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Research Article

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Cluj-Ilmenau index of hexagonal trapezoid system $T_{b,a}$ and triangular benzenoid G_n

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ABSTRACT

Let G(V,E) be a connected molecular graph without multiple edges and loops, with the vertex set V(G) and edge set E(G), and vertices/atoms x,y∈ V(G) and an edge/bond xy∈ E(G). Let m(G,c) be the number of qoc strips of length c (i.e. the number of cut-off edges) in the graph G. The Omega Polynomial Ω(G,x) and the Cluj-Ilmenau index CI(G) for counting qoc strips in G were defined by M.V. Diudea as $\Omega(G,x)=\sum_{c} m(G,c)x^{c}$ *and* $CI(G)=[\Omega(G,x)'^{2}-\Omega(G,x)'-\Omega(G,x)'']_{x=1}$*, respectively. In this paper, we compute an exact formula of these counting topological polynomial and its index for the Benzenoid molecular graphs "Hexagonal Trapezoid system* $T_{b,a}$ *and Triangular Benzenoid* G_n*".*

Keywords: Omega polynomial Ω(G,x), Cluj-Ilmenau index CI(G), Molecular graph, Hexagonal Trapezoid system.

INTRODUCTION

Let *G*(*V*,*E*) be a connected molecular graph without multiple edges and loops, with the vertex set *V*(*G*) and edge set *E*(*G*). In this paper, our notations are standard and mainly taken from [1-3]. A topological index is a numerical value associated with chemical constitution purporting for correlation of chemical structure properties, chemical reactivity or biological activity.

Usage of topological indices in chemistry began in 1947 when chemist *Harold Wiener* developed the most widely known topological descriptor, *Wiener index* [4] and is defined as

$$W(G)=\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} d(u,v)$$

where the distance *d(u,v)* between two vertices *u* and *v* is the number of edges in a shortest path connecting them.
In a connected graph *G*(*V*,*E*), with the vertex set *V*(*G*) and edge set *E*(*G*), two edges *e*=*uv* and *f*=*xy* of *G* are called *co-distant e co f* if they the following relation [5, 6]:

$$d(v,x)=d(v,y)+1=d(u,x)+1=d(u,y)$$

which is reflexive, that is, *e co e* holds for any edge *e* of *G*, and symmetric, *i.e.*, if *e co f* then *f co e* but, in general, relation *co* is not transitive. If "*co*" is also transitive, thus an equivalence relation, then *G* is called a *co-graph* and the set of edges *C(e):={f∈ E(G)| e co f})* is called an *orthogonal cut oc* of *G*, *E*(*G*) being the union of disjoint orthogonal cuts:

$E(G) = C_1 \cup C_2 \cup ... \cup C_{k-1} \cup C_k$ and $C_i \cap C_j = \varnothing$. $i \neq j$.

Klavžar [7] has shown that relation *co* is a theta *Djoković* [8], and *Winkler* [9] relation. Two edges *e* and *f* of a plane graph *G* are in relation *opposite, e op f,* if they are opposite edges of an inner face of *G*. Note that the relation *co* is defined in the whole graph while *op* is defined only in faces/rings. Using the relation *op* the edge set of *G* can be partitioned into *opposite* edge *strips*, *ops.* An *ops* is a quasi-orthogonal cut *qoc*, since *op* is, in general, not transitive. In *co*-graphs, the two strips superimpose to each other, then $C_k=S_k$ for any integer *k*.

The Omega *Polynomial Ω(G,x)* was defined by *M.V.* Diudea on the ground of quasi-orthogonal cut "qoc" edge strips [10]. Denote by *m*(*G*,*c*) the number of *ops* of length $c=|C_k|$ and the Omega polynomial is equal to [10-32]:

$$\Omega(G,x)=\sum_c m(G,c)\,x^c$$

The summation runs up to the maximum length of *qoc* strips in *G*. The first derivative (in *x*=1) equals the number of edges in the graph.

$$\Omega(G,1)'=\sum_c m(G,c)\times c=|E(G)|$$

Recently, the Cluj-Ilmenau *CI*(G) of a molecular graph *G* was defined by *M.V. Diudea* [23] as:

$$CI(G)=[\Omega(G,x)'^2-\Omega(G,x)'-\Omega(G,x)'']_{x=1}.$$

In this study we compute an exact formula of these counting topological polynomial and its index for the Benzenoid molecular graphs "Hexagonal Trapezoid system $T_{b,a}$ and Triangular Benzenoid G_n ($\forall a,b,n\in \mathbb{N}$-{1}, see their structures in Figure 1*)*. Here, we compute the Cluj-Ilmenau index of molecular graphs by using Cut Method and Orthogonal Cut Method. Cut and Orthogonal Cut Methods and their general form were studied by *S. Klavžar* [33] and *P.E. John et.al* [34], respectively.

THE CLUJ-ILMENAU INDEX OF "HEXAGONAL TRAPEZOID SYSTEM $T_{B,A}$"

In this section, we compute the Cluj-Ilmenau index of Benzenoid molecular graph "Hexagonal Trapezoid system $T_{b,a}$" ($\forall a\geq b\in \mathbb{N}$-{1}) by using Cut Method. A hexagonal Trapezoid system $T_{b,a}$ is a hexagonal system consisting $a-b+1$ rows of the Benzenoid chain in which every row has exactly one hexagon less than the immediate row. Reader can see general representation of this family in Figure 1 and Reference [31, 35-37].

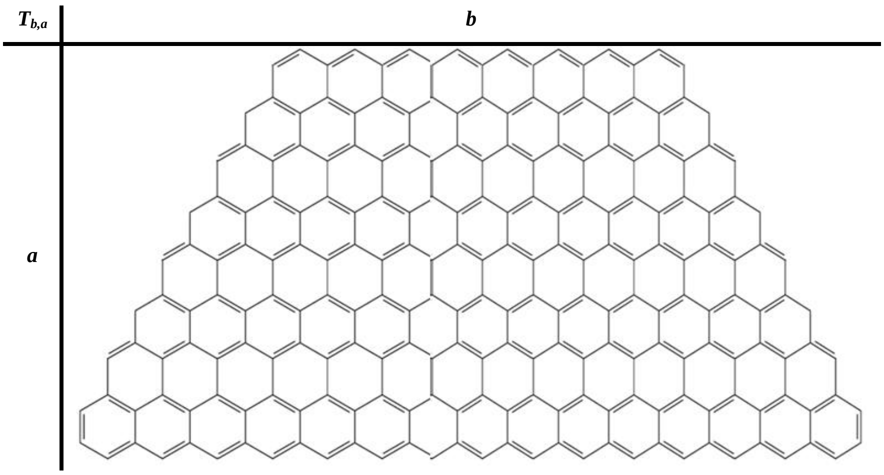

Figure 1. The general representations of this family of the Benzenoid molecular graphs "Hexagonal Trapezoid system $T_{b,a}$" ($\forall a,b\in \mathbb{N}$-{1})

Theorem 1 [36]: The Omega polynomial of the Hexagonal Trapezoid System $T_{b,a}$ ($\forall a\geq b\in \mathbb{N}$-{1}) is equal to :

$$\Omega(T_{b,a},x)=\sum_{i=1}^{a-b+1} x^{a+2-i}+\sum_{i=1}^{a-b} 2x^{i+1}+2bx^{a-b+2}$$

Theorem 2. The Cluj-Ilmenau index of the Hexagonal Trapezoid System $T_{b,a}$ ($\forall a\geq b\in \mathbb{N}-\{1\}$) is as follows:
$CI(T_{b,a})=\frac{1}{4}(9a^4+9b^4+18a^2b^2+50a^3+10b^3+6a^2b-46ab^2+75a^2+11b^2+10ab+10a+6b-16]$

Proof of Theorem 2. Consider the Hexagonal Trapezoid System $T_{b,a}$ for all $a,b\in\mathbb{N}-\{1\}$, with a^2-b^2+4a+2 ($=2a+1+\sum_{i=2b+1}^{2a+1} i$) the number of vertices and $2a+\sum_{i=3b+1}^{3a+1} i=½[3(a^2-b^2)+9a+b+2]$ the number of edges. Also, from Theorem 1, one can see that

$\Omega'(T_{b,a},x)=[x^{a-b+2}+x^{a-b+1}+\ldots+x^{a+1}+x^a+2x^2+2x^3+\ldots+2x^{a-b+1}+2bx^{a-b+2}]'$

$$=\left[\sum_{i=1}^{a-b+1}(a+2-i)\,x^{a-i+1}+\sum_{i=1}^{a-b}2(i+1)x^i+2(a-b+2)bx^{a-b+1}\right]$$

And

$$\Omega''(T_{b,a},x)=\frac{\partial}{\partial x}\left(\sum_{i=1}^{a-b+1}x^{a+2-i}+\sum_{i=1}^{a-b}2x^{i+1}+2bx^{a-b+2}\right)$$

$$=\left[\sum_{i=1}^{a-b+1}(a-i+1)(a-i+2)x^{a-i}+\sum_{i=1}^{a-b}2i(i+1)x^{i-1}+2(a-b+1)(a-b+2)bx^{a-b}\right]$$

And obviously

$$\Omega'(T_{b,a},1)=\sum_{i=1}^{a-b+1}(a+2-i)+\sum_{i=1}^{a-b}2(i+1)+2(a-b+2)b$$

$=(a-b+1)(a+2)-½(a-b+1)(a-b+2)+2(a-b)+(a-b)(a-b+1)+2b(a-b+2)=½[3(a^2-b^2)+9a+b+2]$

Also,

$$\Omega''(T_{b,a},1)=\left[\sum_{i=1}^{a-b+1}(a-i+1)(a-i+2)+\sum_{i=1}^{a-b}2i(i+1)+2(a-b+1)(a-b+2)b\right]$$

$$=\sum_{i=1}^{a-b+1}\left(a^2+i^2-i(2a+3)+3a+2\right)+2\sum_{i=1}^{a-b}\left(i^2+i\right)+2(a-b+1)(a-b+2)b$$

$$=\sum_{i=1}^{a-b}\left(a^2+3i^2-i(2a+1)+3a+2\right)+b(b+1)+2b(a^2+b^2-2ab+3a-3b+2)$$

$$=(a^2+3a+2)(a-b)+3\sum_{i=1}^{a-b}i^2-(2a+1)\sum_{i=1}^{a-b}i+(2a^2b+2b^3-4ab^2+6ab-5b^2+b+4)$$

$=(a^2+3a+2)(a-b)+\frac{3}{6}(a-b)(a-b+1)(2a-2b+1)-½(2a+1)(a-b)(a-b+1)$
$+(2a^2b+2b^3-4ab^2+6ab-5b^2+b+4)$
$=-b(a-b)(a-b+1)+(a^3+3a^2+a^2b+2b^3-4ab^2+3ab-5b^2+2a-b+4)$
$=(a^3+3a^2+b^3-2ab^2+2ab-4b^2+2a-b+4)$.

Table 1 [36]: The number of co-distant edges of the hexagonal Trapezoid system $T_{b,a}$ for all positive integer numbers a,b such that $a\geq b$.

quasi-orthogonal cuts	*The length of qoc strips*	*The number of qoc strips*
C_i $\forall$ $i=1,\ldots,a-b$	$i+1$	2
C_{a-b+1}	$a-b+2$	$2b$
c_i $\forall$ $i=1,\ldots,a-b+1$	$a-i+2$	1

Now, by above mentions formulas for $\Omega'(T_{b,a},x)$ and $\Omega''(T_{b,a},x)$ (x=1) and according to Figure 2 and Tables 1 [26], we can compute the Cluj-Ilmenau index of the Hexagonal Trapezoid System $T_{b,a}$ as follows:

$CI(T_{b,a})=[\Omega'(T_{b,a},x)]^2-[\Omega'(T_{b,a},x)+\Omega''(T_{b,a},x)]_{x=1}$
$=[\Omega'(T_{b,a},1)]^2-[\Omega'(T_{b,a},1)+\Omega''(T_{b,a},1)]$
$=[½(3a^2-3b^2+9a+b+2)]^2-[½(3a^2-3b^2+9a+b+2)+(a^3+3a^2+b^3-2ab^2+2ab-4b^2+2a-b+4)]$

$= \frac{1}{4}(9a^4+9b^4+18a^2b^2+50a^3+10b^3+6a^2b-46ab^2+75a^2+11b^2+10ab+10a+6b-16].$

Here the proof of theorem is completed.■

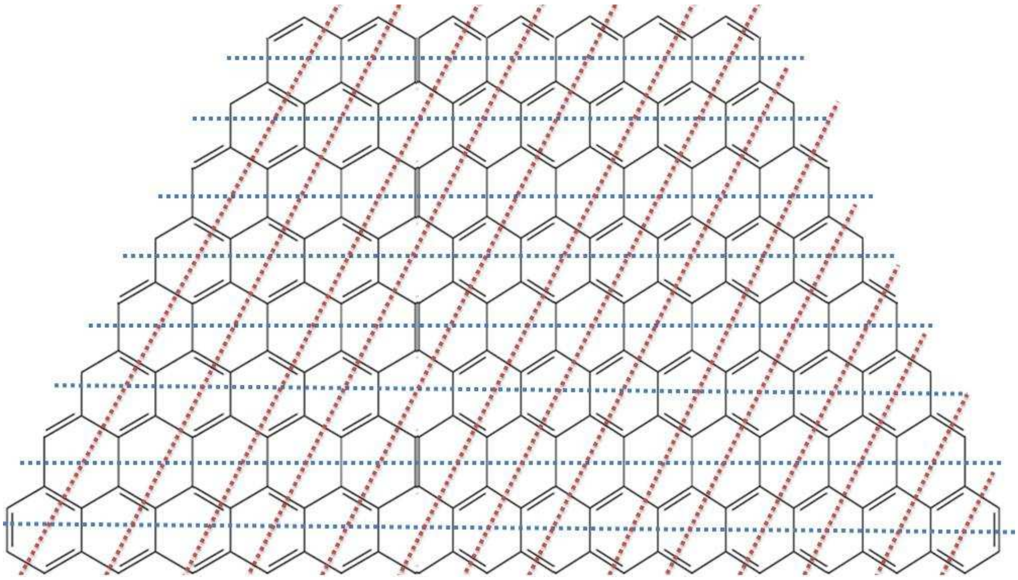

Figure 2: All strips cuts of the Hexagonal Trapezoid System $T_{b,a}$

THE CLUJ-ILMENAU INDEX OF "TRIANGULAR BENZENOID G_N"

The aim of this section is to compute the Cluj-Ilmenau index of the Triangular Benzenoid G_n $(\forall n\in \mathbb{N}-\{1\})$ by using Cut Method. From Figure 3, one can see that the Triangular Benzenoid G_n has exactly n^2+4n+1 vertices/atoms and $\frac{3}{2}n(n+3)$ edges/bonds [31, 35-37].

Now, by according to Figure 3, and using Theorems 1 and 2, we see that there are n strips C_1, C_2, …, C_n of length 2, 3, …, n+1, respectively in a general representation of the Triangular Benzenoid G_n. Thus, the Omega polynomial and the Cluj-Ilmenau index of G_n are as follow:

Theorem 3 [34]. The Omega polynomial of the Triangular Benzenoid G_n $(\forall n\in \mathbb{N}-\{1\})$ is equal to:

$\Omega(G_n,x)=3x^2+3x^3+\ldots+3x^{n+1}$

Theorem 4. The Cluj-Ilmenau index of the Triangular Benzenoid G_n $(\forall n\in \mathbb{N}-\{1\})$ is equal to:

$CI(G_n)= \frac{1}{4}(9n^4+50n^3+99n^2-26n+20].$

Proof of Theorem 4. Consider the Triangular Benzenoid G_n for all positive integer number n. So by using Theorem 2 and definition of G_n, we know that G_n is isomorphs with the Hexagonal Trapezoid System $T_{b,a}$ in case $b=1$ and $a=n$, therefore the Cluj-Ilmenau index of G_n or $T_{1,n}$ is as follows:

$CI(G_n)=[\Omega'(G_n\ x)]^2-[\Omega'(G_n,x)+\Omega''(G_n,x)]_{x=1}=CI(T_{1,n})=$

$= \frac{1}{4}(9n^4+9+18n^2+50n^3+10+6n^2-46n+75n^2+11+10n+10n+6-16].$

$= \frac{1}{4}(9n^4+50n^3+99n^2-26n+20].$

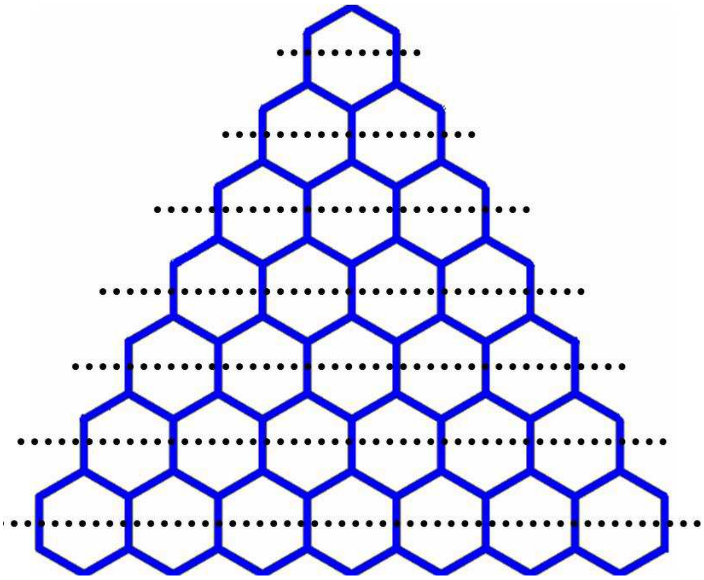

Figure 3 [31]: A general representation of the Triangular Benzenoid G_n or $T_{1,n}$ with all strips cuts

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