Short communication

Computing *Θ(G,x)* and *Π(G,x)* Polynomials of an Infinite Family of Benzenoid

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Abstract

The topological index of a graph *G* is a numeric quantity related to *G* which is invariant under automorphisms of *G*. The Omega polynomial *Ω(G,x)* for counting qoc strips in *G* is defined as $\Omega(G,x) = \Sigma_c\, m(G,c)x^c$ with *m(G,c)* being the number of strips of length *c*. Other three related polynomials can be calculated on ops as $\Theta(G,x) = \Sigma_c m(G,c)cx^c$, $Sd(G,x) = \Sigma_c m(G,c)x^{|E(G,x)|-c}$ and $\Pi(G,x) = \Sigma_c m(G,c)cx^{|E(G)|-c}$. The above polynomials count codistant and non-codistant edges, respectively. In this paper we compute the Theta *Θ(G,x)*, Pi *Π(G,x)* polynomials and the corresponding indices in the circumcoronene series of benzenoids.

Keywords: Circumcoronene Series of Benzenoid, qoc strip, Omega polynomial, Theta polynomial, Pi polynomial.

1. Introduction

Let $G = (V,E)$ be a simple connected graph with the vertex set $V = V(G)$ and the edge set $E = E(G)$, without loops and multiple edges. Two edges $e = uv$ and $f = xy$ of *G* are called codistant (briefly: *e* co *f*) if they obey the topologically parallel edges relation. For some edges of a connected graph *G* there are the following relations satisfied:[1–3]

$$e\ co\ e$$

$$e\ co\ f \Leftrightarrow f\ co\ e$$

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

though the last relation is not always valid. Set $C(e) = \{f \in E(G)\,|\, f\ co\ e\}$, denoting the set of all co-distant edges in *G*. If the relation "co" is transitive on *C(e)* then *C(e)* is called an orthogonal cut "oc" of the graph *G*. Then *G* is called a *co-graph* and *E*(*G*) being the union of disjoint orthogonal cuts.

Let *m(G,c)* be the number of qoc strips of length *c* in the graph *G*. Four counting polynomials have been defined[3–26] on the ground of qoc strips:

$$\Omega(G,x) = \sum_c m(G,c)x^c \tag{1}$$

$$\Theta(G,x) = \sum_c m(G,c)c.x^c \tag{2}$$

$$Sd(G,x) = \sum_c m(G,c)x^{|E(G)|-c} \tag{3}$$

$$\Pi(G,x) = \sum_c m(G,c)c.x^{|E(G)|-c} \tag{4}$$

Ω(G,x) and *Θ(G,x)* polynomials count codistant edges in *G* while *Sd(G,x)* and *Π(G,x)*, non-codistant edges. The first derivative (computed at $x = 1$) of these counting polynomials provide interesting topological indices:

$$\Omega'(G,1) = \sum\nolimits_c m(G,c)\times c = |E(G)| \tag{5}$$

$$\Theta'(G,1) = \sum\nolimits_c m(G,c)\times c^2 \tag{6}$$

$$Sd'(G,1) = \sum\nolimits_c m(G,c)\times(|E(G)|-c) \tag{7}$$

$$\Pi'(G,1) = \sum\nolimits_c m(G,c)\times c(|E(G)|-c) = |E(G)|^2 - \Theta(G) \tag{8}$$

Other indices, called *CI* (Cluj-Ilmenau) and Omega, as[12]

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

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

where d^{th} derivatives is up to the maximum length of qoc strips in G. By definition of Omega and Theta polynomials, one can obtain the Sadhana $Sd(G,x)$ and Pi $\Pi(G,x)$ polynomials by replacing x^c with $x^{|E|-c}$ in Omega and Theta polynomials. Then the Sadhana index will be the first derivative of $Sd(G,x)$ evaluated at $x = 1$. Herein, our notation is standard and taken from the standard book of graph theory.[27]

2. Main Results and Discussion

The aim of this section is to compute the counting polynomials (Omega, Sadhana, Theta and Pi) of codistant of an infinite family Circumcoronene Series of Benzenoid H_k ($\forall k \in \mathbb{N}$) with $6k^2$ vertices/atoms and $9k^2$-$3k$ edges/bonds. A general representation of circumcoronene family is shown in Figure 1.

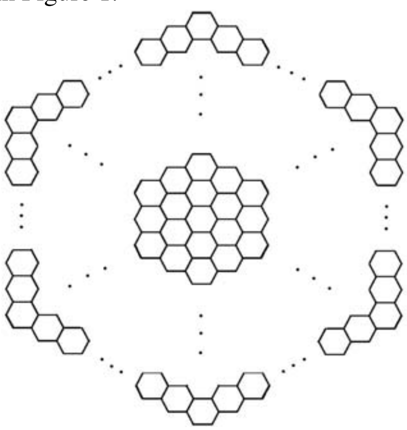

Figure 1. A representation of circumcoronene series of benzenoids H_k $k \geq 1$.

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

– The Omega polynomial of H_k is as follows

$$\Omega(H_k,x) = 6\sum_{i=1}^{k-1} x^{k+i} + 3x^{2k} \tag{9}$$

– The Cluj-Ilmenau index of H_k is equal to

$$CI(H_k) = k(81k^3 - 68k^2 + 12k - 1) \tag{10}$$

– The Omega index of H_k is

$$I_{\Omega}(H_k) = \left(\frac{1}{9k^2-3k}\right) \sum_{d=1}^{2k}\sqrt[d]{6\sum_{i=1}^{k-1}\left(\prod_{j=0}^{d-1}(k+i-j)\right)+3\left(\prod_{j=0}^{d-1}(2k-j)\right)} \tag{11}$$

Theorem 2. The Sadhana polynomial and Sadhana index of circumcoronene series of benzenoids H_k for $k \geq 1$ are as follow:

$$Sd(H_k,x) = \sum_{i=1}^{k-1}\left(6x^{(9k^2-4k-i)}\right) + 3x^{(9k^2-5k)} \tag{12}$$

$$Sd(H_k) = 54k^3 + 11k^2 - 16k \tag{13}$$

Theorem 1 and Theorem 2 were proved by M. R. Farahani, K. Kato and M. P. Vlad in references.[28] So we have following theorem:

Theorem 3. Consider the circumcoronene series of benzenoids H_k for $k \geq 1$; the Theta and Pi polynomials and their indices are calculated by formulas:

$$\begin{aligned}\Theta(H_k,x) &= 6(k+1)x^{k+1} + 6(k+2)x^{k+2} + \ldots \\ &+ 6(2k-2)x^{2k-2} + 6(2k-1)x^{2k-1} + 3(k)x^{2k} \\ &= 6\sum_{i=1}^{k-1}(k+i)x^{k+i} + 6kx^{2k}\end{aligned} \tag{14}$$

$$\Pi(H_k,x) = \sum_{i=1}^{k-1}\left(6(k+i)x^{(9k^2-4k-i)}\right) + 6kx^{(9k^2-5k)}$$

$$\Theta(H_k) = 12k^3 - 15k^2 + k \tag{15}$$

and $\Pi(H_k) = 81k^4 - 66k^6 + 24k^2 - k$

Proof. By Figure 1, there are k distinct cases of *qoc* strips in H_k for $k \geq 1$. We denote the corresponding edges by $e_1, e_2, \ldots, e_{k-1}$ and e_k. Also we denote the orthogonal cut $C(e_i)$ of the molecular graph H_k by C_i such that ($\forall i, j = 1, 2, \ldots, k$ & $i \neq j$; $E(H_k) = C_1 \cup C_2 \cup \ldots \cup C_{k-1} \cup C_k$ and $C_i \cap C_j = \varnothing$, and obviously the circumcoronene series of benzenoids H_k is a *co-graph*. By the reference,[28] it's easy to see that ($\forall i = 1, 2, \ldots, k$ the size of a qoc strip C_i ($= C(e_i)$) is equal to $k+i = c_i$ and $m(H_k,c_i) = 6$ for $i = 1,2,\ldots,k-1$ and $m(H_k,c_k) = 3$. *Then*

$$\begin{aligned}\Theta(H_k,x) &= \sum_c m(H_k,c) \times cx^c \\ &= \sum_{c_i=k+i,\, i=1}^{k} m(H_k,c_i) \times c_i x^{c_i} \\ &= \sum_{i=1}^{k-1}\left(6c_i x^{c_i}\right) + 3c_k x^{c_k} \\ &= \sum_{i=1}^{k-1}\left(6(k+i)x^{k+i}\right) + 6kx^{2k}\end{aligned}$$

and

$$\begin{aligned}\Theta(H_k) &= \Theta'(H_k,1) = 6\sum_{i=1}^{k-1}(k+i)^2 + 3(2k)^2 \\ &= 6\sum_{i=1}^{k-1}\left(k^2 + 2ki + i^2\right) + 12k^2 \\ &= 6k^2(k-1) + 12k\sum_{i=1}^{k-1} i + 6\sum_{i=1}^{k-1} i^2 \\ &+ 12k^2 = 12k^3 - 15k^2 + k\end{aligned}$$

Finally, the Pi polynomial *($\Pi(H_k,x)$)* will be

$$\Pi\left(H_k,\mathrm{x}\right)=\sum\nolimits_{c} m\left(H_k,c\right)\times c.\mathrm{x}^{\left|E(H_k)\right|-c}$$

$$=\sum_{c_i=k+i,i=1}^{k} m\left(H_k,c_i\right)\times c_i\,\mathrm{x}^{\left|E(G)\right|-c_i}$$

$$=\sum_{i=1}^{k-1}\left(6(k+i)\mathrm{x}^{\left(9k^2-3k-k-i\right)}\right)+3\left(2k\right)x^{\left(9k^2-5k\right)}$$

and $\Pi(H_k)$ is equal to

$$\Pi'(H_k,1)=\sum_{c_i=k+i,i=1}^{k} m\left(H_k,c_i\right)\times c_i\left(\left|E\left(H_k\right)\right|-c_i\right)$$

$$=\left|E\left(H_k\right)\right|^2-\Theta\left(H_k\right)$$

$$=\left(9k^2-3k\right)^2-\left(12k^3-15k^2+k\right)$$

$$=81k^4-66k^6+24k^2-k$$

Here the proof is completed.

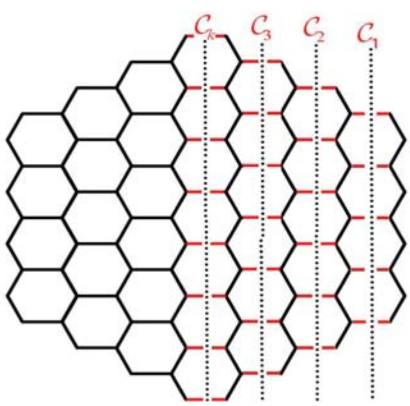

Figure 2. The presentation of quasi-orthogonal cuts qoc strips of H_4.

3. Conclusions

We demonstrated the determination of two topological polynomials and their topological indices of the molecular graphs of circumcoronene series of benzenoids. . The new topological indices are useful to characterize the structure of molecular graphs by counting *qoc* strips. The indices developed contribute to the pool of topological indices that can be used as molecular structure descriptors for modeling physicochemical, toxicological, biological and other properties of chemical compounds, including the analysis of nano structures. Arguably, the best known of these polynomials is the Omega polynomial $\Omega(G,x)$ and three related polynomials: the Sadhana Sd(G,x), Pi $\Pi(G,x)$ and Theta $\Theta(G,x)$ polynomials. The Omega polynomial was defined recently by M. V. Diudea and this subject became a challenge for many scientific research groups.

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Povzetek

Topološki indeks grafa G je numerična vrednost grafa G, ki je invariantna glede na avtomorfizme grafa. Omega poliniom $\Omega(G,x)$ za enumeracijo pasov v G je definiran kot $\Omega(G,x) = \Sigma_c\, m(G,c)x^c$, kjer je $m(G;c)$ število pasov dolžine c. Ostali trije podobni polinomi so $\Theta(G,x) = \Sigma_c m(G,c)cx^c$, $Sd(G,x) = \Sigma_c m(G,c)x^{|E(G,x)|-c}$ in $\Pi(G,x) = \Sigma_c m(G,c)cx^{|E(G)|-c}$. Omenjeni polinomi preštevajo enako oddaljene oz. različno oddaljene povezave. V tem članku izračunamo $\Theta(G,x)$ in $\Pi(G,x)$ ter pripadajoče indekse za neskončno družino cirkumkoronenov.