Omega and related Polynomials of phenylenes and their hexagonal squeezes

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Omega polynomial of a graph G is defined on the ground of "opposite edge strips" *ops*. The Sadhana, Theta and PI polynomial can also be calculated by *ops* counting. In this paper we compute these polynomials of phenylenes and of the corresponding hexagonal squeeze. Also an efficient formula for calculating the Sadhana index of phenylenes and their hexagonal squeeze is given.

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1. Introduction

Graph polynomials were introduced in mathematical chemistry to give further insights into the structure and properties of chemical graphs. In particular, the first derivative of such polynomials computed at a given value returns a corresponding topological index of interest.
A graph polynomial, also called a counting polynomial, can be written as $P(G,x)=\sum_k m(G,k)x^k$, with the exponents showing the extent of partitions $p(G)$, $\bigcup p(G)=P(G)$ of a graph property $P(G)$ while the coefficients $m(G,k)$ are related to the number of partitions of extent k.

Counting polynomials have been introduced, in the Mathematical Chemistry literature, by Hosoya[12] to count independent edge sets (the Z-polynomial) and the distances in the graph (the Wiener polynomial, latter called the Hosoya polynomial and denoted $H(G,x)$[9,19] Other counting polynomials are the sextet polynomials[13,14], *independence*, [10,11,21] *domino*, [20] *star[8] and clique[15]* polynomials. More about polynomials the reader can find in ref [3]

Let $G=(E,V)$ be a connected graph, with the vertex set $V(G)$ and edge set $E(G)$. Two edges $e = uv$ and $f = xy$ of G are called *codistant e co f* if they obey the following relation: [16]

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

where d is the usual shortest-path distance function. Relation *co* is reflexive, that is, *e co e* holds for any edge *e* of *G*; it is also symmetric, if *e co f* then *f co e*. In general, relation *co* is not transitive, an example showing this fact is the complete bipartite graph $K_{2,n}$. If "*co*" is also transitive, thus an equivalence relation, then *G* is called a *co-graph* and the set of edges $C(e)=\{f\in E(G)\mid f\ co\ e\}$ is called an *orthogonal cut oc* of G, $E(G)$ being the union of disjoint orthogonal cuts:

$$E(G)=C_1\cup C_2\cup\cdots\cup C_k,\ C_i\cap C_j=\phi,\ i\neq j\ .$$

Klavžar in [18] has shown that relation *co* is a theta Djoković-Winkler relation, see [7,23].

Let $e = uv$ and $f = xy$ be two edges of G which are *opposite* or topologically parallel and denote this relation by *e op f*. A set of opposite edges, within the same face/ring, eventually forming a strip of adjacent faces/rings, is called an *opposite* edge *strip ops*, which is a quasi-ortogonal cut *qoc* (*i.e.*, the transitivity relation is not necessarily obeyed). Note that *co* relation is defined in the whole graph while *op* is defined only in a face/ring. The length of *ops* is maximal irrespective of the starting edge.

Let $m(G,c)$ be the number of *ops* strips of length c. The Omega polynomial [4] is defined as

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

Other polynomial also related to the ops in G, but counting the non-opposite edges is the *Sadhana Sd* polynomial [1] defined as

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

Let now the set of edges codistant to edge *e* of *G* be *C(e).* A Θ-polynomial [5] of *G*, counting the edges equidistant to the all reference edges *e*, is written as

$$\Theta(G;x)=\sum_{e\in E(G)} x^{|C(e)|}.$$

If the polynomial counts the edges non-equidistant to the all reference edges *e*, it is called the Π-polynomial [5] and is defined as

$$\Pi(G;x) = \sum_{e \in E(G)} x^{|E(G)|-|C(e)|}.$$

Suppose now G is a *co*-graph; then [6]

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

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

The first derivative (computed at x = 1) of these counting polynomials give interesting inter-relations and valuable information on the graph

$$\Omega'(G;1) = \sum_c m(G,c) \cdot c = |E(G)|.$$

$$Sd(G,1) = \sum_c m(G,c) \cdot (|E(G)| - c) = Sd(G),$$

$$\Theta'(G;1) = \sum_c m(G,c) \cdot c^2 = \Theta(G)$$

$$\Pi'(G;1) = \sum_c m(G,c) \cdot c(|E(G)| - c) = \Pi(G)$$

Let G be a connected graph, u and v be vertices of G and $e = uv$. The number of edges of G lying closer to u than to v is denoted by $n_{eu}(e|G)$ and the number of edges of G lying closer to v than to u is denoted by $n_{ev}(e|G)$. The PI polynomial of G is defined as

$$PI(G;x) = \sum_{\{u,v\} \subseteq V} x^{N(u,v)} ,$$

where $N(u,v) = n_{eu}(e|G) + n_{ev}(e|G)$, if $e = uv$; and = 0, otherwise.

Now If G be a bipartite *co*-graphs it is well known fact that [17]

$$PI(G,x) = \sum_c m(G,c) \cdot c \cdot x^{|E(G)|-c} = \Pi(G,x)$$

2. Main results and discussion

Phenylenes are a class of chemical compounds in which the carbon atoms form 6- and 4-membered cycles. Each 4-membered cycle (=square) is adjacent to two disjoint 6-membered cycles (=hexagons), and no two hexagons are adjacent. Their respective molecular graphs are also referred to as phenylenes. By eliminating, “squeezing out,” the squares from a phenylene, a catacondensed hexagonal system (which may be jammed) is obtained, called the hexagonal squeeze of the respective phenylene [22]. Clearly, there is a one-to-one correspondence between a phenylene (PH) and its hexagonal squeeze (HS). Both possess the same number (h) of hexagons. In addition, a PH with n hexagons possesses $h - 1$ squares. The number of vertices of PH and HS are 6h and 4h +2, respectively; The number of edges of PH and HS are 8h −2 and 5h +1, respectively. An example of PH and its HS is shown in Fig. 2.

Let we introduce some conceptions in a PH analogously in a hexagonal system. The linear chain PH is a PH without kinks (see Fig. 1), where the kinks are the branched or angularly connected hexagons. A segment of a PH is a maximal linear chain in the PH, including the kinks and/or terminal hexagons at its end. The number of hexagons in a segment S is called its length and is denoted by *l(S)*. For any segment S of a PH, $2 \le \ell(S) \le n$.

Particularly, a PH is a full kink one if and only if the lengths of its segment are all equal to 2.

A PH consists of a sequence of segments $S_1, S_2, \ldots, S_s$, $s \ge 1$, with Lengths $\ell(S_i) \equiv \ell_i$, $i = 1,2,\ldots,s$, where $\sum_{i=1}^{s} \ell_i = n + s - 1$, since two neighboring segments have always one hexagon in common.

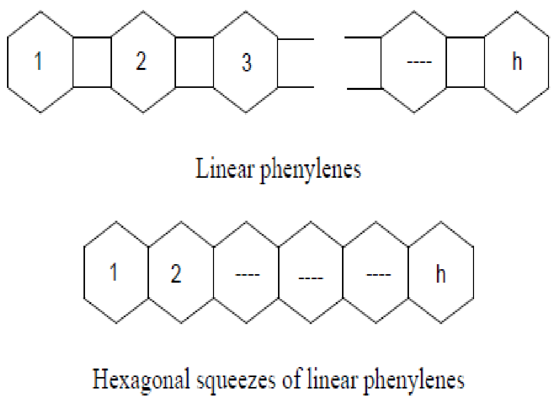

Fig. 1. The linear chain of phenylenes and its hexagonal squeezes

In this section, we will give efficient formulas for calculating the Omega and related polynomials of PHs and of the corresponding HS.

Theorem 1. Let PH be a phenylene with h hexagons consisting of $s \ge 1$ segments $S_1, S_2, \ldots, S_s$ with lengths $\ell_1, \ell_2, \ldots, \ell_s$. Then

$$\Omega(PH,x) = (3h - s)x^2 + \sum_{i=1}^{s} x^{2l_i}$$

$$\Theta(PH,x) = 2(3h - s)x^2 + \sum_{i=1}^{s} 2l_i x^{2l_i}$$

$$Sd(PH,x) = (3h - s)x^{8h-4} + \sum_{i=1}^{s} x^{8h-2-2l_i}$$

$$PI(PH,x) = 2(3h - s)x^{8h-4} + 2\sum_{i=1}^{s} l_i x^{8h-2-2l_i}$$

Proof. Let us first observe that the edges of PH fall into two distinct classes, namely the ones which are cut across by the straight line passing through the centers of the hexagonal and squares of S_i and those which are not. We denote the edges of the first type contained in S_i by $E_c(S_i)$.

The edges $E_c(S_i)$ $(1 \le i \le s)$ in each S_i form a strip C_i of length $2\ell_i (1 \le i \le s)$. On other hand two opposite edges in each hexagonal and squares (except the edges belong to $E_c(S_i)$) form a strip C_0 of length 2, see Fig. 2. Thus the number of strips of length 2 is equal to

$$m(PH,2) = \tfrac{1}{2}(|E(G)| - \sum_{i=1}^{s} |E_c(S_i)|)$$

$$= 4h - 1 - \sum_{i=1}^{s} \ell_i = 3h - s.$$

Using definition of mentioned polynomials, the result is follow.

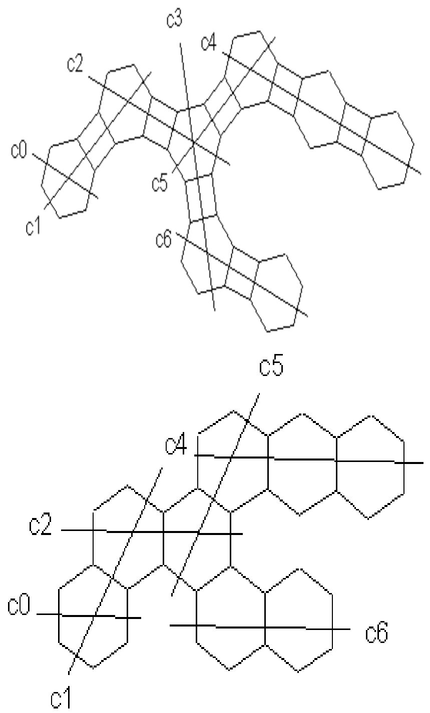

Fig. 2. The Strips of a phenylene (PH) and its hexagonal squeeze (HS)

In comparing with PH, graph HS has h-1 squares less than PH. So $|E_c(S_i)| = \ell_i + 1$. On other hand, Since two opposite edges in every square form a strip of length 2, so $m(SH,2) = 2h - s + 1$.

Theorem 2. Let PH be phenylene and HS its hexagonal squeeze, both having h Hexagons consisting of $s \ge 1$ segments $S_1, S_2, \ldots, S_s$ with lengths $\ell_1, \ell_2, \ldots, \ell_s$. Then

$$\Omega(HS,x) = (2h - s + 1)x^2 + \sum_{i=1}^{s} x^{l_i+1}$$

$$\Theta(HS,x) = (2h - s + 1)x^2 + \sum_{i=1}^{s} (l_i + 1)x^{l_i+1}$$

$$SH(HS,x) = (2h - s + 1)x^{8h-4} + \sum_{i=1}^{s} x^{8h-3-l_i}$$

$$PI(HS,x) = 2(2h - s + 1)x^{8h-4} + 2\sum_{i=1}^{s} (l_i + 1)x^{8h-3-l_i}$$

In following tables we give formulas for mentioned polynomials of linear chain and full kink of phenylenes and of corresponding hexagonal squeeze.

Table 1. The mentioned polynomials of linear chain of phenylene PH

polynomial	**PH**
Ω	$(3h-1)x^2 + x^{2h}$
Θ	$2(3h-1)x^2 + 2hx^{2h}$
Sd	$(3h-1)x^{8h-4} + x^{6h-2}$
PI	$2(3h-1)x^{8h-4} + 2hx^{6h-2}$

Table 2. The mentioned polynomials of linear chain of phenylene HS

polynomial	**HS**
Ω	$2hx^2 + x^{h+1}$
Θ	$4hx^2 + (h+1)x^{h+1}$
Sd	$2hx^{8h-4} + x^{7h-3}$
PI	$4hx^{8h-4} + 2(h+1)x^{7h-3}$

Table 3. The mentioned polynomials of full kink of phenylene PH

polynomial	**PH**
Ω	$(3h-s)x^2 + sx^4$
Θ	$2(3h-s)x^2 + 4sx^4$
Sd	$(3h-s)x^{8h-4} + sx^{8h-6}$
PI	$2(3h-s)x^{8h-4} + 4sx^{8h-6}$

Table 4. The mentioned polynomials of full kink of phenylene HS

polynomial	HS
Ω	$(2h-s+1)x^2+sx^3$
Θ	$2(2h-s+1)x^2+3sx^3$
Sd	$(2h-s+1)x^{8h-4}+sx^{8h-5}$
PI	$2(2h-s+1)x^{8h-4}+6sx^{8h-5}$

THE SD INDEX OF PH AND HS

Aziz and at.al. [2] computed Sadhana index of phenylenes only for linear chain of pH. They proved that

$$Sd(L(PH))=(3h-1)(8h-2)$$

In this section, we give exact formulas for Sd index of arbitrary phenylenes and their hexagonal squeeze. By derivative of Sd polynomial and computed at x = 1, we obtain

$$Sd(PH)=Sd'(PH,1)=24h^2-14h+2$$

$$Sd(PH)=Sd'(HS,1)=16h^2-h-3$$

The above text implies that Sadhana index of phenylenes and their hexagonal squeeze only depends on the number of Hexagos and dose not depends on the length and number of segments. Thus we have the following result.

Corollary 3. Let $L(PH)$ and $F(PH)$ be the *linear chain* and *full kink* of phenylene PH, respectively. Then

$$Sd(PH)=Sd(L(PH))=Sd(F(PH))$$

$$Sd(HS)=Sd(L(HS))=Sd(F(HS))$$

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