$=4ab+(⅔+2\sqrt{2})a+(4\sqrt{2}-10/3)b-8/3.$$

And $GA(B_{a,b})=\sum_{uv\in E(B_{a,b})}\frac{2\sqrt{d_ud_v}}{d_u+d_v}$

$$=\sum_{uv\in E_9^*}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{uv\in E_6^*}\frac{2\sqrt{d_ud_v}}{d_u+d_v}+\sum_{uv\in E_4^*}\frac{2\sqrt{d_ud_v}}{d_u+d_v}$$
$$=2|E_9^*|\frac{\sqrt{9}}{6}+2|E_6^*|\frac{\sqrt{6}}{5}+2|E_4^*|\frac{\sqrt{4}}{4}$$
$$=(6ab+a-5b-4)+\sqrt{6}/5\times(4a+4b-4)+(4b+4)$$
$$=6ab+(4\sqrt{6}/5+1)a+(4\sqrt{6}/5-1)b-4\sqrt{6}/5$$

Here, we complete the proof of the Theorem 1.■

CONCLUSIONS

In Theoretical Chemistry, the topological indices and molecular structure descriptors are used for modeling physico-chemical, toxicologic, biological and other properties of chemical compounds and nano steucture analyzing.
In this paper, we counting two connectivity topological indices of an infinite family of Benzenoid Systems and called *jagged-rectangle* $B_{a,b}$ $(\forall a,b\in\mathbb{N})$.

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