# A Study on the Wiener Polynomials for the Paraffin Polynomial-Rings

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## Abstract

In this paper, we find the Wiener polynomial of multi-circles of Paraffin structural. We prove that this obtained formula is better than the formulas, which are previously presented. Also, we evaluate the coefficients for any limited power of $x$ without depending on the number of circles, and we find the Wiener index and average distance for this structural. On the other hand, we build a MATLAB program to evaluate the Wiener polynomial coefficient, Wiener index, and average distance.

**Keywords:** Weiner index; Wiener polynomial; Polynomial ring; Paraffin structural

## 1. Introduction

In many chemical structures, we notice the existence of data from the hexagonal systems, which consists of hexagonal rings connected to each other, and that any two rings in this system are either shared by an edge or not shared.

By matching each hexagonal ring with a vertex, and connecting any two of the resulting vertices with an edge when the two rings have an edge in common, the resulting statement is called the characteristic graph of the hexagonal system.

A hexagonal system is said to be Catacondensed if there are no three hexagonal rings sharing one vertex.

Types of Catacondensed unbranched hexagonal systems contain data such that each characteristic statement is equivalent to a trail statement ([6], [2], [8-9]).

A non-branched Catacondensed hexagonal ring system is said to be a multi-circles of paraffin structural, which is sometimes called a hexagonal ring band graph if every edge common to any two rings is the same as all edges common to any two rings of the same system, as shown in Figure -1-

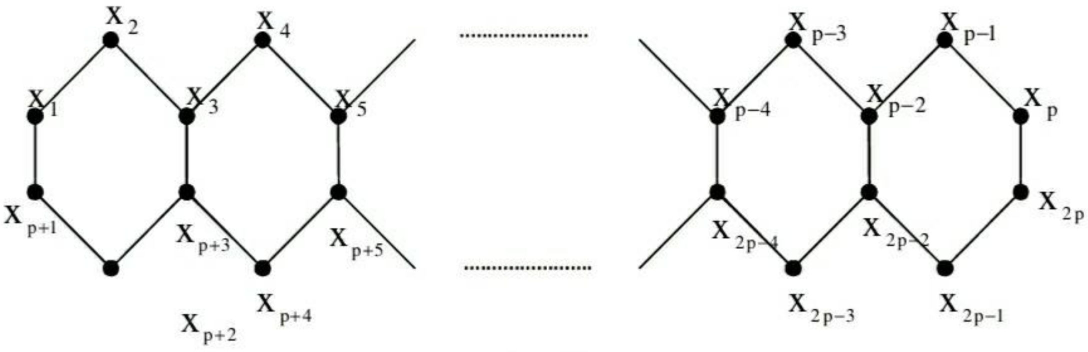

**Figure 1.** Multi-circles of paraffin structural

DOI: https://doi.org/10.54216/GJMSA.0110202
Received: December 04, 2023 Revised: March 29, 2024 Accepted: July 25, 2024

We will code this type of compound with $\boldsymbol{H_{2p}}$, since 2p represents the number of carbon atoms corresponding to the rank of the statement, and p is always an odd number.

In the statement related to G, the number of pairs of vertices of G that are on the dimension K of each other is denoted by the symbol d(G,k) where $k = 0,1,2,\ldots,\delta$

The wiener polynomial [3] of G is defined as:

$\boldsymbol{W(G;x) = \sum_{k=0}^{\delta} d(G;k)x^k;}$

The Wiener index is defined by the statement G: is the sum of the distances between all pairs of vertices in G, that is:

$$\boldsymbol{W(G) = \sum_{\{u,v\}} d(u,v)}$$

The sum is taken on each of two different vertices u or v in G.

The Wiener proof based on the Wiener polynomial can be expressed as the derivative of the Wiener polynomial for x, when x=1, that is:

$$\boldsymbol{W(G) = W'(G;x)|_{x=1} = \sum_{k=1}^{\delta} kd(G;k)}$$

Where $\boldsymbol{W'(G;x)}$represents the derivative of the Wiener polynomial.

If the number of vertices in the connected statement G is p, then there are $\frac{1}{2}p(p-1)$ unordered pairs of different vertices in the statement. We can now define the average distance [1] of G as the product of dividing the Wiener proof of G by 1/2 p (p-1), and the average distance of G is denoted by $\boldsymbol{\overline{D}(G)}$, that is:

$$\boldsymbol{\overline{D}(G) = \frac{W(G)}{p(p-1)/2}}$$

We must mention that the Scientist H.Wiener [3] was the first to study the total distance in the data he observed in the structures of chemical molecules, as his results and contributions were well known to specialized chemists, but mathematicians ' knowledge of them was limited. And that the usefulness of the Wiener polynomial is to obtain the total distance, which represents the Wiener index, which has wide uses in Chemistry [1].

## 2. The Main Theorem

The Wiener polynomial of a paraffin polynomial-rings $\boldsymbol{H_{2p}}$ of rank 2p is:

$$\boldsymbol{W(H_{2p};x) = \sum_{k=0}^{\delta} d(H_{2p};k)x^k}$$

Where:

$$\boldsymbol{d(H_{2p},0) = 2p;}$$

$$\boldsymbol{d(H_{2p},1) = \frac{1}{2}(5p-3);}$$

$$\boldsymbol{d(H_{2p},k) = 4(p-k) + 2 + R; \qquad k = 2,3,\ldots.,\delta} \qquad (1)$$

Thus:

$$\boldsymbol{R = \begin{cases} (p-1)/2 & when\ k = 3 \\ 0 & other\ wise \end{cases}}$$

And that the diameter is p, and δ=p.

**Proof:**

Suppose that the headers of the statement $\boldsymbol{H_{2p}}$ are tagged with the formula.

$$V_1 = \{x_1, x_2, \ldots, x_p\}$$
$$V_2 = \{x_{p+1}, x_{p+2}, \ldots, x_{2p}\}$$

DOI: https://doi.org/10.54216/GJMSA.0110202
Received: December 04, 2023 Revised: March 29, 2024 Accepted: July 25, 2024

We will denote the distance between any two vertices in $V_i$ at a distance k from each other by $\boldsymbol{d}(\boldsymbol{H_{2p}},\boldsymbol{k})V_i$,since i=1,2, and denote the distance between a vertex of $V_1$ with a vertex of $V_2$ at a distance k from each by $\boldsymbol{d}(\boldsymbol{H_{2p}},\boldsymbol{k})V_1V_2$.

We note that:

$$d(H_{2p},k)V_i = d(P_p,k) = p-k \qquad ; \qquad i = 1,2$$

For each k = 0,1,2,…, $p$

Where $\boldsymbol{P_p}$ is a trail of rank p.

It is clear that $\boldsymbol{d}(\boldsymbol{H_{2p}},\boldsymbol{0}) = \boldsymbol{d}(\boldsymbol{H_{2p}},\boldsymbol{0})V_1 + \boldsymbol{d}(\boldsymbol{H_{2p}},\boldsymbol{0})V_2 = p+p = 2p$ and:

$$\boldsymbol{d(H_{2p},1)} = \boldsymbol{d(H_{2p},1)}V_1 + \boldsymbol{d(H_{2p},1)}V_2 + \boldsymbol{d(H_{2p},1)}V_1V_2$$

$$= \boldsymbol{(p-1)+(p-1)+\frac{1}{2}(p+1) = \frac{1}{2}(5p-3)}$$

Where:

$$\boldsymbol{d(H_{2p},1)}V_1V_2 = \sum_{\boldsymbol{i=1}}^{\boldsymbol{(p+1)/2}} \boldsymbol{d(x_{2i-1},H_{2p},1)}V_2 = \sum_{\boldsymbol{i=1}}^{\boldsymbol{(p+1)/2}} \boldsymbol{1 = \frac{1}{2}(p+1)}$$

Now, we follow the method of mathematical induction to prove the relationship (1) at k=2, then:

$$\boldsymbol{d(H_{2p},2)} = \boldsymbol{d(H_{2p},2)}V_1 + \boldsymbol{d(H_{2p},2)}V_2 + \boldsymbol{d(H_{2p},2)}V_1V_2$$

$$= \boldsymbol{(p-2)+(p-2)+2+2(p-2) = 4(p-2)+2}$$

Where:

$$\boldsymbol{d(H_{2p},2)}V_1V_2 = \sum_{\boldsymbol{i=1}}^{\boldsymbol{p}} \boldsymbol{d(x_i,H_{2p},2)}V_2 = 1 + \sum_{\boldsymbol{i=2}}^{\boldsymbol{p-1}} \boldsymbol{d(x_i,H_{2p},2)}V_2 + \boldsymbol{1}$$

$$= \boldsymbol{1 + \sum_{i=2}^{p-1} 2 + 1 = 2 + 2(p-2)}$$

When k=3, then:

$$\boldsymbol{d(H_{2p},3)} = \boldsymbol{d(H_{2p},3)}V_1 + \boldsymbol{d(H_{2p},3)}V_2 + \boldsymbol{d(H_{2p},3)}V_1V_2$$

$$= \boldsymbol{(p-3)+(p-3)+4+2(\frac{p-1}{2})+3(\frac{p-5}{2})}$$

$$= \boldsymbol{4(p-3)+2+(p-1)/2}$$

Where:

$$\boldsymbol{d(H_{2p},3)}V_1V_2 = \sum_{\boldsymbol{i=1}}^{\boldsymbol{p}} \boldsymbol{d(x_i,H_{2p},3)}V_2 = 1+2+\sum_{\boldsymbol{i=3}}^{\boldsymbol{p-2}} \boldsymbol{d(x_i,H_{2p},3)}V_2 + \boldsymbol{2+1}$$

$$= \boldsymbol{1+2+}\sum_{\boldsymbol{j=2}}^{\boldsymbol{(p-1)/2}} \boldsymbol{d(x_{2j-1},H_{2p},3)}V_2 + \sum_{\boldsymbol{j=2}}^{\boldsymbol{(p-3)/2}} \boldsymbol{d(x_{2j},H_{2p},3)}V_2 + \boldsymbol{2+1}$$

$$= \boldsymbol{3 + \sum_{j=2}^{(p-1)/2} 2 + \sum_{j=2}^{(p-3)/2} 3 + 3 = 4 + 2(\frac{p-1}{2}) + 3(\frac{p-5}{2})}$$

When k=4, then:

$$\boldsymbol{d(H_{2p},4)} = \boldsymbol{d(H_{2p},4)}V_1 + \boldsymbol{d(H_{2p},4)}V_2 + \boldsymbol{d(H_{2p},4)}V_1V_2$$

$$= \boldsymbol{(p-4)+(p-4)+2+2(p-4) = 4(p-4)+2}$$

Where:

DOI: https://doi.org/10.54216/GJMSA.0110202
Received: December 04, 2023 Revised: March 29, 2024 Accepted: July 25, 2024

$$d(H_{2p},4)V_1V_2=\sum_{i=1}^{3} d(x_i,H_{2p},4)V_2+\sum_{i=4}^{p-3} d(x_i,H_{2p},3)V_2+\sum_{i=p-2}^{p} d(x_i,H_{2p},3)V_2$$

$$=\sum_{i=1}^{3} 1+\sum_{i=4}^{p-3} 2+\sum_{p-2}^{p} 1=3+2(p-6)+3=2+2(p-4)$$

We assume that Formula (1) is true when k=r, thus:

$$d(H_{2p},r)=4(p-r)+2$$

Now we will prove that Formula (1) is true when k=r+1

$$d(H_{2p},r+1)=d(H_{2p},r+1)V_1+d(H_{2p},r+1)V_2+d(H_{2p},r+1)V_1V_2$$

$$=\big(\mathrm{p}-(\mathrm{r}+1)\big)+\big(\mathrm{p}-(\mathrm{r}+1)\big)+2+2\big(\mathrm{p}-(\mathrm{r}+1)\big)$$

$$=4(p-(r+1))+2$$

thus:

$$d(H_{2p},r+1)V_1V_2=\sum_{i=1}^{r} d(x_i,H_{2p},r+1)V_2+\sum_{i=r+1}^{p-r} d(x_i,H_{2p},r+1)V_2+\sum_{i=p-r+1}^{p} d(x_i,H_{2p},r+1)V_2$$

$$=\sum_{i=1}^{r} 1+\sum_{i=r+1}^{p-r} 2+\sum_{i=p-r+1}^{p} 1=r+2(p-2r)+r$$

$$=2+(p-(r+1))+2$$

## 3. The result

Wiener's proof of the paraffin polytope-the $H_{2p}$ rings of rank 2p are:

$$W(H_{2p})=\frac{1}{3}p(p+1)(2p+1)-1$$

And that the average distance of this compound is not more than $\frac{1}{3}(p+3)$

**Proof:**

$$W\big(H_{2p}\big)=W'\big(H_{2p};x\big)\big|_{x=1}$$

$$=\frac{1}{2}(5p-3)+8(p-2)+4+12(p-3)+6+\frac{3}{2}(p-1)+\sum_{k=4}^{p} 4k(p-k)+2k$$

The above formula can be written in the following form:

$$W\big(H_{2p}\big)=-1+\sum_{k=1}^{p} 4k(p-k)+2k$$

$$=-1+2(2p+1)\sum_{k=1}^{p} k-4\sum_{k=1}^{p} k^2$$

$$=-1+2(2p+1)(\frac{p(p+1)}{2})-4(\frac{p(p+1)(2p+1)}{6})$$

$$=-1+\frac{1}{6}p(p+1)(2p+1)(6-4)=\frac{1}{3}p(p+1)(2p+1)-1$$

And that the average distance:

$$\bar{D}(H_{2p})=\frac{W(H_{2p})}{2p(2p-1)/2}$$

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$$= \frac{\boldsymbol{p(p+1)(2p+1)-3}}{\boldsymbol{3p(2p-1)}}$$

And after simplifying the amount, we get:

$$\boldsymbol{\bar{D}(H_{2p}) = \frac{1}{3}(p+2) + \frac{(p-1)}{p(2p-1)}}$$

We note that the magnitude $\frac{(p-1)}{p(2p-1)}$ is no more than $\frac{1}{3}$, whatever the value of p. (Since p is always greater than or equal to 3 in these compounds).

Then:

$$\boldsymbol{\bar{D}(H_{2p}) < \frac{1}{3}(p+2) + \frac{1}{3} = \frac{1}{3}(p+3)}$$

Where the magnitude $\boldsymbol{\frac{1}{3}(p+3)}$represents the upper bound of the average distance for $\boldsymbol{H_{2p}}$ and does not represent the upper limit constraint.

For example, if the value of p is 7, then:

$W(H_{14}; x) = 14 + 16x + 22x^2 + 21x^3 + 14x^4 + 10x^5 + 6x^6 + 2x^7$

$W(H_{14}; x) = 279$

$\boldsymbol{\bar{D}(H_{2p}) = 279/91 \cong 3.0659 < 3.3333}$

Finally, we designed a program in the MATLAB language to calculate the coefficients of the Wiener polynomials as a sequence of numbers starting with the coefficient for powers of zero and ending with the coefficient for powers of p, as well as giving Wiener's proof and the average distance once a p value is entered.

To verify the accuracy of the program, we entered p=7 and the results were matched, starting from the coefficients for the Wiener polynomial, the Wiener proof and the distance parameter.

## 4. The Main Algorithm

**1.** Start.

**2.** Enter the value of p (which represents the number of carbon atoms).

**3.** Create the adjacency matrix A (by dividing the matrix A into four partial matrices and defining these matrices and then performing some operations on them), It is known that matrix A is a symmetric matrix.

**4.** Definition of a zero-initial Matrix B and a zero-initial Matrix s.

**5.** Put k=1.

**6.** Put s(k)=0.

**7.** Calculation of the matrix C, C=A^k.

**8.** Put i=1

**9.** Put j=i+1.

**10.** If $A(i,j) \neq 0$and B (i, j) = 0, then:

$B(i, j) = k$ $\quad\quad$ $s(k) = s(k)+1$

**11.** Put j=j+1.

**12.** If j<=2*p go to step 10 otherwise make i=i+1.

**13.** If i<=2*p-1 Go to step 9 otherwise make k=k+1.

**14.** If k<=p go to step 6.

**15.** We print Wiener polynomial coefficients [2*p s(1) s(2) s(3) … s(p)] (Starting from the coefficient for forces zero to the coefficient for forces p).

**16.** We print the Wiener index guide $index = \sum_{k=1}^{p} ks(k)$

**17.** We print the average distance average = index / p(2*p-1)

**18.** The end.

## 5. The program

```
% Program to evaluate Coefficients of Wiener Polynomial, Wiener index and Average distance for multi-circles of paraffin structural G of order 2*p.(p is positive odd integer number).
p=input(' input p = ');
a=ones(1,p-1);
b=diag(a,1)+diag(a,-1);
c=eye(p,p);
for i=2:2:p-1
c(:,i)=0;
end
% A is adjacency matrix of the graph.
A=[b c;c b];
B=zeros(2*p,2*p);
s=zeros(1,p);
for k=1:p
s(k)=0;
C=A^k;
for i=1:2*p-1
for j=i+1:2*p
if (C(i,j)~=0)&(B(i,j)==0)
B(i,j)=k;
s(k)=s(k)+1;
end
end
end
end
%coefficient stands for the Wiener polynomial coefficients. coefficients=[2*p,s]
% [2*p,s]is given matrix with size (1,p+1) such that the first element is
% 2*p, and other elements are matrix elements s.
% Wiener index of G is given by index.
index=sum(polyder(fliplr(coefficients)))
% average distance of G is given by average.
average=index/(p*(2*p-1))
```

RUN

```
input p = 7
coefficients =
14 16 22 21 14 10 6 2
index =
279
average =
3.0659
```

DOI: https://doi.org/10.54216/GJMSA.0110202
Received: December 04, 2023 Revised: March 29, 2024 Accepted: July 25, 2024

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DOI: https://doi.org/10.54216/GJMSA.0110202
Received: December 04, 2023 Revised: March 29, 2024 Accepted: July 25, 2024