Wiener Numbers of Pericondensed Benzenoid Molecule Systems

W.C. Shiu[†] *and Peter, C.B. Lam*[‡]

Abstract

The Wiener number W of a molecular graph, or more generally of a connected graph, is equal to the sum of distances between all pairs of its vertices. There is correlation between W and a variety of physico-chemical properties of alkanes and of benzenoid hydrocarbons. One important problem is to calculate W of a general (molecular) graph, especially of polycyclic graphs. In this paper, we shall summarize results obtained in this respect, and apply a new method to find the Wiener number of another series — the irregular hexagonal nets.

Key words and phrases: Wiener number, hexagonal net, benzenoid

AMS 1991 Subject Classifications: 05C12, 05C90

1. Introduction

An important invariant of connected graphs is called Wiener number (or Wiener index) W. This number is equal to the sum of distances between all pairs of vertices of the respective graph. American physico-chemist Harold Wiener first examined the quantity W in 1947 and 1948 [15-19]. It is one of the most extensively studied graph-theoretical structure-descriptors. Wiener, and after him numerous other researchers, reported the existence of correlation between W and a variety of physico-chemical properties of alkanes; details of its theory and its chemical applications can be found in the recent reviews [7, 9], in which also references to previous research on W are given. Considerable attention was paid to the Wiener number of benzenoid hydrocarbons. Until 1992 only catacondensed benzenoid systems could be treated [2-6]. A breakthrough in this area was achieved in 1995 by the present authors, who introduced an infinite graph called wall and a useful lemma for finding general expressions for W of homologous series of compact pericondensed systems [10].

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In this article, we summarize all the Wiener numbers of homologous series of compact pericondensed benzenoid molecules which are hexagonal parallelograms, hexagonal rectangles, hexagonal jagged-rectangles, hexagonal trapeziums and hexagonal bitrapeziums and particularly regular hexagonal polygons including hexagons, quadrangles (rhombus) and triangles. All the results are found in [10-14].

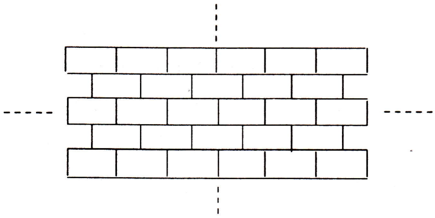
Recently, I. Gutman and S. Klavžar [8] introduced another method to find the Wiener number of benzenoid hydrocarbons. In section 4 we shall use this method to find the Wiener of irregular hexagonal nets.

2. Graph Theory Model

In this article, $\mathbb{Z}$ denotes the set of integers. Notation and terminology for graph theory used in this paper are those in the book of Bondy and Murty [1].

Definition: Let $G=(V,E)$ be a graph. For $v,w\in V$ let $\rho(v,w)$ be the distance between v and w. The *Wiener number* of G is defined by $W(G)=\frac{1}{2}\sum_{v,w\in V}\rho(v,w)$.

Definition: Let $G=(V,E)$ be an infinite graph where $V=\mathbb{Z}\times\mathbb{Z}$ and $\{(x_1,y_1),(x_2,y_2)\}\in E$ if (1) $y_1=y_2$ and $|x_1-x_2|=1$, or, (2) $x_1=x_2$, $|y_1-y_2|=1$ and $x_1+y_1+x_2+y_2\equiv 1\pmod 4$. This graph was first introduced in [10] and called the *wall.*



A useful lemma was shown in [10], it is

Lemma 2.1: *Suppose $d\geq b$. The distance, $\rho((a,b),(c,d))$, of two vertices in the wall (a,b) and (c,d) is*

$$\begin{cases} 2(d-b) & \text{if } |c-a|\leq(d-b) \text{ and } c+d\equiv a+b \pmod 2 \\ 2(d-b)+1 & \text{if } |c-a|\leq(d-b),\ c+d\equiv 0 \text{ and } a+b\equiv 1 \pmod 2 \\ 2(d-b)-1 & \text{if } |c-a|\leq(d-b),\ c+d\equiv 1 \text{ and } a+b\equiv 0 \pmod 2 \\ (d-b)+|c-a| & \text{if } |c-a|\geq(d-b) \end{cases}$$

Moreover, a shortest path between (a,b) and (c,d) lies in the rectangle spanned by these two vertices.

W.C. Shiu, P.C.B. Lam, C.S. Tong and I. Gutman [10-14] used this lemma to treat several homologous series of compact pericondensed systems. All the results are referenced in the next section.

3. Wiener Numbers of Some Pericondensed Benzenoid Molecules

In this section, we shall summarize the Wiener numbers of homologous series of compact pericondensed benzenoid molecules obtained in [10-14]. Some particular sharp of these molecules are shown in the Appendix.

Definition: A graph formed by a row of n hexagonal cells is called an *n-hexagonal chain.* A graph consisting of m n-hexagonal chains forming the shape of a parallelogram is called an $n \times m$ *hexagonal parallelogram*, and is denoted by $Q_{n,m}$ (it was denoted by $Q_{m,n}$ in [11]). $Q_{n,n}$ is called a *hexagonal n-quadrangle* and is denoted by Q_n.

Since $Q_{n,m} \cong Q_{m,n}$, we assume $m \geq n$.

Theorem 3.1: *For* $m \geq n \geq 1$ *the Wiener number of* $Q_{n,m}$ *is*

$$\tfrac{1}{15}\{20(n+1)^2 m^3 + 10n(n^2+9n+8)m^2$$
$$+5(n^4+8n^3+16n^2+2n-1)m - n(n^4-20n+4)\}.$$

Since $Q_{n,1}$ is an n-benzenoid chain, we have the following corollary which is a previously known result [3].

Corollary 3.2: *The Wiener number of the n-benzenoid chain* ($n \geq 1$) *is* $\frac{1}{3}(16n^3+36n^2+26n+3)$.

Theorem 3.3: *The Wiener number of* Q_n *is*

$$\tfrac{1}{15}(34n^4+170n^3+200n^2+10n-9)n, \; n \geq 1.$$

Definition: A graph consisting of m n-hexagonal chains forming the shape of a rectangle is called an $n \times m$ *hexagonal rectangle*, and is denoted by $R_{n,m}$ [12].

It should be noted that $R_{1,n}$ and $R_{n,1}$ are not isomorphic to each other.

Theorem 3.4: *When* $1 \leq m \leq 2n$ *the Wiener of* $R_{n,m}$ *is*

$$\tfrac{1}{60}\{-m^5+5(2n+1)m^4+5(8n^2+24n+11)m^3$$
$$+5[16n^3+72n^2+78n+5]m^2+[160n^3+320n^2+140n-25-31(-1)^m]m$$
$$+5[16n^3+(12(-1)^m-16)n+3((-1)^m-1)]\}.$$

When $m \geq 2n$ *the Wiener of* $R_{n,m}$ *is*

$$\tfrac{1}{15}\{20(n+1)^2m^3+60n(n+1)m^2+(20n^4+80n^3+155n^2+60n-5)m$$
$$+(-8n^4-20n^3+30n^2-25n-22)n\}.$$

There are other types of hexagonal rectangle called the *hexagonal jagged-rectangles* (*HJR*) [14]. In hexagonal rectangle every hexagonal chain is of the same length n. In the HJR the numbers of hexagonal cells in each chain alternative between n and $n-1$. These result in 3-types of HJR. If the top and bottom rows are longer we shall call it HJR of type I and denoted by $I^{n,m}$. If the top and bottom rows are shorter we shall call it HJR of type K and denoted by $K^{n,m}$. The last one is called HJR of type J and denoted by $J^{n,m}$.

Theorem 3.5: *The Wiener number of* $I^{n,m}$ *is*

$$\tfrac{1}{15}(80mn^3+80m^2n^2+120mn^2-20n^2+40m^3n+80m^2n$$
$$+30mn-20n-8m^4+20m^3+30m^2-20m-7)m$$

if $1 \leq m \leq n$, *and*

$$\tfrac{1}{15}(-8n^5+40mn^4-20n^4+80mn^3-10n^3+160m^3n^2$$
$$+10mn^2+20n^2+160m^3n-60mn+18n+40m^3-25m)$$

if $n \leq m$.

Theorem 3.6: *The Wiener number of* $J^{n,m}$ *is*

$$\tfrac{2}{15}(40m^2n^3+40mn^3+10n^3+40m^3n^2+120m^2n^2+20mn^2-15n^2$$
$$+20m^4n+80m^3n+45m^2n-15mn+5n-4m^5+5m^3-45m^2-31m)$$

if $1 \leq m \leq n$, *and*

$$\tfrac{2}{15}(-4n^5+20mn^4+40mn^3-5n^3+80m^3n^2+120m^2n^2$$
$$+65mn^2+80m^3n-45mn+9n+20m^3-30m^2-35m)$$

if $n-1 \leq m$.

Theorem 3.7: *The Wiener number of* $K^{n,m}$ *is*

$$\tfrac{1}{15}(80m^2n^3+160mn^3+80n^3+80m^3n^2+360m^2n^2+220mn^2$$
$$-60n^2+40m^4n+240m^3n+270m^2n-40mn+10n-8m^5-20m^4$$
$$-50m^3-280m^2-197m-15)$$

if $1 \leq m \leq n-1$, *and*

$$\tfrac{1}{15}(-8n^5+40mn^4+20n^4+80mn^3-10n^3+160m^3n^2+480m^2n^2+490mn^2$$
$$+100n^2+160m^3n-360mn-132n+40m^3-120m^2-55m+45)$$

if $n-1 \leq m$.

Definition: A graph consisting of m s-hexagonal chains, where s runs from n to $n-m+1$, forming the shape of a trapezium is called an *$n\times m$ hexagonal trapezium* [13]. A graph obtained by merging the base n-hexagonal chains of two $n\times m$ hexagonal trapeziums, forming a convex 6-sided polygon, is called an *$n\times m$ hexagonal bitrapezium* [13]. An $n\times m$ hexagonal trapezium and an $n\times m$ hexagonal bitrapezium are denoted by $T_{n,m}$ and $S_{n,m}$, respectively.

Theorem 3.8: *When $1\le m\le \frac{1}{2}(n+1)$, the Wiener number of $S_{n,m}$ is*

$$\tfrac{1}{15}\{-28m^4+20(n+1)m^3-10(4n^2+8n+3)m^2$$
$$+10(8n^3+24n^2+23n+7)m-(20n^2+40n+17)\}m\,.$$

When $\frac{1}{2}(n+1)\le m\le n$, the Wiener number of $S_{n,m}$ is

$$\tfrac{1}{15}\{36m^5-140(n+1)m^4+10(12n^2+24n+13)m^3-10(n+1)m^2$$
$$+(20n^4+80n^3+100n^2+40n-1)m+2n(n^4+5n^3+10n^2+10n+4)\}\,.$$

Definition: A graph formed by a hexagon in the centre, surrounded by r rings of hexagonal cells, is called an *n-hexagonal net*, and is denoted by H_r [10].

The Wiener number of H_r was shown in [10] previously. It is a special case of Theorem 3.5 when taking $n=2r-1$ and $m=r$ for $r\ge 1$.

Corollary 3.9: *The Wiener number of H_r is $\frac{1}{5}(164r^5-30r^3+r)$, $r\ge 1$.*

Theorem 3.10: *The Wiener number of $T_{n,m}$, $1\le m\le n$, is*

$$\tfrac{1}{30}\{-8m^5+20m^4n-5(8n^2+16n+7)m^3+5(8n^3+24n^2+24n+9)m^2$$
$$+4(20n^3+55n^2+45n+7)m+20n(2n^2+3n+1)\}\,.$$

Definition: A graph with n k-hexagonal chains, where k ranges from 1 to n, in the shape of an equilateral triangle is called an *n-hexagonal triangle* and denoted by T_n [12].

The Wiener number of T_n was found by Shiu, Tong and Lam in [12] previously. But it is a special case of Theorem 3.10 when taking $m=n$.

Corollary 3.11: *The Wiener number of the n-hexagonal triangle T_n is*

$$\tfrac{1}{10}(4n^3+36n^2+79n+16)(n+1)n\,.$$

4. Wiener Number of Irregular Hexagonal Nets

In 1996, I. Gutman and S. Klavžar [8] introduced another method to calculate the Wiener numbers of benzenoid hydrocarbons. In the following we shall modify their definitions and their Theorem. We shall use this method to find the Wiener of irregular hexagonal nets.

Let B be a benzenoid system B. We viewed B as a plane graph in which each of its faces are the same regular hexagon. Choose an edge $e \in \partial B$, where ∂B is the boundary of B. Draw a straight line L through the midpoint P of e and orthogonal on e. Let Q be the first intersection point of L with ∂B. Then the line segment C with endpoints P and Q is called the *elementary cut pertaining to e* (see Figure 1 for example). For convenience, we identify the elementary cut C with the set of edges of B which are crossed by C. The set of all elementary cuts of B is called the *complete set of elementary cuts* (CSEC) of B. Note that any edge of B belongs to one and only one elementary cut.

Let C be an elementary cut of B. Then $B-C$ consists two components, denoted by $B'(C)$ and $B''(C)$ (see Figure 2 for example).

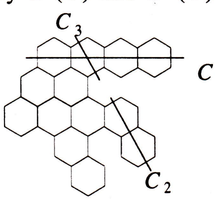


Figure 1: C_1, C_2 and C_3 are elementary cuts

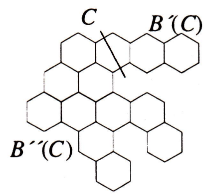


Figure 2

Then we have the following modified Theorem (the original Theorem is stated in [8] without proof).

Theorem 4.1: *Let B be a benzenoid system such that ∂B is a cycle. Then the Wiener number of B is*

$$W(B) = \sum_{C} n(B'(C))n(B''(C)) = \sum_{C} n(B'(C))\{n(B) - n(B'(C))\} \qquad (4\text{-}1)$$

where $n(G)$ denotes the order of G, and the summation runs over the CSEC of B.

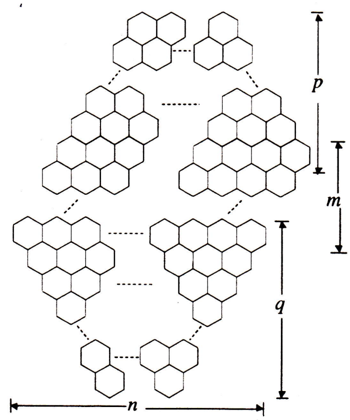
Proof: For $u, v \in V(B)$, let $P_{u,v}$ be a given shortest $(u,v)-$path in B. Since the family of all CSEC of B is a disjoint partition of $E(B)$, it follows that

$$W(B) = \sum_{\{u,v\}\in S} |P_{u,v}| = \sum_{C} \sum_{\{u,v\}\in S} |P_{u,v} \cap C|,$$

where S is the set of all unordered pairs of V. Now given and elementary cut C, then $P_{u,v} \cap C = \emptyset$, i.e., $|P_{u,v} \cap C| = 0$, if u and v belong to the same component of $B-C$, otherwise $|P_{u,v} \cap C| = 1$. Therefore

$$\sum_{\{u,v\}\in S} \left|P_{u,v} \cap C\right| = n(B'(C))n(B''(C)),$$

and (4-1) follows. □



$H_{n,m,p,q}$

Definition: A graph obtained by merging the base n-hexagonal chains of $T_{n,p}$ and $T_{n,q}$ with two base n-hexagonal chains of $Q_{n,m}$ forming a convex 6-sided polygon, is called an *irregular hexagonal net* and denoted by $H_{n,m,p,q}$ (see the figure), where $1 \le p, q \le n$ and $m \ge 1$. By reflection it is easy to see that $H_{n,m,p,q} \cong H_{n,m,q,p}$. Therefore, we may assume that $q \ge p$.

Now we consider $B = H_{n,m,p,q}$ and draw it in the normal direction (as the above figure). We separate CSEC of B into three groups, namely Γ_0, Γ_1 and Γ_2, where Γ_i is the set of elementary cut that cut the graph B in an angle $60i°$ to the horizontal in clockwise direction, $i = 0,1,2$. Then

$$W(B) = f_0 + f_1 + f_2$$

where

$$f_0 = \sum_{C\in\Gamma_0} n(B'(C))\{n(B) - n(B'(C))\} = f(n,m,p,q), \tag{4-2}$$

$$f_1 = \sum_{C\in\Gamma_1} n(B'(C))\{n(B) - n(B'(C))\},$$

$$f_2 = \sum_{C\in\Gamma_2} n(B'(C))\{n(B) - n(B'(C))\}.$$

It is easy to see that $n(B) = n(H_{n,m,p,q}) = 2(m+p+q-1)(n+1) - (p^2+q^2)$. Since

$$f_1 = \begin{cases} f(n, m+p+q-n-1, n-p+1, n-q+1) & \text{if } p+q \ge n-m+2 \\ f(m+p+q-2, -m-p-q+n+3, m+q-1, m+p-1) & \text{if } p+q \le n-m+2 \end{cases}$$

and

$$f_2 = \begin{cases} f(n+m-1, p+q-n, n-p+1, n-q+1) & \text{if } p+q \ge n+1 \\ f(m+p+q-2, n-p-q+2, q, p) & \text{if } p+q \le n+1. \end{cases}$$

Thus it suffices to calculate f_0. Let C_z be the elementary cut of B which passes through the z-th layer of B (the bottom layer is the first layer and the top one is the

$(p+q+m-2)$-th layer) and let $B'(C_z)$ be the subgraph of B that under the elementary cut C_z. Then $n(B'(C_z))$ is equal to

$\sum_{y=0}^{z-1}(2n-2q+2y+3)$ if $1 \le z \le q$,

$\sum_{y=0}^{q-1}(2n-2q+2y+3)+\sum_{y=m+q-2}^{z-1}(2n+2)$ if $q \le z \le m+q-1$, and

$\sum_{y=0}^{q-1}(2n-2q+2y+3)+\sum_{y=q}^{z-1}(2n+2)+\sum_{y=q+m-1}^{z-1}(2n+2m+2q-2y-1)$

if $m+q \le z \le m+q+p-2$.

Hence

$$n(B'(C_z))=\begin{cases} z(z+2n-2q+2) & \text{if } 1 \le z \le q \\ 2nz+2z-q^2 & \text{if } q \le z \le m+q-1 \\ 2(m+q)(z-q+1)+2nz-z^2-m^2-1 & \text{if } m+q \le z \le m+q+p-2. \end{cases}$$

Substitute the above results into (4-2) we have f_0 equal to

$$\begin{aligned} &\tfrac{1}{30}\{20m(m-1)(m-2)(n+1)^2 \\ &\quad +(p+q)[(60m^2-120m+40)n^2+(120m^2-230m+70)n+(60m^2-110m+31)] \\ &\quad +20pq(6mn+6m-6n-5)(n+1) \\ &\quad +10(p^2+q^2)[6(m-1)n^2-(3m^2-18m+13)n-(3m-12m+7)] \\ &\quad +pq(p+q)(60n^2-60mn+180n-60m+115) \\ &\quad +(p^3+q^3)(20n^2-40mn+80n-40m+55) \\ &\quad +30p^2q^2(m-2n-3)-40pq(p^2+q^2)(n+1)-20(p^4+q^4)(n+1) \\ &\quad +20p^2q^2(p+q)+4(p^5+q^5)\}. \end{aligned}$$

Therefore we get the following Theorem:

Theorem 4.2: *The Wiener number of* $H_{n,m,p,q}$ *is*

$$\begin{aligned} &\tfrac{1}{30}\{2(20n^3m^2+10n^2m^3+5nm^4-m^5-40n^3m+30n^2m^2+10m^4+20n^3 \\ &\qquad -100n^2m+20nm^2-20m^3+60n^2-80nm+20m^2+55n-24m+15) \\ &\quad +(p+q)(80n^3m+60n^2m^2+40nm^3-10m^4-80n^3+120n^2m+80m^3 \\ &\qquad -200n^2+90nm-120m^2-170n+90m-57) \\ &\quad +20pq(4n^3+6n^2m+6nm^2-2m^3+6n^2+12m^2+5n-12m+5) \\ &\quad +10(p^2+q^2)(4n^3-2m^3+12n^2+6m^2+12n-5m+5) \\ &\quad -5(p^3+q^3)(8n^2+4m^2+16n-8m+11)-5pq(p+q)(12m^2-24m+11) \\ &\quad +20(p^4+q^4)(n-m+2)-40pq(p^2+q^2)(m+1)-20pq(p^3+q^3)-8(p^5+q^5)\} \end{aligned}$$

if $p+q \le n-m+2$;

$$\tfrac{1}{30}\{2(-n^5+5n^4m+10n^3m^2+20n^2m^3-10n^4-30n^2m^2+40nm^3-20n^3$$
$$+20n^2m-100nm^2+20m^3-20n^2+80nm-60m^2-24n+55m-15)$$
$$+(p+q)(10n^4+40n^3m+120n^2m^2-120n^2m+240nm^2+40n^2$$
$$-390nm+120m^2+150n-230m+101)$$
$$+20pq(2n^3+12n^2m-6n^2+24nm-19n+12m-11)$$
$$+10(p^2+q^2)(2n^3+6n^2m-6nm^2+24nm-6m^2-12n+19m-11)$$
$$-60p^2q^2(n-m+2)-5(p^3+q^3)(4n^2+8nm+8m-5)$$
$$+5pq(p+q)(12n^2-24nm+48n-24m+37)+10(p^4+q^4)(n-m+2)$$
$$-40pq(p^2+q^2)(n+1)+20p^2q^2(p+q)-10pq(p^3+q^3)-6(p^5+q^5)\}$$
if $n-m+2\le p+q\le n+1;$

$$\tfrac{1}{30}\{2(-2n^5+5n^4m+10n^3m^2+20n^2m^3-15n^4-30n^2m^2+40nm^3-30n^3$$
$$+20n^2m-100nm^2+20m^3-30n^2+80nm-60m^2-28n+55m-15)$$
$$+(p+q)(20n^4+40n^3m+120n^2m^2+40n^3-120n^2m+240nm^2+100n^2$$
$$-390nm+120m^2+190n-230m+109)$$
$$+20pq(12n^2m-12n^2+24nm-25n+12m-13)$$
$$+10(p^2+q^2)(6n^2m-6nm^2-6n^2+24nm-6m^2-18n+19m-13)$$
$$-60p^2q^2(2n-m+3)-5(p^3+q^3)(8nm-8n+8m-9)$$
$$+5pq(p+q)(24n^2-24nm+72n-24m+49)-10(p^4+q^4)(m-1)$$
$$-80pq(p^2+q^2)(n+1)+40p^2q^2(p+q)-4(p^5+q^5)\}$$
if $n+1\le p+q$.

Note that $H_{n,m,1,1}=Q_{n,m}$, $H_{n,1,m,m}=S_{n,m}$ and $H_{n,1,1,m}=T_{n,m}$. Theorem 4.2 can be verified by these special cases.

Acknowledgement

We thank Fox K.H. Woo for his programming work.

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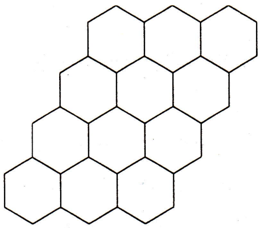
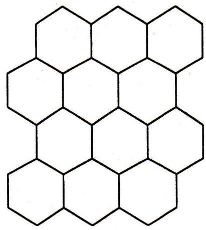
Appendix

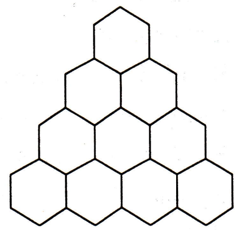
The followings are some compact pericondensed benzenoid molecule graphs which are defined in this paper.



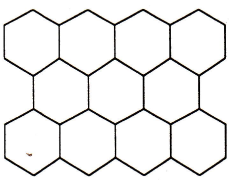
$Q_{3,4}$



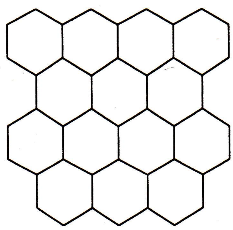
$R_{3,4}$



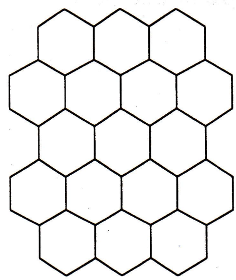
T_4



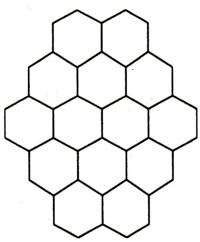
$I^{4,2}$



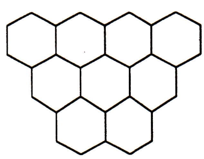
$J^{4,2}$



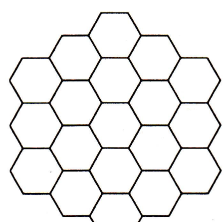
$K^{4,2}$



$S_{4,3}$



$T_{4,3}$



H_3