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THE WIENER POLYNOMIAL OF LINEAR CHAIN PHENYLENES AND OF THE CORRESPONDING HEXAGONAL SQUEEZES

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Abstract. The Wiener index is a graphical invariant and is the sum of distances between all pairs vertices in a connected graph G. We define a generating function, which we call the Wiener polynomial, whose derivative is a *x*-analog of the Wiener index. In this paper we find formulae for the Wiener polynomial of linear phenylenes and of the corresponding hexagonal squeeze. Also efficient formulae for calculating the Wiener index of mentioned molecular graphs are given.

Keywords: Wiener Polynomial, Linear chain, Phenylen, hexagonal squeeze**.**

AMS Subject Classification: 05C07, 13A99.

1. Introduction

Let$G$ be a simple connected graph with vertex set V and edge set E. The distance between two vertices u and v of V is the length of the shortest path between u and v and is denoted by $d(u,v)$. The Wiener index of G is defined by

$$W(G) = \sum_{\{u,v\}\subseteq V} d(u,v).,$$

On the numerous chemical applications of the Wiener index see the reviews [3,4,6,7] and the references quoted therein; on its mathematical properties see the reviews [1,2].

We wish to define and study a related generating function. If x is a parameter, then the Wiener polynomial of G is

$$W(G;x) = \sum_{\{u,v\}\subseteq V} x^{d(u,v)} .$$

It is easy to see that the derivative of $W(G;x)$ is a x-analog of $W(G)$, i.e.,

$$W'(G;1) = W(G) .$$

The Wiener Polynomial is initially defined by Hosoya [5], and so termed in honour of Harold Wiener who coined the earlier index. It is often called the Hosoya Polynomial and appears in slightly different forms in the literature.

Let the set $V = \{v_1, v_2, \ldots, v_n\}$ be vertices of G. Then by the definition the Wiener polynomial we obtain

$$W(G;x)=\sum_{\{u,v\}\subseteq V} x^{d(u,v)}=\sum_{i=2}^{n} x^{d(v_1,v_i)}+\sum_{i=3}^{n} x^{d(v_2,v_i)}+\cdots+\sum_{i=n-1}^{n} x^{d(v_{n-2},v_i)}$$
$$+x^{d(v_{n-1},v_n)}=\sum_{j=1}^{n-1}\sum_{i=j+1}^{n} x^{d(v_j,v_i)}.$$

The set of distances the vertex v_1 of V with the other vertices of V we denote by $D_{v_1}^{V\setminus v_1}=\{d(v_1,v_2),d(v_1,v_3),\ldots,d(v_1,v_n)\}$. Also if $S=\{u_1,u_2,\ldots,u_m\}$ is the subsequent of V, then the set of distances the vertices of S with themselves denoted by $D_S^S=\left\{D_{u_1}^{S\setminus\{u_1\}},D_{u_2}^{S\setminus\{u_1,u_2\}},\ldots,D_{u_{m-1}}^{S\setminus\{u_1,\ldots,u_{m-1}\}}\right\}$.

Thus by the above notations the Wiener polynomial of G is given by

$$W(G;x)=\sum_{k\in D_V^V} N(k)x^k \tag{1}$$

where $N(k)$ is the number of $k\in D_V^V$.

Usingthis technique, we compute the wiener polynomial of linear chain phenylens.

2. 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 [2]. 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.

Let we introduce some conceptions in a PH analogously in a hexagonal system. The linear chain PH is a PH without kinks (see figure 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, $2\le \ell(S)\le n$.

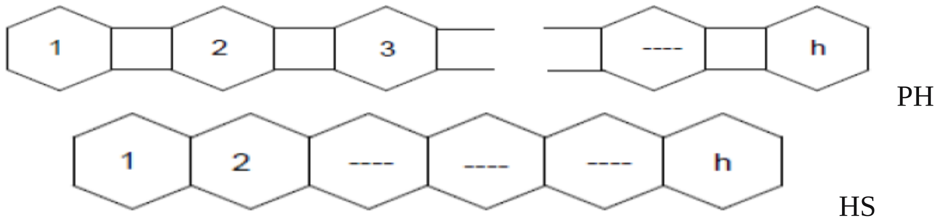

Figure 1. The linear phenylenes (PH) and its hexagonal squeezes (HS)

In this section, we will give efficient formulas for calculating the wiener polynomials of linear phenylenes and of the corresponding hexagonal squeezes.

Theorem 1. The Wiener polynomial of linear phenylene $L_h(PH)$ with h hexagons is

$$W(L_h(PH);x)=\sum_{k=0}^{3h-4}(4k+2)x^{3h-k}+(13h-10)x^3+(12h-6)x^2+(8h-2)x.$$

Proof. The number of vertices of PH is 6h, which we show by $V=\{v_1,v_2,\ldots,v_{6h}\}$, see Fig 2. It is easy to see that

$$D_{v_{6k+1}}^{V\backslash\{v_1,v_2\ldots,v_{6k+1}\}}=\{1,1,2,2,3,3,4,4,\ldots,3(h-k)-1,3(h-k)-1,3(h-k)\},0\le k\le h-1,$$

$$D_{v_{6k+2}}^{V\backslash\{v_1,v_2\ldots,v_{6k+2}\}}=\{1,2,2,3,3,4,4,\ldots,3(h-k)-1,3(h-k)-1,3(h-k)\},0\le k\le h-1,$$

$$D_{v_{6k-1}}^{V\backslash\{v_1,v_2\ldots,v_{6k-1}\}}=\{1,1,2,2,3,3,4,4,\ldots,3(h-k),3(h-k),3(h-k)+1\},1\le k\le h-1,$$

$$D_{v_{6k-2}}^{V\backslash\{v_1,v_2\ldots,v_{6k-2}\}}=\{1,2,2,3,3,4,4,\ldots,3(h-k)+1,3(h-k)+1,3(h-k)+2\},1\le k\le h,$$

$$D_{v_{6k}}^{V\backslash\{v_1,v_2\ldots,v_{6k}\}}=\{1,2,2,3,3,4,4,\ldots,3(h-k),3(h-k),3(h-k)+1\},1\le k\le h-1,$$

$$D_{v_{6k-3}}^{V\backslash\{v_1,v_2\ldots,v_{6k-3}\}}=\{3,1,2,2,3,3,4,4,\ldots,3(h-k)+1,3(h-k)+1,3(h-k)+2\},1\le k\le h,$$

and

$$D_{v_{6h-1}}^{V\backslash\{v_1,\ldots,v_{6h-1}\}}=\{1\}.$$

Now by the formula (1), to calculate the Wiener polynomial of $L_h(PH)$, it is enough to count $N(1),N(2),\ldots,N(3h)$, which we show them in following table.

Table 1. Value of *N(k)*

k	1	2	3	4	5	6	….	3*h*-1	3*h*
N(k)	8*h*-2	12*h*-6	13*h*-10	12*h*-14	12*h*-18	12*h*-22	…	6	2

Therefore

$$W(L_h(PH);x) = (8h-2)x + (12h-6)x^2 + (13h-10)x^3 + (12h-14)x^4 +$$
$$(12h-18)x^5 + (12h-22)x^6 + \cdots + 6x^{3h-1} + 2x^{3h}.$$

The proof is completed.

Similar tothe proof ofthe previous theorem, we havethe following result.

Theorem 2. Let $L_h(PH)$ be linear chain phenylene and $L_h(HS)$ its hexagonal squeeze, both having h Hexagons. Then

$$W(L_h(HS);x) = \sum_{k=0}^{2h-3}(4k+2)x^{2h+1-k} + (9h-6)x^3 + (8h-2)x^2 + (5h+1)x.$$

In following tables, we compute the Wiener polynomial of linear chain phenylens and of the corresponding hexagonal squeezes for some h.

Table 2. Wiener polynomial of linear phenylene $L_h(PH)$ for some h.

h	$W(L_h(PH);x)$
2	$2x^6 + 6x^5 + 10x^4 + 16x^3 + 18x^2 + 14x$
3	$2x^9 + 6x^8 + 10x^7 + 14x^6 + 18x^5 + 22x^4 + 19x^3 + 30x^2 + 22x$
4	$2x^{12} + 6x^{11} + 10x^{10} + 14x^9 + 18x^8 + 22x^7 + 26x^6 + 30x^5 + 34x^4 + 42x^3 + 42x^2 + 30x$

Table 3. Wiener polynomial of linear chain of *HS* for some *h*.

h	$W(L_h(HS);x)$
2	$2x^5 + 6x^4 + 12x^3 + 14x^2 + 11x$
3	$2x^7 + 6x^6 + 10x^5 + 14x^4 + 21x^3 + 22x^2 + 16x$
4	$2x^9 + 6x^8 + 10x^7 + 14x^6 + 18x^5 + 22x^4 + 30x^3 + 30x^2 + 21x$

The derivative eof Wiener polynomial (computed at $x = 1$), wehave the following result.

Theorem 3. Let $L_h(PH)$ be linear phenylene and $L_h(HS)$ its hexagonal squeeze, both having h Hexagons. Then

$$W(L_h(PH)) = 18h^3 + 9h^2,$$

$$W(L_h(HS)) = \frac{1}{3}(16h^3 + 36h^2 + 26h + 3).$$

Table 3. The Wiener index of $L_h(PH)$ and $L_h(HS)$ for some h

h	1	2	3
$W(L_h(PH))$	180	567	1296
$W(L_h(HS))$	109	279	569

3. Conclusion

In this paper we have calculated the Wiener polynomial of the phenylenes and its hexagonal squeezes only for linear chains. On the other hand, by using the Wiener polynomial we give formulas for Wiener index of linear phenylenes. The computation of Wiener polynomial for random phenylene chains can be done in future studies.

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Fenilenin xətti zəncirinin və müvafiq altıbuçaqlı sıxılmanın Viner çoxhədlisi

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XÜLASƏ

Viner indeksi qrafik invariantdır və G əlaqəli qrafın bütün təpələrinin cütləri arasındakı məsafələrin cəmidir. Biz Viner polinomu adlandırdığımız törədici funksiyanı təyin edirik ki, bunun da törəməsi Viner indeksinin x-analoqudur. Bu məqalədə biz xətti fenilenlərin Viner çoxhədlisi üçün düsturlar və müvafiq altıbucaqlı sıxılmanı müəyyən etmişik. Bundan bağqa göstərilən molekulyar qrafların Viner indeksinin hesablanması üçün effektiv düsturlar verilmişdir.

Açar sözlər: Viner polinomu, xətti zəncir, fenilen, altıbucaqlı cıxılma.

Многочлен Винера линейной цепочки фенилена и соответствующего шестиугольного сжатия

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РЕЗЮМЕ

Индекс Винера является графическим инвариантном и суммой расстояний между всеми парами вершин в связном графе G. Мы определяем производящую функцию, которую мы называем полином Винера, производная которой является x-аналогом индекса Винера. В этой статье мы найдем формулы для полинома Винера линейных фениленов и соответствующего шестиугольного сжатия. Кроме того, приведены эффективные формулы для расчета индекса Винера указанных молекулярных графов.

Ключевые слова: полином Винера, линейная цепочка, фенилен, шестиугольное сжатие.