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OMEGA POLYNOMIAL OF A BENZENOID SYSTEM

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ABSTRACT. The Omega polynomial *Ω(G,x)* is defined as the collection of the equidistant, topologically parallel opposite edge stripes in the molecular graph. This polynomial was introduced by *Diudea* in 2006. In this paper, we compute the Omega polynomial of an important class of benzenoid system.

Keywords: *Molecular graph, Omega polynomial, Opposite edge strip, Benzenoid systems.*

INTRODUCTION

Let *G* be a simple connected graph in the Chemical Graph Theory. The vertex set and edge set of the molecular graph G are denoted by *V(G)* and *E(G)* respectively and its vertices correspond to the atoms while the edges correspond to the covalent bonds [1,2].

A topological index of *G* is a numeric quantity, derived following certain rules, which can be used to characterize the property of molecules and is invariant under the automorphism of the graph. Usage of topological indices in chemistry began in 1947 when *Harold Wiener* developed the most widely known topological descriptor, *Wiener index* [3], defined as

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

where the topological distance *d(u,v)* between two vertices *u* and *v* is the number of edges in the shortest path connecting them.

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Let *G*(*V*,*E*), be a molecular graph; two edges *e*=*uv* and *f*=*xy* of *G* are called co-distant (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 [4-7]

e co e

e co f ↔ *f co e*

e co f & *f co h* → *f co h*

though the last relation is not always valid.

Set *C(e):={f∈E(G)| e co f}*. If the relation "co" is transitive on *C(e)* then C(e) is called an *orthogonal cut "oc"* of the graph *G*. The graph *G* is called co-graph if and only if the edge set *E(G)* is the union of disjoint orthogonal cuts.

$$E(G) = \mathcal{C}_1 \cup \mathcal{C}_2 \cup ... \cup \mathcal{C}_{k-1} \cup \mathcal{C}_k \text{ and } \mathcal{C}_i \cap \mathcal{C}_j = \varnothing,$$

for *i≠j and i, j=1, 2, …, k.*

The Omega polynomial *Ω(G,x)* counts the "quasi-orthogonal cut' strips, qoc strips (because the relation is not always transitive, see above) in *G* and was defined by *M.V. Diudea* (2006) as

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

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

The first derivative of Omega polynomial (in *x=1*), equals the number of edges in *G* (see also the papers [8-16]):

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

Herein, our notations are standard and taken from the standard books of Graph Theory [1,2]. The aim of this study is to compute the Omega polynomial of an important class of benzenoid system called hexagonal system $B_{m,n}$ (Figure1).

RESULTS AND DISCUSSION

The Omega polynomial of an infinite family of benzenoid system was computed as described above.

Shui Ling-Ling et al.[17] defined a new hexagonal system named jagged-rectangle. An *a*×*b* hexagonal jagged-rectangle whose shape forms a rectangle and the number of hexagonal cells in each chain alternate *a* and $a-1$. For two independent positive integer numbers $a\geq 2$ & $b\geq 1$, the vertex set of $B_{a,b}$ *is* defined as (see Figure1 and [17, 18]).

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

This graph has $4ab+4a+2b-2$ vertices, since $|V(B_{a,b})|=2b(2a+1)+(2a-1)+(2a-1)$. It is easy to see that $\forall a\in \mathbb{N}-\{1\}$, $B_{a,a}$ has exactly $4a^2+6a-2$ vertices and $6a^2+6a-4$ edges. A general representation of this hexagonal system is shown in Figure 1.

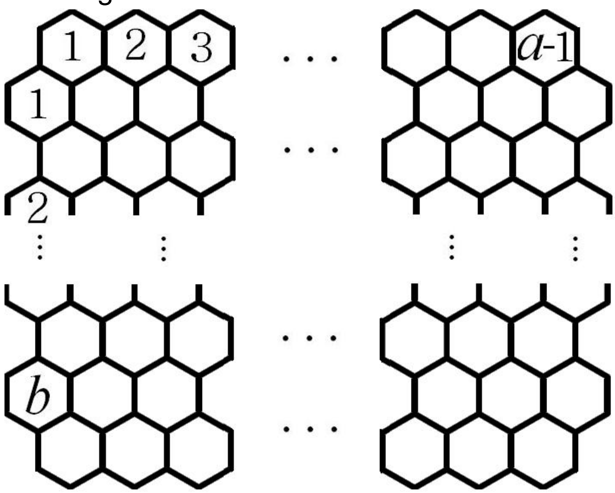

Figure 1. A general representation of the Benzenoid system $B_{a,b}$ ($\forall a,b\geq 1$).

Theorem 1. The Omega polynomial of the hexagonal system $B_{a,b}$ $\forall a,b\in \mathbb{N}$, is as follows:

If $a\geq b+2$:
$$\Omega\left(B_{a,b},\mathrm{x}\right)=(b+1)x^{a}+bx^{a+1}+\sum_{i=1}^{b}\left(4\mathrm{x}^{2i+1}\right)+2\left(a-b-1\right)x^{2b+2}$$

If $a\leq b+1$:
$$\Omega\left(B_{a,b},\mathrm{x}\right)=(b+1)x^{a}+bx^{a+1}+\sum_{i=1}^{a-1}\left(4\mathrm{x}^{2i+1}\right)+2(b-a+1)x^{2a}$$

***Proof*.** Let $G=B_{a,b}$ be the hexagonal system, with $4ab+4a+2b-2$ vertices. To compute the Omega polynomial of G it is enough to calculate $C(e)$ for every e in $E(G)$. Now, by using the *Cut Method,* and by using the Tables 1 and 2 and Figure 2, the proof is easily. The *Cut Method* in its general form was studied by *S. Klavžar* [19] and used in paper series [20-30].

So, from Table 1 we have

$$\Omega\left(B_{a,b},\mathrm{x}\right)=\sum_{c}\mathrm{m}\left(B_{a,b},c\right)\mathrm{x}^{c}$$
$$=(b+1)x^{a}+bx^{a+1}+\sum_{i=1}^{b}\left(4\mathrm{x}^{2i+1}\right)+2\left(a-b-1\right)x^{2b+2}$$

Table 1. The number of co-distant edges, when *a≥b+2*

quasi-orthogonal cuts	Number of co-distant edges	No
C_{2i+1} ∀ *i=0,…,b*	1	*a*
C_{2i} ∀ *i=1,…,b*	1	*a+1*
$\mathcal{C}_i$ ∀ *i=1,…,b*	4	*2i+1*
$\mathcal{C}_{b+1}$	*2(a-b-1)*	*2b+2*

On other hands, from Table 2, ∀*a≤b+1*:

$$\Omega\left(B_{a,b},\mathrm{x}\right)=(b+1)x^{a}+bx^{a+1}+\sum_{i=1}^{a-1}\left(4\mathrm{x}^{2i+1}\right)+2(b-a+1)x^{2a}$$

Table 2. The number of co-distant edges, when *a≤b+1*

quasi-orthogonal cuts	Number of co-distant edges	No
C_{2i+1} ∀ *i=0,…,b*	1	*a*
C_{2i} ∀ *i=1,…,b*	1	*a+1*
$\mathcal{C}_i$ ∀ *i=1,…,a-1*	4	*2i+1*
$\mathcal{C}_a$	*2(b-a+1)*	*2a*

and this completes the proof.

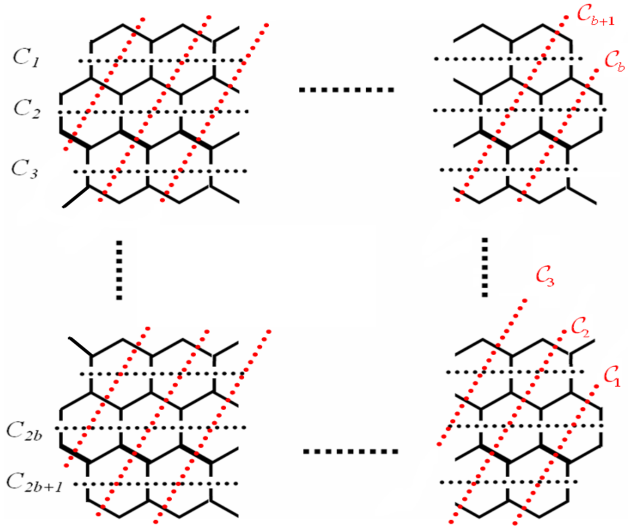

Figure 2. The presentation of quasi-orthogonal cuts (qoc strips) of $B_{a,b}$.

From Theorem 1, one can to see that the number of edges in G is equal to

$$\left|E\left(B_{a,b}\right)\right| = \Omega'\left(B_{a,b}, \mathrm{x}\right)|_{x=1}$$

$$= \frac{\partial\left((b+1)x^a + bx^{a+1} + \sum_{i=1}^{b}\left(4\mathrm{x}^{2i+1}\right) + 2\left(a-b-1\right)x^{2b+2}\right)}{\partial x}|_{x=1}$$

$$= a(b+1) + b(a+1) + 4\sum_{i=1}^{b}(2i+1) + 2\left(a-b-1\right)\left(2b+2\right)$$

$$= ab + a + ab + b + 4\left(\frac{2b(b+1)}{2} + b\right) + 4ab - 4b^2 + 4a - 8b - 4$$

$=6ab+5a+b-4.$

And also $\left|E\left(B_{a,b}\right)\right| = \dfrac{\partial\left((b+1)x^a + bx^{a+1} + \sum_{i=1}^{a-1}\left(4\mathrm{x}^{2i+1}\right) + 2(b-a+1)x^{2a}\right)}{\partial x}|_{x=1}$

$$= a(b+1) + b(a+1) + 4\sum_{i=1}^{a-1}(2i+1) + 2\left(b-a+1\right)\left(2a\right)$$

$$= 2ab + a + b + 4\left(\frac{2a(a-1)}{2} + a - 1\right) + 4ab - 4a^2 + 4a$$

$=6ab+5a+b-4.$

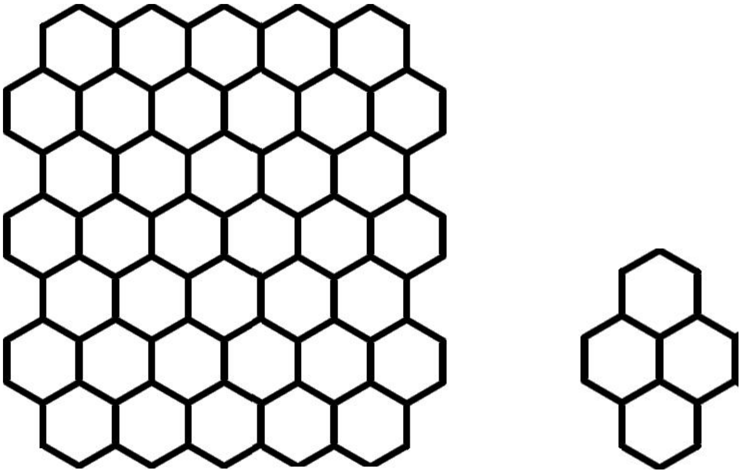

Figure 3. The hexagonal systems $B_{6,3}$ and $B_{2,1}$ (the first member of this hexagonal systems).

Example 1. By using Theorem 1, the Omega polynomial of the hexagonal system $B_{6,3}$ (Figure 3) is equal to $\Omega(B_{6,3},x)=4x^3+4x^5+4x^6+7x^7+4x^8$.

Example 2. From the second equation in Theorem 1, it's easy to see that the Omega polynomial of $B_{2,1}$ (Figure 3) is $\Omega(B_{6,3},x)=2x^2+5x^3$.

Example 3. By using Theorem 1 one can see that the Omega polynomial of the hexagonal system $B_{3,1}$ or the coronene H_2 (Figure 4) is equal to $\Omega(B_{6,3},x)=2x^3+x^4+4x^3+2x^4=6x^3+3x^4=\Omega(H_2,x)$.

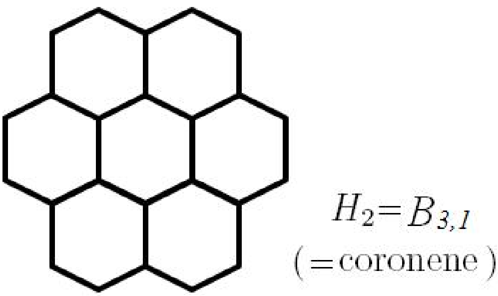

Figure 4. The hexagonal system $B_{3,1}$ ("coronene H_2" the second member of the circumcoronene series of benzenoid).

Theorem 2. The Omega polynomial of the hexagonal system $B_{a,a}$ $\forall a \in$, is equal to

$$\Omega\left(B_{a,a}, \mathrm{x}\right) = (a+1)x^{a} + ax^{a+1} + \sum_{i=1}^{a-1}\left(4\mathrm{x}^{2i+1}\right) + 2x^{2a}$$

$$= ax^{3} + 4x^{5} + \ldots + (a+1)x^{a} + ax^{a+1} + \ldots + 4x^{2a-1} + 2x^{2a}$$

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