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OMEGA POLYNOMIALS AND CLUJ-ILMENAU INDEX OF CIRCUMCORONENE SERIES OF BENZENOID

MOHAMMAD REZA FARAHANI[1, *], KATALIN KATO[2], MIRANDA P. VLAD[3]

ABSTRACT. The "Omega" Ω(G,x) polynomial was defined by Diudea on the ground of quasi-orthogonal cut "qoc" edge strips. Two topological indices CI(G) (Cluj-Ilmenau index) and Omega index I_Ω are defined on the above polynomial. The goal of this paper is to compute the Omega polynomial and the corresponding indices in the circumcoronene series of benzenoids.

Keywords: *Omega polynomial, Cluj-Ilmenau index, Circumcoronene.*

INTRODUCTION

Let *G*=(*V*,*E*) be a molecular graph, with the vertex set *V*=*V*(*G*) and edge set *E*=*E*(*G*). Two edges *e*=*uv* and *f*=*xy* of G are called co-distant, "e co f", if and only if they obey the following relation [1]

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

where the distance d(x,y) between x and y is defined as the length of a shortest path between x and y. For some edges of *G* the following relations are satisfied [1,2]

$$e\ co\ e$$
$$e\ co\ f \Leftrightarrow f\ co\ e$$
$$e\ co\ f\ \&\ f\ co\ h \Rightarrow e\ co\ h$$

though the last relation is not always valid. In other words, relation *co* is not transitive, in general and if *co* is also transitive, the above relations represent an equivalence; then *G* is called a *co-graph* and $C(e)=\{f \in E(G);\ f\ co\ e\}$, denoting the set of edges in *G*, co-distant to the edge $e \in E(G)$, is called an *orthogonal cut* (denoted by oc) of *G*, *E*(*G*) being the union of disjoint orthogonal cuts

[1] *Department of Mathematics of Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran.* [*] *Mr_Farahani@Mathdep.iust.ac.ir*
[2] *Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, 400028, Aranj Janos 11, Cluj, Romania*
[3] *Faculty of Economic Sciences Cluj, Dimitrie Cantemir University, Bucharest*

$$\mathrm{E}(\mathrm{G}) = \mathcal{C}_1 \cup \mathcal{C}_2 \cup ... \cup \mathcal{C}_{k-1} \cup \mathcal{C}_k \text{ and } \mathcal{C}_i \cap \mathcal{C}_j = \varnothing,$$
$$\text{for } i \neq j \quad \text{and} \quad i,j = 1,2,..,k.$$

If any two consecutive edges *e* and *f* of a plane graph *G* of an edge-cut sequence are topologically parallel within the same face of the covering, such a sequence is called a quasi-orthogonal cut qoc strip. Obviously, any orthogonal cut strip is a qoc strip but the reverse is not always true. This means the transitivity relation of the *co* relation is not necessarily obeyed [1, 3-5].

The *Omega Polynomial Ω(G,x)* for counting qoc strips in G was defined by *M.V. Diudea* [6] as

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

where m(G,c) denote the number of qoc strips of length c. The summation runs up to the maximum length of qoc strips in G.

Also, first derivative of Omega polynomial (in *x*=1) equals the number of edges in the graph G (see also [1-4, 6-9])

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

An index, called *CI* (Cluj-Ilmenau), is derived from and its first and second derivatives, in *x*=1, as [5]

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

CI index is eventually equal to the well-known *Padmakar-Ivan index* (PI) [1, 10], in polycyclic graphs embedded in the plane. *PI* index of G is an important topological descriptor in chemical graph theory and is defined as

$$PI(G) = \sum_{e \in E(G)} \left(m_u(e|G) + m_v(e|G)\right)$$

where $m_u(e|G)$ is the number of edges of G lying closer to u than to v and $m_v(e|G)$ is the number of edges of G lying closer to v than to u.

Another single number descriptor is calculable from the Ω(*G,x*) derivatives *d*, in *x*=1, and normalized to the first polynomial derivative. The Omega index is equal to

$$I_\Omega(G) = \frac{1}{\Omega'(G,\mathrm{x})} \sum_d \sqrt[d]{\Omega^d(G,\mathrm{x})}\Bigg|_{x=1}$$

In fact, d is up to the maximum length of qoc strips in G.

The aim of this study is to compute the Omega polynomial, Omega and Cluj-Ilmenau index of Circumcoronene series of benzenoidd H_k, with *k* being a positive integer number. A general representation of circumcoronene family is shown in Figure 1.

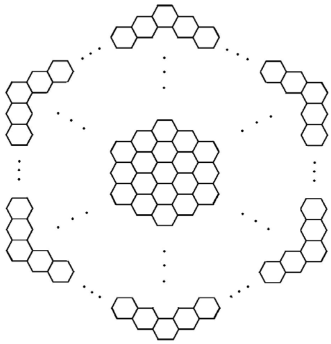

Figure 1. A view of circumcoronene series of benzenoids $H_k, k \geq 1$.

RESULTS AND DISCUSSION

The aim of this paper is to compute the Omega polynomial and Omega and Cluj-Ilmenau indices of Circumcoronene series of benzenoids. We know that the general case of this molecular graph has $6k^2$ vertices and $9k^2-3k$ edges (Figure 1).

Theorem 1. Consider the molecular graph of Circumcoronene series of benzenoids $H_k, \forall k \in \mathbb{N}$, then

- The Omega polynomial of H_k is as follows

$$\Omega(H_k, x) = 6\sum_{i=1}^{k-1} x^{k+i} + 3x^{2k}$$

- The Cluj-Ilmenau index of H_k is equal to

$$CI(H_k) = k(81k^3 - 68k^2 + 12k - 1)$$

- The Omega index of H_k is

$$I_\Omega(H_k) = \left(\frac{1}{9k^2-3k}\right)\sum_{d=1}^{2k} \sqrt[d]{6\sum_{i=1}^{k-1}\left(\prod_{j=0}^{d-1}(k+i-j)\right) + 3\left(\prod_{j=0}^{d-1}(2k-j)\right)}$$

Proof. Let $G = H_k$ be the Circumcoronene series of benzenoids. This graph has $6k^2$ vertices. *Cut Method* and its general form was studied by *S. Klavzar* [11] and others [5, 12]. Now, by using this method and Figure 1, there are k distinct cases of qoc strips. Obviously, Circumcoronene series of benzenoids is a co-graph, thus the size of a qoc strip $\mathcal{C}_i$ for every $(\mathrm{i}=1,\dots,\mathrm{k}-1)$

is equal to $k+i=c_i$ since $\forall e \in \mathcal{C}_i$ there are k+i-1 co-distant edges with e (see Figure 2.) and the number of repetitions of these quasi-orthogonal cuts $\mathcal{C}_i$ $\forall \mathrm{i}=1,\dots,\mathrm{k}-1$ is six times $\left(\mathrm{m}(H_k, c_i)=6\right)$. The number of repetitions of qoc $\mathcal{C}_k$ is three times $\left(\mathrm{m}(H_k, c_k)=3\right)$, respectively. This implies that

$$3|\mathcal{C}_k|+6|\mathcal{C}_{k-1}|+\dots+6|\mathcal{C}_1|=6\sum_{i=1}^{k}[k+i]-6k=9k^2-3k=\left|E(H_k)\right|.$$

So, we have

$$\begin{aligned}\Omega(H_k,\mathrm{x}) &= \sum\nolimits_c \mathrm{m}(H_k,c)\,\mathrm{x}^c \\ &= \sum_{\substack{i=1\\ c_i=k+i}}^{k} \mathrm{m}(H_k,c_i)\,\mathrm{x}^{c_i} \\ &= \sum_{i=1}^{k-1}\left(\mathrm{m}(H_k,c_i)\,\mathrm{x}^{c_i}\right)+\mathrm{m}(H_k,c_k)\,\mathrm{x}^{c_k} \\ &= \sum_{i=1}^{k-1}\left(6\mathrm{x}^{k+i}\right)+3x^{2k}\end{aligned}$$

Now, we can calculate the Cluj-Ilmenau index of H_k as

$$\begin{aligned}CI(H_k) &= \left[\Omega'(H_k,\mathrm{x})\right]^2-\left[\Omega'(H_k,\mathrm{x})+\Omega''(H_k,\mathrm{x})\right]_{x=1} \\ &= \left[\left(\sum_{i=1}^{k-1}\left(6\mathrm{x}^{k+i}\right)+3x^{2k}\right)'\right]^2-\left[\left(\sum_{i=1}^{k-1}\left(6\mathrm{x}^{k+i}\right)+3x^{2k}\right)'+\left(\sum_{i=1}^{k-1}\left(6\mathrm{x}^{k+i}\right)+3x^{2k}\right)''\right]_{x=1} \\ &= \left[6\sum_{i=1}^{k-1}(k+i)\,\mathrm{x}^{(k+i-1)}+6kx^{2k-1}\right]^2- \\ &\quad -\left[6\sum_{i=1}^{k-1}(k+i)\,\mathrm{x}^{(k+i-1)}+6kx^{2k-1}+6\sum_{i=1}^{k-1}(k+i)(k+i-1)\,\mathrm{x}^{(k+i-2)}+6k(2k-1)\,x^{2k-2}\right]_{x=1} \\ &= \left[6\sum_{i=1}^{k-1}(k+i)+6k\right]^2-\left[6\sum_{i=1}^{k-1}(k+i)+6k+6\sum_{i=1}^{k-1}(k+i)(k+i-1)+6k(2k-1)\right] \\ &= k(81k^3-68k^2+12k-1)\end{aligned}$$

Now, we compute the Omega index of Circumcoronene series of benzenoids as

$$I_\Omega(H_k)=\frac{1}{\Omega'(H_k,\mathrm{x})}\sum_d \sqrt[d]{\Omega^d(H_k,\mathrm{x})}\Bigg|_{x=1}$$

since $$\Omega^d(H_k,\mathrm{x}) = 6\sum_{i=1}^{k-1}\left(\prod_{j=0}^{d-1}(k+i-j)\right)\mathrm{x}^{(k+i-d)} + 3\left(\prod_{j=0}^{d-1}(2k-j)\right)x^{2k-d}$$

In final, for every integer k, $I_\Omega(H_k)$ will be

$$I_\Omega(H_k) = \left(\frac{1}{9k^2-3k}\right)\sum_{d=1}^{2k}\sqrt[d]{6\sum_{i=1}^{k-1}\left(\prod_{j=0}^{d-1}(k+i-j)\right)+3\left(\prod_{j=0}^{d-1}(2k-j)\right)}$$

Thus completing the demonstration.

Lemma 2. By refering to the definition of I_Ω it is easy to see that $I_\Omega(G) \geq 1$.

Since $$I_\Omega(G) = \underbrace{\frac{1}{\Omega'(G,\mathrm{x})}\sqrt[1]{\Omega'(G,\mathrm{x})}\Bigg|_{x=1}}_{=1} + \underbrace{\frac{1}{\Omega'(G,\mathrm{x})}\sum_{d\in\mathbb{N}-\{1\}}\sqrt[d]{\Omega^d(G,\mathrm{x})}\Bigg|_{x=1}}_{\geq 0}$$

The second part of the above equation is positive, because polynomial $\Omega(\mathrm{G},\mathrm{x}) = \sum_c \mathrm{m}(\mathrm{G},c)\,\mathrm{x}^c$ and its all derived of order d have positive integer coefficients. Of course, if s is the maximum length of qoc strips in G, then $\Omega^d(G,\mathrm{x}) = 0, \forall d \geq s$.

Obviously, this lower bound of $I_\Omega(G)$ holds if and only if G is the complete graph K_2 or path P_2.

Conjecture 1. For every molecular graph G, the upper bound of $I_\Omega(G)$ is two. Thus, we have

$$\frac{1}{\Omega'(G,\mathrm{x})}\sum_{d\in\mathbb{N}-\{1\}}\sqrt[d]{\Omega^d(G,\mathrm{x})}\Bigg|_{x=1} < 2$$

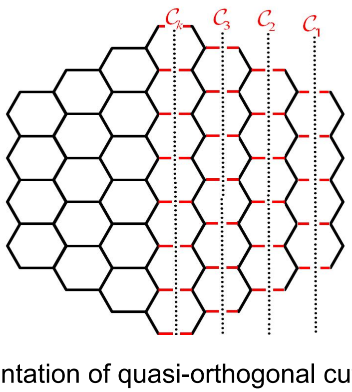

Figure 2. The presentation of quasi-orthogonal cuts qoc strips of H_4.

Example 1. By Figure 2, it is obvious that the Omega polynomial of H_4 is as follows:

$$\Omega(H_4, x) = 6x^5 + 6x^6 + 6x^7 + 3x^8$$

Also, the CI and I_Ω indices of H_4 are equal to $CI(H_4) = 16572$ and $I_\Omega(H_4) =$ 1.586

CONCLUSIONS

In this paper, we obtained the Omega polynomial, Omega and Cluj-Ilmenau indices of molecular graph Circumcoronene series of benzenoids H_k $(k \geq 1)$ and for the first time and we conjectured the lower and upper bounds for I_Ω of any molecular graph G, as $1 \leq I_\Omega(G) < 2$.

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