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Domination in Benzenoids

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A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science at Virginia Commonwealth University.

by

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Contents

Abstract

DOMINATION IN BENZENOIDS

By Nisreen A. Bukhary, Master of Science.

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A benzenoid is a molecule that can be represented as a graph. This graph is a fragment of the hexagon lattice. A dominating set D in a graph G is a set of vertices such that each vertex of the graph is either in D or adjacent to a vertex in D. The domination number $\gamma = \gamma(G)$ of a graph G is the size of a minimum dominating set. We will find formulas and bounds for the domination number of various special benzenoids, namely, linear chains $L(h)$, triangulenes T_k, and parallelogram benzenoids $B_{p,q}$. The domination ratio of a graph G is $\frac{\gamma(G)}{n(G)}$, where $n(G)$ is the number of vertices of G. We will use the preceding results to prove that the domination ratio is no more than $\frac{1}{3}$ for the considered benzenoids. We conjecture that is true for all benzenoids.
Keywords: benzenoid, domination number, packing number, linear chain, triangulene, benzenoid parallelgoram, domination ratio.

Benzenoids, Domination, and Introduction

1.1 Introduction

1.1.1 Key Definitions

A *graph* $G = (V, E)$ consists of a set of vertices $V = V(G)$ and a set of edges $E = E(G)$ together with an incidence relation which associates each edge in E to two distinct vertices in V. A graph can be thought of as "dots and lines". In the graph G in Fig. 1.1, $V(G) = \{v_1, v_2, v_3, v_4, v_5, v_6, v_7\}$ and $E(G) = \{v_1v_2, v_1v_3, v_3v_4, v_4v_5, v_5v_2, v_3v_6, v_1v_6, v_4v_6, v_1v_7, v_2v_7, v_5v_7\}$. Our graphs are *simple*: they do not have loops or more than one edge between any pair of vertices.

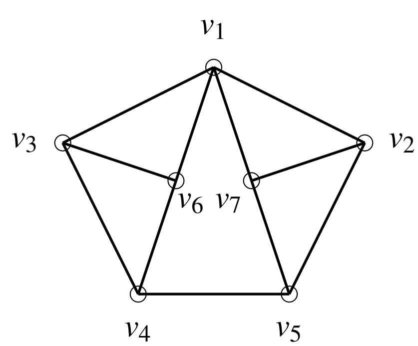

Figure 1.1: A graph G with 7 vertices, packing number $\rho(G) = 1$, and domination number $\gamma(G) = 2$. The set $P = \{v_1\}$ is a maximum packing set, and the set $D = \{v_2, v_3\}$ is a minimum dominating set.

What follows are, in alphabetical order, definitions of some of the key concepts occurring in this thesis. Other concepts are defined as they appear in the thesis.

DEFINITION 1.1. Let C be a cycle on the hexagonal lattice. A *benzenoid* or *benzenoid graph* is formed by the vertices in edges lying on C and in the interior of C [7]. Benzene (see Fig. 1.2) is the simplest example. Benzenoid graphs are also called benzenoid systems, hexagonal systems and hexagonal animals.

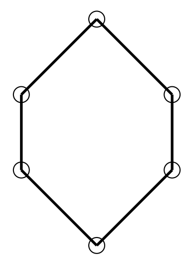

Figure 1.2: The graph of benzene, C_6.

DEFINITION 1.2. A set D in a graph G is a *dominating set* if each vertex is either in D or adjacent to a vertex in D. The *domination number* $\gamma = \gamma(G)$ is the cardinality of a minimum dominating set. Furthermore, D is an *efficient dominating set* if $|N[v] \cap D| = 1$ for every vertex $v \in D$. Not every graph has an efficient dominating set. The graph G is *efficient* if and only if has an efficient dominating set [8].

If D is a dominating set, D is said to dominate itself as well as its neighbors. For instance, for the graph in Fig. 1.1, the set $D = \{v_2, v_3\}$ is a minimum dominating set and $\gamma(D) = 2$. Note that D is not an efficient dominating set; so this graph is not efficient. Furthermore, for the complete graph K_n, any vertex dominates itself and the remaining vertices, so $\gamma(K_n) = 1$. For any cycle C_n, the reader may check, $\gamma(C_n) = \lceil \frac{n}{3} \rceil$.

DEFINITION 1.3. The *domination ratio* is the ratio of the domination number $\gamma(G)$ to the number of vertices $n(G)$, such that $\frac{\gamma(G)}{n(G)}$.

In Fig. 1.1, the domination ratio is $\frac{\gamma(G)}{n(G)} = \frac{2}{7}$. Also, for example for the cycle C_4, the domination ratio is $\frac{2}{4}$. C_4 is an example of a graph whose domination ratio is greater than $\frac{1}{3}$.

For the graphs considered in this thesis we conjecture that the domination ratio is no more than $\frac{1}{3}$, and we prove this in special cases.

DEFINITION 1.4. An *independent set* is a set of vertices S in a graph G which no two vertices in S are adjacent. Furthermore, the *independence number* $\alpha = \alpha(G)$ is the size of largest set of vertices such that no two are adjacent.

For the graph G in Fig. 1.1, the set $S = \{v_6, v_7\}$ is an maximum independent set and $\alpha(G) = 2$. For the complete bipartite graph $K_{n,n}$, for example, the independence number is $\alpha(K_{n,n}) = n$, and for the complete graph K_n the independence number is $\alpha(K_n) = 1$.

DEFINITION 1.5. In a graph G, the *degree* of a vertex v of a graph G is the number of edges incident to the vertex. The degree of a vertex v is denoted $deg(v)$. The *maximum degree* of a graph G, denoted by $\Delta = \Delta(G)$, and the *minimum degree* of a graph G, denoted by $\delta = \delta(G)$, are the maximum and minimum degree of its vertices.

In the graph G in Fig. 1.1, the maximum degree is $\Delta(G) = 4$ and the minimum degree is $\delta(G) = 3$. For the complete graph K_n, for example, the maximum degree and the minimum degree are equal; $\Delta(K_n) = \delta(K_n) = n-1$.

DEFINITION 1.6. For every vertex v, the *open neighborhood* of v is $N(v) = \{w \in V(G) | wv \in E(G)\}$. The *closed neighborhood* $N[v]$ for any vertex $v \in V(G)$ is the open neighborhood of v together with the vertex v itself. So $N[v] = \{v\} \cup N(v)$.

For example, in Fig. 1.1, the open neighborhood for v_1 is $N(v_1) = \{v_2, v_7, v_6, v_3\}$, and the closed neighborhood is $N[v_1] = \{v_1, v_2, v_7, v_6, v_3\}$.

DEFINITION 1.7. A set P is a *packing set* or *packing* if for any two vertices $u, v \in P$, $N[v] \cap N[u] = \phi$. The *packing number* $\rho = \rho(G)$ is the cardinality of maximum packing set.

In Fig. 1.1, $P = \{v_1\}$ is a maximum packing set and $\rho(G) = 1$. For the complete graph K_n, for example, any vertex dominates itself and the remaining vertices, it will be also a packing set; so $\rho(K_n) = 1$.

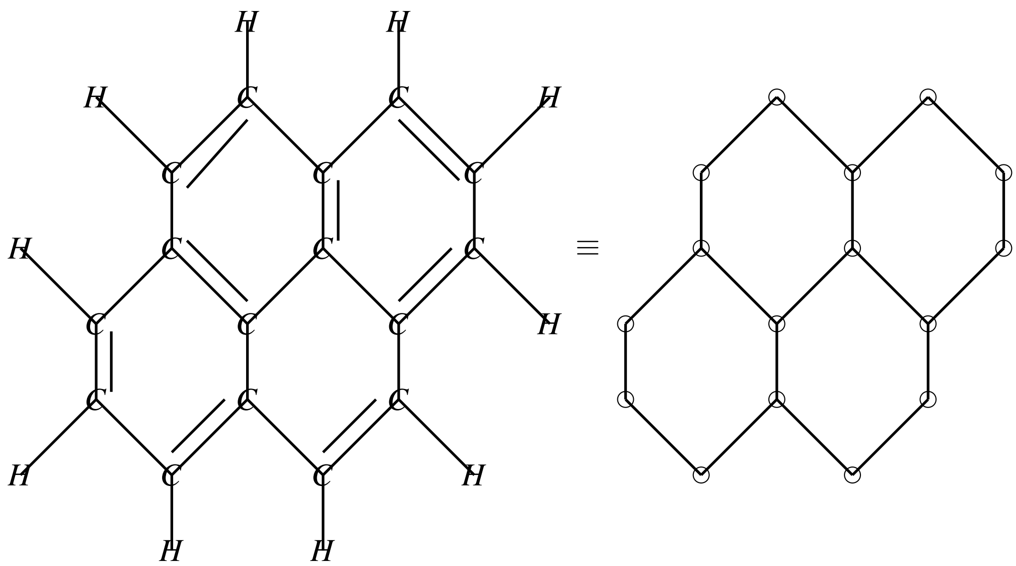

Figure 1.3: A structural diagram of a benzenoid hydrocarbon.The carbon atoms with free electrons on the outer edge of the benzenoid are bonded with hydrogen atoms. For the present purposes, we consider the graph on the right formed by removing these hydrogens. The resulting graph is the “carbon framework” of the benzenoid.

1.1.2 Chemistry

The chemical properties of benzenoids are of great and practical interest. The investigation of the mathematical properties of benzenoids may lead to insights regarding their chemical properties. This has occurred with related investigations.

Benzenoid hydrocarbons are condensed polycyclic unsaturated fully conjugated hydrocarbons consisting of benzene rings C_6 (see Fig. 1.3) according to the definition of the International Union of Pure and Applied Chemistry $IUPAC$. The German chemist Kekule discovered the structure for benzene in the $19th$ century. It is not known how many of these compounds exist in nature, but it is probably in the thousands. It is not easy to answer this question and determine the number of benzenoid hydrocarbons because of separation, isolation, purification, and identification of any benzenoid hydrocarbons [7].

Benzenoids are commonly found in the environment. Tons are produced in car exhausts [5]. In 1933, scientists reported a benzo[a]pyrenemany as a carcinogenic costituent of coal. After that they discovered that other benzenoid hydrocarbons are carcinogenic. Many of the smaller benzenoids have now been classified as either carcinogenic or non-carcinogenic. Some work has been done on a general theory of which benzenoids are carcinogenic [1]. More work remains to be done.

The thrust of this thesis is a mathematical investigation of the domination number and domination number of the graphs of these chemical molecules. Similar investigations have led to chemical insights. It is our hope that this investigation will lead to chemical insights. Following an investigation of the Graffiti conjecture-making program, Fajtlowicz and Larson showed that minimization of the independence number of a fullerene graph is a very good predictor of the stability of fullerene molecules [6]. Relatedly Pepper pointed out that minimization of the independence number of a benzenoid is a predictor of benzenoid stability [9][10]. Furthermore, Pepper found an upper bound for the independence ratio of a benzenoid. He found that, for every benzenoid G, $\alpha(G) \leq \frac{11n(G)-2}{20}$, so that the independence ratio is never more than $\frac{11}{20}$ [10]. We expect that the following investigation of the domination number and domination ratio will lead to similar correlation with chemical properties.

Results on Domination

2.0.3 The history of the domination number.

In 1862, the problem of determining the domination numbers of graphs first occurs in the paper of de Jaenisch. He wanted to find the minimal number of queens on a chessboard, such that every square is either occupied by a queen or can be reached by a queen with a single move [4]. Domination as a theoretical area in graph theory was formalized by Berge in 1958 and by Ore in 1962 [8]. One early result that we will use (Theorem 2.4) is due to Ore [2].

Furthermore, the theory of packing sets and the packing number is closely related to the theory of dominating sets and the domination number. In particular, it is proved in Theorem 2.2 that, for any graph which has a packing that dominates all vertices in the graph, the packing number $\rho(G)$ is equal to the domination number $\gamma(G)$. So we have that $\rho(G) = \gamma(G)$. Furthermore, for any graph $\rho(G) \leq \gamma(G)$. So in investigating the domination number of a graph it is a useful tool to construct packings. This is used in several of the following proofs.

2.0.4 Some useful results.

LEMMA 2.1. (Rubalcaba, Schneider and Slater [11]). For any graph G, $\rho(G) \leq \gamma(G)$.

Proof. Let P be a maximum packing set, and D is a minimum dominating set. Each vertex $v \in P$ is either in D or can be associated to a unique vertex v' in $D \setminus P$. Note that vertices

$v, w \in P$ can not both be adjacent to the same vertex in D since, for every $v, w \in P$, we have $N[v] \cap N[w] = \phi$. So $|P| \leq |D|$; thus, $\rho(G) \leq \gamma(G)$. $\square$

Earlier, we defined efficient dominating sets. These sets can be thought of as dominating sets where each vertex in the graph is dominated by exactly one vertex in the set. Recall that $\rho(G)$ is the packing number of G and that $\gamma(G)$ is the domination number of G.

THEOREM 2.2. (Rubalcaba, Schneider and Slater [11]). If a graph G has an efficient dominating set, then $\rho(G) = \gamma(G)$.

Proof. Let G be a graph, and let S be an efficient dominating set of G. So $\gamma(G) \leq |S|$. It also follows from the definition that S is a packing. Thus, $|S| \leq \rho(G)$. So, $\gamma(G) \leq \rho(G)$. By Lemma 2.1, $\rho(G) \leq \gamma(G)$. Thus $\rho(G) = \gamma(G)$. $\square$

However, later it will be useful to prove bounds on the domination number in terms of the numbers of vertices n, and the maximum degree $\Delta(G)$. Recall that the upper bound and the lower bound on the domination number is restricted by the number of vertices in the graph. So we will prove two theorems for upper and lower bounds on the domination number.

THEOREM 2.3. (Walikar, Acharya, Sampathkumar [8], See p.50). For any graph G, $\left\lceil \frac{n}{1+\Delta(G)} \right\rceil \leq \gamma(G)$.

Proof. Let D be a minimum dominating set of G. Each vertex $v \in D$ dominates at most $\Delta(D)$ other vertices. That is $|N(D)| \leq |D| \cdot \Delta(G)$. Since D is a dominating set, we have $D \cup N(D) = V(G)$. Hence, $|V| \leq |D| + |N(D)|$, which implies $n \leq |D| \cdot \Delta(G) + |D|$. So $n \leq \gamma(\Delta(G)+1)$. Thus, $\left\lceil \frac{n}{1+\Delta(G)} \right\rceil \leq \gamma(G)$. $\square$

THEOREM 2.4. (Ore, [8], See p.41). If G is a graph of order n without isolated vertices, then $\gamma(G) \leq \frac{n}{2}$.

Proof. Let S be a minimum dominating set of a graph G with no isolated vertices. We will show that $V(G)-S$ is also a dominating set. Let $v \in S$. So it must be shown that there is a vertex $w \in V(G)-S$, such that w is adjacent to v. Note that v is adjacent to some vertex in G since G has no isolated vertices. If v is only adjacent to vertices in S, then $S-\{v\}$ is dominating set, which contradicts of the minimality of S. So v is adjacent to some vertex $w \in V(G)-S$, and $V(G)-S$ is a dominating set. Thus, $\gamma(G) \leq min\ \{|S|,|V(G)-S|\}$. Since $|S|+|V(G)-S|=n$, it follows that, $\gamma(G) \leq \frac{n}{2}$. □

Benzenoid Domination Main Results

3.1 Linear Benzenoid Chains.

A *linear benzenoid chain* is a collection of hexagons arranged on a horizontal line where each pair of adjecent hexagons share a vertical edge. Let $L(h)$ be the linear benzenoid chain with h hexagons. Benzene, represented by an isolated hexagon, is $L(1)$. See Fig. 3.1 for $L(5)$.

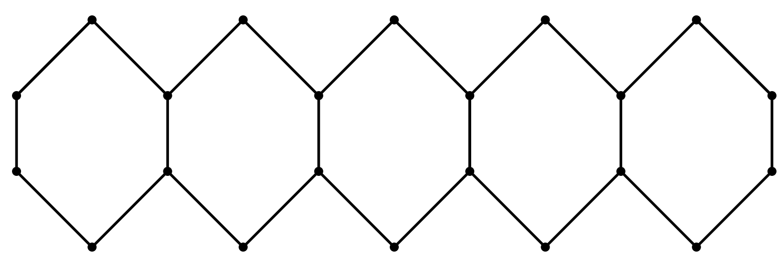

Figure 3.1: The linear benzenoid chain $L(5)$.

In order to represent the vertices of $L(h)$ by coordinates we can view the linear chain as being situated on two horizontal lines. See Fig. 3.2.

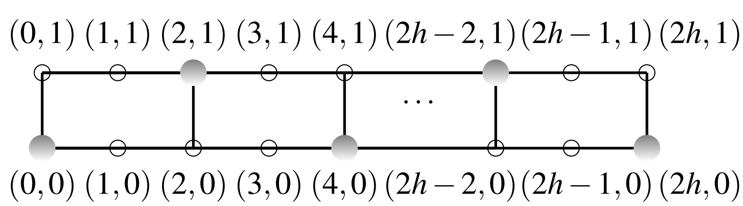

Figure 3.2: Coordinate system for the linear chain.

In the following two results, we will calculate the number of vertices $n(L(h))$ and the domination number $\gamma(L(h))$ of the linear benznoid chain with h hexagons.

PROPOSITION 3.1. If $L(h)$ is a linear benzenoid chain with h hexagons, then $n(L(h)) = 4h+2$.

Proof. First, we note by inspection that the lemma is true for a linear benzenoid chain $L(h)$ with $h=1$. Now, assume the lemma is true for a linear benzenoid chain $L(h-1)$ with $h-1$ hexagons. So assume the number of vertices is $n(L(h-1)) = 4(h-1)+2 = 4h-2$. We will now show that the lemma follows for a linear benzenoid chain with h hexagons. See Fig. 3.3. Note that by removing the vertices $(2h-2,1),(2h,1),(2h-1,0),(2h,0)$ we are left with a linear benzenoid chain with $h-1$ hexagons. Thus, $n(L(h)) = n(L(h-1))+4$. So by the inductive assumption, the number of vertices for $n(L(h)) = (4h-2)+4 = 4h+2$, proving the corollary. $\square$

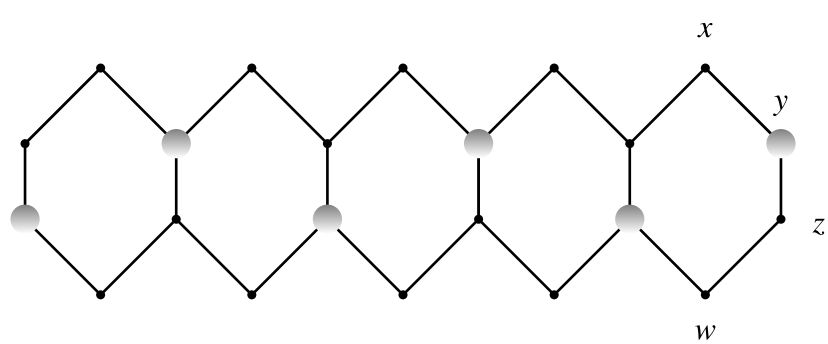

Figure 3.3: The shaded vertices are a minimum dominating set for the linear benzenoid chain $L(5)$. The shaded vertices are also a maximum packing.

THEOREM 3.2. If $L(h)$ is a linear benzenoid chain with h hexagons, then $\gamma(L(h)) = h+1$.

Proof. Let $L(h)$ be a linear chain with h hexagons. We represent the vertices of $L(h)$ by the coordinate system described above. Let $S_h = \{(2x, \frac{1+(-1)^{x+1}}{2})|x = 0,1,...,h\}$. The vertices in this set correspond to the shaded vertices in Fig. 3.3. It is easy to check that S_1 is an efficient dominating set for $L(1)$. Assume S_{h-1} is an efficient dominating set for $L(h-1)$. We will now show that S_h is an efficient dominating set for $L(h)$. Note that $S_h = S_{h-1} \cup \{(2h, \frac{1+(-1)^{h+1}}{2})\}$. We will show that each vertex in $(2h-2,1), (2h,1), (2h-1,0), (2h,0)$ is dominated by exactly one vertex in S_h. We know $(2h-2,0)$ is in S_h and $(2h-2,0)$ dominates $(2h-1,0)$. We also know $(2h,1)$ is in S_h and it dominates itself as well as $(2h-1,1)$ and $(2h,0)$. So each vertex in $L(h)$ is dominated exactly once. Thus, by Theorem 2.2, S_h is a miniumum dominating set and $\gamma(L) = |S_h| = h+1$. □

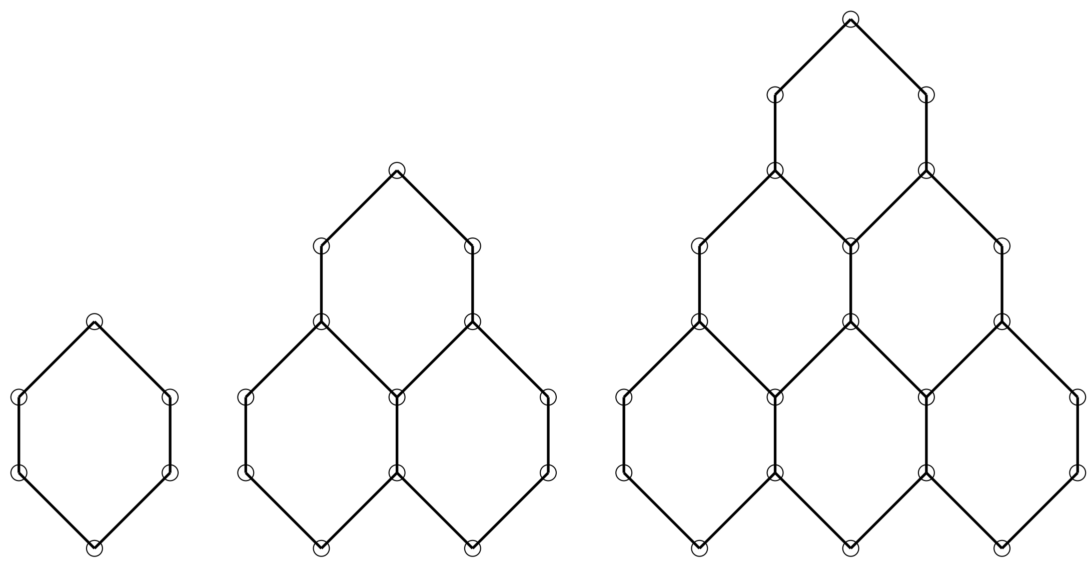

Figure 3.4: The first three triangulenes; T_1, T_2, and T_3.

3.2 Triangulenes

Let us now represent another simple class of benzenoid graphs, (see Fig. 3.4), group of benzenoid triangulenes. The *triangulene* T_k, with $k \geq 1$ levels of hexagons, is arranged in the form of an equilateral triangle, which have the same number of hexagons in each side. These triangulene consists of k rows, and k hexagons on the last bottom row, and the k rows are placed in a grid of horizontal lines, and these lines are noted by $1,2,3,\cdots,2k$ or $2k+1$. Furthemore, depending on the number of rows, we can divide the class of triangulenes in to *even triangulenes* with $2k$ levels, or *odd triangulenes* with $2k+1$ levels. Moreover, this class of benzenoids is not new, where it was noted by Clar [3]. The different classes of the triangulenes were used to show that the independence number can be arbitrarily larger than the matching number, $\alpha(G)-\mu(G)$ [7]. Actually, because of the difference between triangulenes with even and odd number of rows following Pepper in [10], we will consider these cases seperately. For even triangulenes, we will find an exact forrmula for the domination number; for the odd triangulenes, we will find an upper bound.

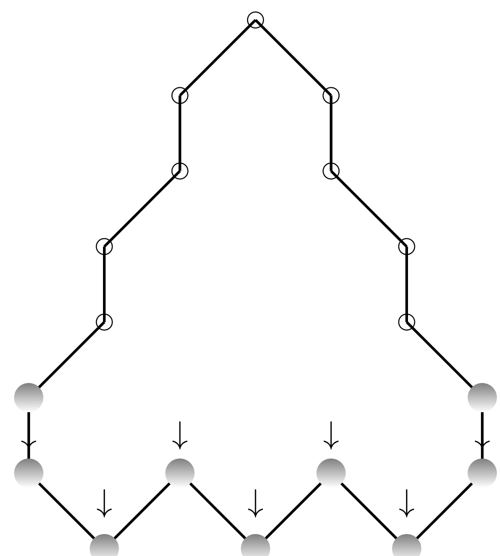

Figure 3.5: The bottom row of the triangulene T_k contains $2k+3$ vertices. The $2(3)+3=9$ shaded vertices are the bottom row of T_3.

LEMMA 3.3. For every triangulene T_k with $k \geq 2$, there are $2k+3$ vertices belonging to the bottom row of hexagons, which do not belong to any other row of hexagons.

Proof. Let T_k be a triangulene with k levels, $k \geq 2$. So there is a bottom row of hexagons with one or more rows above this row. Also note that, for a triangulene with k levels, there are k hexagons on the bottom row. Each of these hexagons has a negatively sloping bottom edge adjacent to two vertices, totaling $2k$ vertices. Moreover, the left-most hexagon on the bottom row also contains one other vertex not belonging to this set, or to any of the hexagons in the rows above, and the right-most hexagon contains two vertices not belonging to this set or to any of the hexagons in the rows above. Thus, together these are totally $2k+3$ vertices (see Fig. 3.5). □

PROPOSITION 3.4. For any triangulene T_k with k levels, $k \geq 2$, there are $n(T_k) = k^2+4k+1$ vertices.

Proof. Clearly, $n(T_1) = (1)^2+4(1)+1 = 6$ since T_1 is benzene, the six-cycle. Now, assume the result of the lemma is true for T_l where $l \geq 2$. Let T_{l+1} be a triangulene with $l+1$ levels. The vertices in T_{l+1} consist of the vertices in the first l levels together with the vertices on the bottom $(l+1)th$ row, which do not belong to any previous level. By the inductive assumption, the first l levels of T_{l+1} have $n(T_l) = l^2+4l+1$ vertices. Furthermore, by Lemma 3.3 there are $2(l+1)+3$ vertices on the last row, which do not belong to any previous row. Thus, $n(T_{l+1}) = (l^2+4l+1)+[2(l+1)+3] = l^2+6l+6 = (l+1)^2+4(l+1)+1$, which was to be shown. □

3.2.1 Even Triangulenes

An *even triangulene* is a benzenoid with an even number of levels; denoted by T_{2k} for an integer $k \geq 1$. See Fig. 3.7 for an example of an even triangulene with 6 levels, such that $T_{2k} = T_{2(3)}$ where k is the number of even rows.

LEMMA 3.5. For every triangulene with an even number of levels, denoted by T_{2k} for an integer k, and $k \geq 1$, there is a packing which dominates all the vertices of T_{2k}.

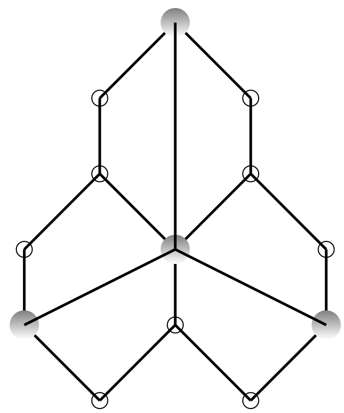

Figure 3.6: The shaded vertices are a packing of T_2, which dominates all the vertices of T_2; so $\rho(T_2) = \gamma(T_2) = 4$.

Proof. The lemma can be verified for $T_2 = T_{2k}$, which is $k = 1$. By inspection: the shaded set in Fig. 3.6 is a packing which dominates all the vertices in T_2. For an even triangule T_{2n} consider the set P_{2n} described as follows; note that each even row consists of consecutive pairs of hexagons (since there are an even number of hexagons). Let P_{2n} consist of the apex (the vertex at the very top) together with the lower left vertex of the left hexagon and the lower right vertex of the right hexagon of each of these packing og hexagons, plus the vertex of the two shared vertices of theis pair. Assume P_{2n} is a packing for T_{2n}. We will show that $P_{2(n+1)}$ is a packing set for $T_{2(n+1)} = T_{2n+2}$. By the construction, $P_{2(n+1)}$ is a packing of the last bottom row (which is an even row). It remains to show that every vertex in the second row from the bottom is dominated, but every vertex in this row belongs to either the row above it or below it except the upper left vertex of the left-most hexagon and the upper right vertex of the right-most hexagon. By the construction, $P_{2(n+1)}$ contains the lower left vertex of the left-most hexagon of the third row from the bottom and the lower right vertex of the right-most hexagon of this row. It can be checked that these dominate the remaining two vertices from the second row from the bottom. $\square$

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THEOREM 3.6. For every even triangulene T_{2k} with $k \geq 1$, the domination number of T_{2k} is $\gamma(T_{2k}) = (k+1)^2$.

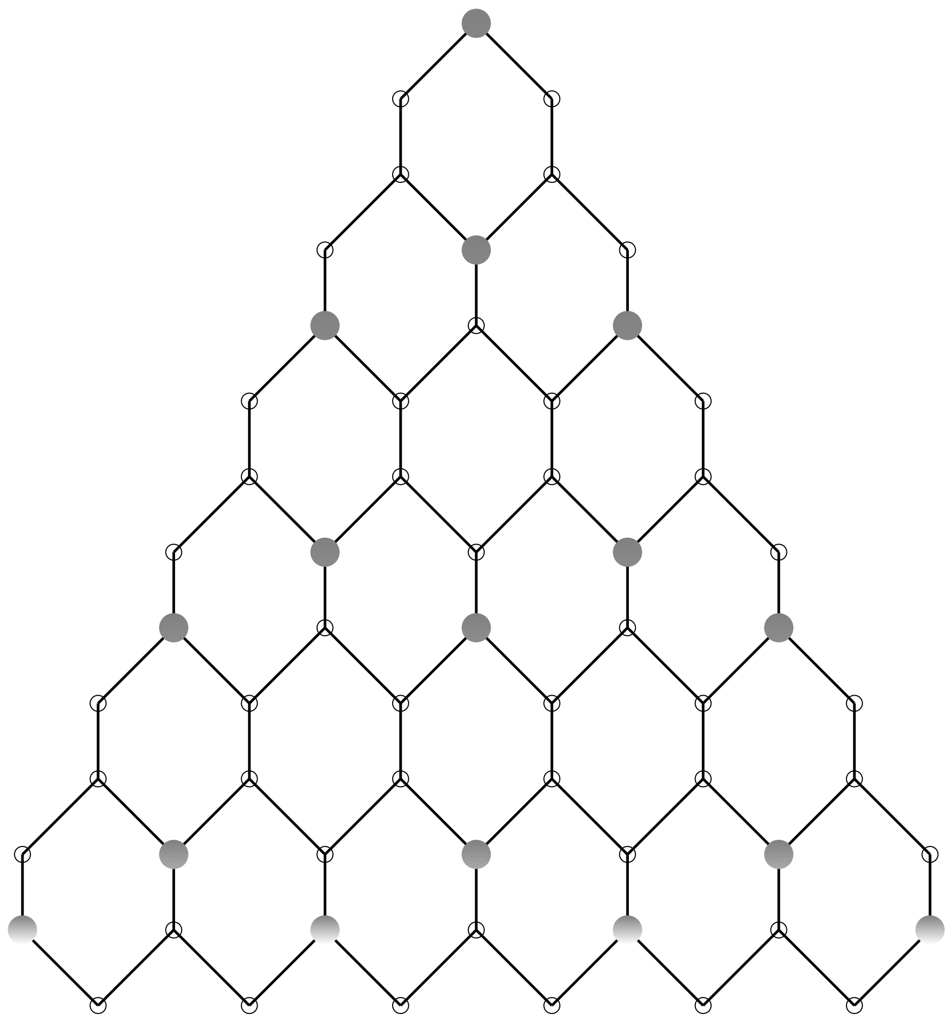

Figure 3.7: The shaded vertices are a dominating set for the even triangulene T_6. This set is also a packing. Here $\gamma(T_6) = \gamma(T_{2(3)}) = (3+1)^2 = 16$.

Proof. It can be seen from Fig. 3.6 for T_{2k} with $k = 1$, that $\gamma(T_2) = (1+1)^2 = 4$. Now, assume that $\gamma(T_{2k}) = (k+1)^2$ is true. Note that $\gamma(T_{2(k+1)}) = (T_{2k+2}) = ((k+1)+1)^2 = (k+2)^2$. Let S be a packing of T_{2k+2} guaranteed by the Lemma 3.5. Furthermore, by the construction of this packing, S consists of a packing of T_{2k} together with $2k+3$ vertices from the "bottom row" namely the $(2k+2)$nd row of hexagons. However, since the packing set S is a dominating set, then Theorem 2.2 guarantees that $\rho(T_{2k}) = \gamma(T_{2k})$. By assumption $\gamma(T_{2k}) = (k+1)^2$; hence, $\rho(T_{2k+2}) = \rho(T_{2k}) + (2k+3) = (k+1)^2 + (2k+3) = (k+2)^2$. Thus, by the construction, this packing is a dominating set, and $\gamma(T_{2k+2}) = \rho(T_{2k+2}) = (k+1)^2$, proving the theorem. □

3.2.2 Odd Triangulenes

An *odd triangulene* is a benzenoid with an odd number of levels; denoted by T_{2k+1} with $k \geq 1$. In Fig.3.8 is an example of an odd triangulene with 5 levels. There is some difficulty to get an exact formula for the domination number. We are not able to use the same packing we used for the even triangulenes T_{2k} to define the dominating set for T_{2k+1}, but we will conjecture a close bound.

THEOREM 3.7. For any odd triangulene T_{2k+1}, $\gamma(T_{2k+1}) \leq (k+1)^2 + k$.

Proof. As what was proved above, we already know that a triangulene with even levels, T_{2k}, has a minimum dominating set which is a maximum packing set with $(k+1)^2$ vertices, and $\gamma(T_{2k}) = (k+1)^2$. Now, we will use this fact to form an upper bound for a triangulene with $2k+1$ levels. One, not necessarily minimum, dominating set of T_{2k+1} consists of dominating set of T_{2k} together with sufficiently many vertices to dominate the "bottom row" of T_{2k+1}. It is clear that $\gamma(T_{2k}) \leq \gamma(T_{2k+1})$ since T_{2k+1}consists of T_{2k} plus an additional vertices. Let S be the packing of T_{2k} guaranteed by Lemma 3.5. Then it can be easily checked that S together with the bottom vertex of each hexagon in the bottom row is a dominating set of T_{2k+1}. So $\gamma(T_{2k+1}) \leq \gamma(T_{2k})$ + one vertex from each hexagon on the bottom row, which equals to $\gamma(T_{2k}) + k$. Therefore, by Theorem 3.6, $\gamma(T_{2k}) = (k+1)^2$, and we have $\gamma(T_{2k+1}) \leq (k+1)^2 + k = k^2 + 4k + 2$, which we need to show as approximate bound for the odd triangulene. □

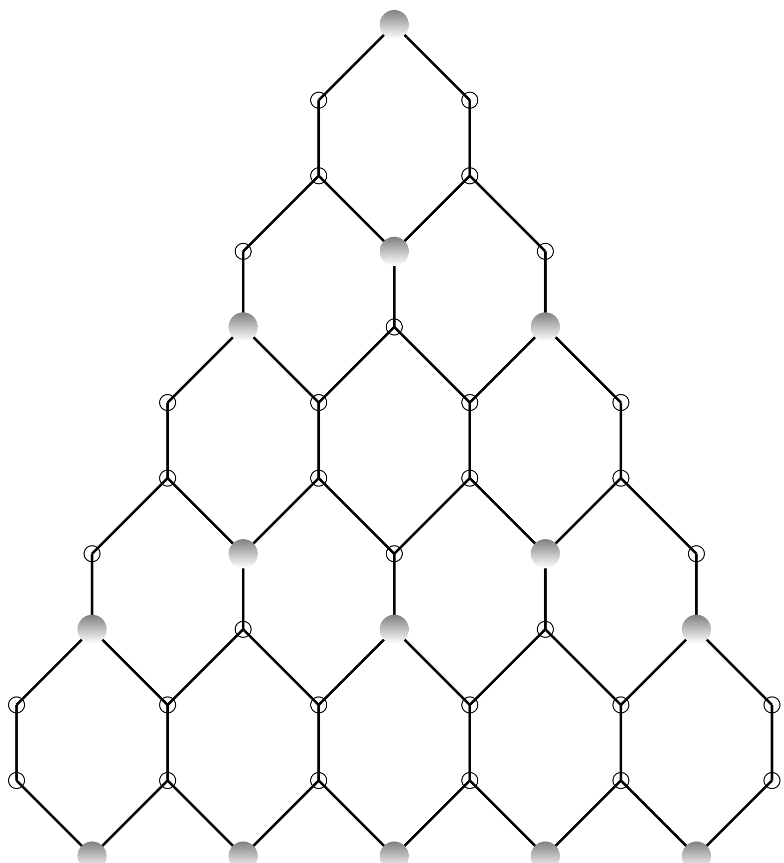

Figure 3.8: The shaded vertices are a dominating set for T_5; which is an example of T_{2k+1} with $k = 2$, corresponding to the construction in the proof of Theorem 3.8. This dominating set has 14 vertices.

3.3 Parallelogram Benzenoids

In Fig. 3.9, we see a new type of benzenoid called a *parallelogram benzenoid*. Let $p \geq 1$ and $q \geq 1$ be an integers. The parallelogram $B_{p,q}$ is a benzenoid that consists of $p \cdot q$ hexagons: these regular hexagons are arranged in shape of p rows, and each row has q benzene rings, which are shifted by half benzene ring to the right from the row immediately below (see Fig. 3.9). We will find a formula for the domination number of these parallelogram benzenoids.

However, the parallelogram benzenoid $B_{p,q}$ can have either even or odd number of rows. For the difference even and odd rows in $B_{p,q}$, we will note that is difficult to deduce a formula for the domination number for $B_{p,q}$ with even p or q, but we can find an exact formula for the domination number for $B_{p,q}$ with odd p and q. Hence, we will consider cases, depending on whether p and q are odd or even, and we will define an upper bound for these cases where we do not have an exact formula.

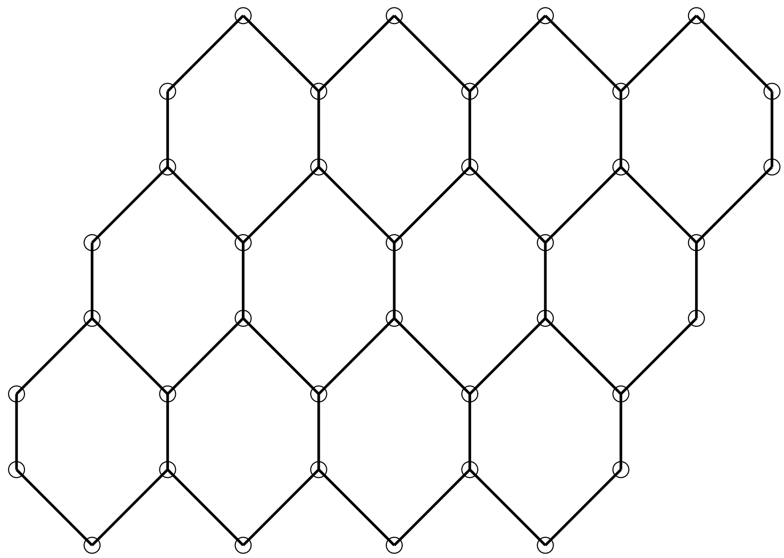

Figure 3.9: Benzenoid parallelogram $B_{p,q}$ where in this figure the number of rows are $p = 3$, and the number of hexagons in each row is $q = 4$.

PROPOSITION 3.8. For any benezenoid parallelogram, $B_{p,q}$, the number of vertices of $B_{p,q}$ is $n(B_{p,q}) = 2pq + 2p + 2q$.

Proof. A linear chain is a special parallelogram benzenoid, where $p = 1$. So we know by Proposition 3.1, that $n(B_{1,q}) = 2(1)q + 2(1) + 2q = 4q + 2$. Now, assume that $n(B_{p,q}) = 2pq + 2p + 2q$. We must show that $n(B_{p+1,q}) = 2(p+1)q + 2(p+1) + 2q = 2pq + 4q + 2p + 2$. The number of vertices of $B_{p+1,q}$ is $n(B_{p+1,q}) = n(B_{p,q}) +$ the vertices on the bottom row. The negatively sloped edge of each hexagon in the bottom row contains two vertices for a total of $2q$ vertices. Furthermore, the left-most and the right-most hexagon each contain one vertex not belonging to $B_{p,q}$ or a negatively sloped edge. So the total vertices on the bottom row is $2q+2$. Thus, $n(B_{p+1,q}) = n(B_{p,q}) + (2q+2) = (2pq+2p+2q) + (2q+2) = 2pq+4q+2p+2$, which was to be shown. □

Recall, the domination number of a linear benzenoid chain is $\gamma(L(h)) = h+1$, where h is the number of hexagons. Since each row P_i, of the chemical structure in $B_{p,q}$ is a linear chain, then for each row $\gamma(P_i) \leq h+1 = q+1$, where h=q. Now, we will consider the following six cases, and find an approximate upper bound for each case:

1. $p = 2$ and $q \geq 4$.

2. p is even and $q \geq 4$.

3. $p = 3$ and q is even.

4. p and q are both odd.

5. p and q are both even.

6. The remaining special cases: $B_{2,2}$, $B_{4,4}$, and $B_{4,6}$.

Case 1. $p = 2$ and $q \geq 4$.

THEOREM 3.9. For any benzenoid parallelogram $B_{p,q}$, with $p = 2$ and $q \geq 4$, then $\gamma(B_{2,q}) \leq 2q$.

Proof. In this case, we have a benzenoid parallelogram $B_{p,q}$ with $p = 2$ rows and $q \geq 4$ of columns. First, $B_{2,q}$ can be divided into two disjoint copies of T_2 (call them T_{p_1} and T_{p_2}) with remaining vertices (see Fig. 3.10). Now, the two triangulenes T_{p_1} and T_{p_2} have dominating sets that are packings. Note, using the construction of the dominating set for T_{2k} from Theorem 3.6, the union of these sets dominates $B_{2,4}$. Now, let D be the dominating set which includes these dominating sets for T_{p_1} and T_{p_2}, and the "valleys" vertices from the top row and the "peaks" from the bottom row (see the example on the right in Fig. 3.10.) Let D_q be the described set corresponding to $B_{2,q}$. Clearly, D_4 dominates $B_{2,4}$. Assume D_n dominates $B_{2,n}$ for $n \geq 4$. Furthermore, $B_{2,n+1}$ consists of $B_{2,n}$ together with one more one more column, and D_{n+1} consists of D_n together with the upper and lower right vertices of $B_{2,n+1}$. By assumption D_n dominates $B_{2,n}$. It can easily be checked that the other two vertices in D_{n+1} dominate the 6 vertices added in creating $B_{2,n+1}$ from $B_{2,n}$. So D_{n+1} dominates $B_{2,n+1}$. This proves that D_q dominates $B_{2,q}$ for $q \geq 4$. By construction, $|D_q| = 8+2(q-4) = 2q$. So, $\gamma(B_{2,q}) \leq 2q$. □

Furthermore, this idea of $B_{2,q}$ when $p = 2$ and $q \geq 4$, can be extended to the case where p even. We follow the same procedure of Theorem 3.9 in the Case 1.

Case 2. p is even and $q \geq 4$.

THEOREM 3.10. For any benzenoid parallelogram $B_{p,q}$, with p even and $q \geq 4$, then $\gamma(B_{p,q}) \leq \frac{pq}{2} + \frac{p}{2} + q - 1$

Proof. As what proved in previous case, we already know that a parallelogram benzenoid $B_{2,q}$ with $p = 2$ and $q \geq 4$, has upper bound $\gamma(B_{2,q}) \leq 2q$. Now, we will use this upper bound for the $B_{2,q}$ with $q \geq 4$, to form an upper bound for $B_{p,q}$ with p even and $q \geq 4$ (See Fig. 3.10). Note that, we will extend the construction of the dominating set for $B_{2,q}$ from Theorem 3.9. Let D_2 be the constructed set. Now, let D_p be the dominating set with even p constructed in Theorem 3.9. The pth row, which can be viewed as a linear chain. Let D be the union of these sets. By construction D dominates every vertex in the first and second rows and every vertex in the every even row. It remains to show that D dominates every vertex in the third rows. Note that there are only two vertices in each odd row which does not belong to the previous of following even rows. These two vertices are the upper left-most vertex of this odd row and the lower right-most vertex of this row. The upper left-most vertex of this odd row is dominated by the lower left-most vertex of the row above (which belongs to D by our construction). The lower right-most vertex of the odd row is dominated by the upper right-most vertex of the even row below it (which belongs to D by our construction). Note there are $\frac{p}{2}$ even rows, and $\frac{p}{2}-1$ even rows other than the second row. See the left example in Fig.3.10. Thus, by construction, $|D| = |D_2| + (\frac{p}{2}-1)\cdot|D_p| = 2q + (\frac{p}{2}-1)(q+1) = \frac{pq}{2} + \frac{p}{2} + q - 1$. So, $\gamma(B_{p,q}) \leq \frac{pq}{2} + \frac{p}{2} + q - 1$, which proves the result. □

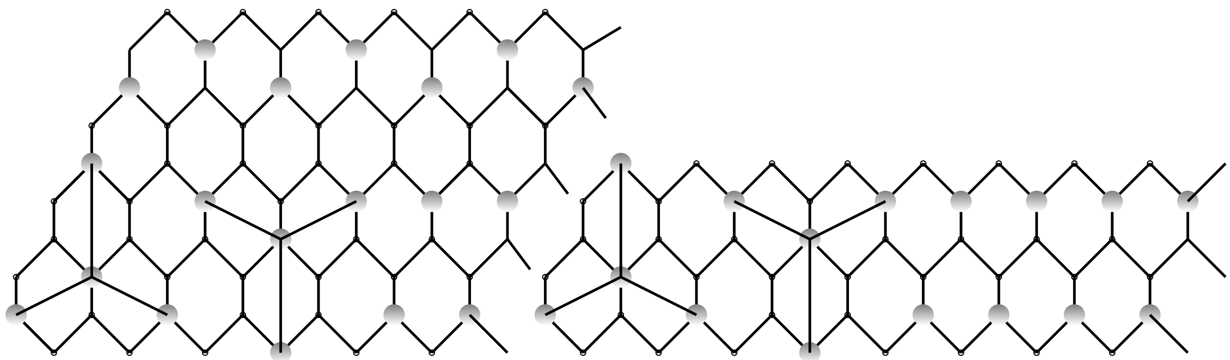

Figure 3.10: On the right, the construction in the proof of Theorem 3.9, for $B_{2,q}$ with $p=2$ and $q \geq 4$. In the left, the construction in the proof of Theorem 3.10, for $B_{4,q}$ with $p=4$ and $q \geq 7$. Furthermore, the shaded vertices are a dominating set for $B_{2,q}$ and $B_{4,q}$, respectively.

Case 3.$p=3$ and q is even.

THEOREM 3.11. For any benzenoid parallelogram $B_{p,q}$ with $p=3$ and q even, then $\gamma(B_{3,q}) \leq 2q+3$.

Proof. In this case, we have a benzenoid parallelogram $B_{p,q}$ with $p=3$ rows and q even. Since we have two odd rows in $B_{3,q}$ corresponding to a linear chain, then each row has a dominating set with $(q+1)$ vertices. Let D_i be the dominating set of the ith odd row constructed in Theorem 3.2 for the linear chains.

For the even row of $B_{3,q}$, the vertices of this row belong to either to first odd row below and second odd row above this even row except two vertices. The first vertex is the upper left-most vertex of the left hexagon in the even row, which is dominated by the lower right-most vertex of this row above it (which belongs to D by our construction). For the second vertex is the lower right vertex of the right-most hexagon of the even row, but it is not dominated by any other vertices in D_1 or D_3. Let D be the set consisting of the union of D_1, D_3 and this vertex. We have argued that D is a dominating set for $B_{3,q}$ (see our construction in Fig.3.11).

So, $\gamma(B_{3,q}) \leq |D| = 2(q+1)+1 = 2q+3$, which proves our result. $\square$

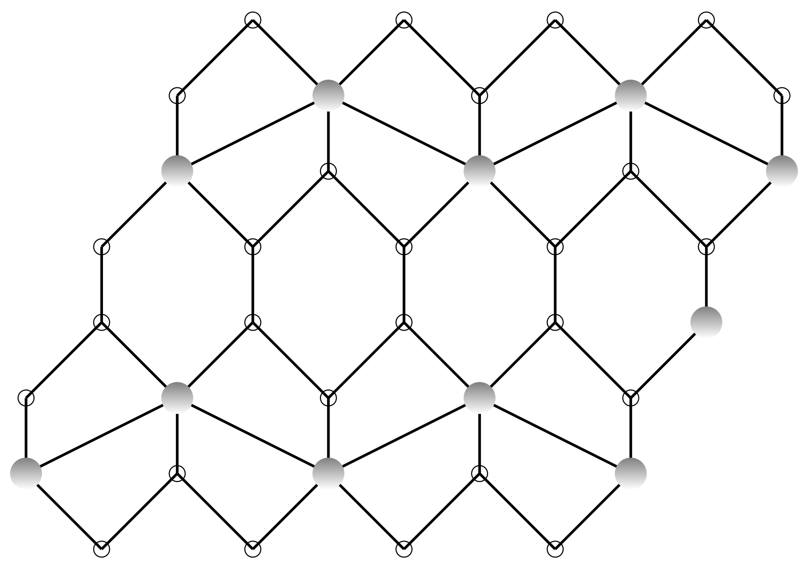

Figure 3.11: The shaded vertices are a dominating set for $B_{3,4}$; which an example of $B_{3,q}$ with $p=3$ and q even, corresponding to the construction in the proof of Theorem 3.11. This dominating set has $\gamma(B_{3,4}) = 2(4)+3 = 11$.

Case 4. p and q are both odd.

THEOREM 3.12. For any benzenoid parallelogram $B_{p,q}$ with p and q both odd, then $\gamma(B_{p,q}) = \frac{1}{2}(p+1)(q+1)$.

Proof. In this case, let O represent the odd rows (counting rows from the bottom proceeding up for $B_{p,q}$). Note that each row in O corrseponds to a linear chain. So each odd row has a dominating set with $(q+1)$ vertices. We will use these dominating sets from the odd rows to construct a dominating set D for $B_{p,q}$ which is a packing. For each odd row there are odd

q hexagons, and each odd row has a maximum packing set which is a dominating set with $q+1$ vertices (see Fig. 3.12). D will be the union of the dominating sets for the odd rows. For each odd row O_i, let D_i be the dominating set constructed in Theorem 3.2. Let D be the union of these D_i's. The set D_i has been shown to be a dominating set and a packing in the proof of Theorem 3.2. Hence, $\gamma(B_{1,q}) = \frac{1}{2}(1+1)(q+1) = q+1$. Consider any of the even rows of $B_{p,q}$. All but two of the vertices of this row belong either to odd rows above and below this row.

The remaining vertices are the upper left-most vertex of this row and the lower right-most vertex of this row (see the right example in Fig. 3.12). The upper left-most vertex of this row is dominated by the lower right-most vertex of the row above it (which belongs to D by our construction). The lower right-most vertex of this row is dominated by the upper right-most vertex of the row below it (which belongs to D by our construction). All the other vertices in this even row belong to odd rows above and below it and are hence dominated by D.

Now, we will show D is a packing of $B_{p,q}$. Consider any odd row of $B_{p,q}$. Let D_i be the constructed dominating set for this row. By the construction of D_i, D_i does not contain any of the "peaks" of the vertices along the top of this row. Hence, D_i does not dominate any vertex in the odd rows above it. Also, D_i does not contain any of the "valleys" of the vertices along the bottom of this row. Hence, D_i does not dominate any vertex in the odd rows below this row. Thus, no vertex is dominated by two different vertices. So D is a packing. Since D is a dominating set and a packing, Theorem 2.2 implies that $\gamma(B_{p,q}) = |D|$. Since there are $\frac{p+1}{2}$ odd rows, then $|D| = (\frac{p+1}{2})(q+1) = \frac{1}{2}(p+1)(q+1)$, which proves the result. □

Case 5. p and q are both even.

THEOREM 3.13. For any benzenoid parallelogram $B_{p,q}$, with p and q both even, and $p,q \geq 4$, then $\gamma(B_{p,q}) \leq \frac{p}{2}(q+1) + \frac{p}{2} + q$.

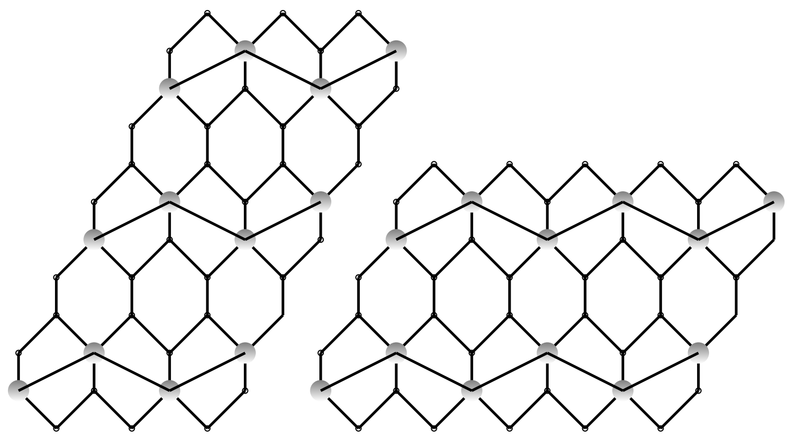

Figure 3.12: The shaded vertices are a dominating set for $B_{3,5}$ or $B_{5,3}$; which is an example of $B_{p,q}$ with odd p and q, corresponding to the construction in the proof of Theorem 3.12. This dominating set has $\gamma(B_{3,5}) = \frac{1}{2}(3+1)(5+1) = \frac{24}{2} = 12$ vertices.

Proof. As previous case, we count the odd rows (from the bottom to the top for $B_{p,q}$). Since each odd row corresponds to a linear chain, then each row has a dominating set with $(q+1)$ vertices. Let D_i be the dominating set of the ith odd row constructed in Theorem 3.2 for the linear chains. Let D be the union of the dominating sets for the D_i's. By this theorem, $|D_i| = \frac{1}{2}(1+1)(q+1) = q+1$. Since p is even, there are $\frac{p}{2}$ odd rows. So, $\sum |D_i| = \frac{p}{2}(q+1)$ for the odd rows.

For the even rows of $B_{p,q}$, the vertices of this row belong either to odd rows above and below this row except for two vertices. These two remaining vertices are the upper left-most vertex of this row and the lower right-most vertex of this row (see example in Fig. 3.13). The upper left-most vertex of this row is dominated by the lower right-most vertex of the row above it (which belongs to D by our construction), but the lower vertex of the right-most hexagon of this row is not dominated by any other vertices in D. For that, we will dominate these vertices by $\frac{p}{2}$ vertices. These vertices are the lower right vertex from the right-most hexagon from each even row. Since there are $\frac{p}{2}$ of these, then $|D_q| = \frac{p}{2}$ (see our construction in Fig. 3.13). The other vertices in the even row belong to odd rows above and below it and are dominated by D. Note that, in the last top even row of hexagons can be dominated by the "peaks" of this row. Let S be the set of these row peaks for this row in D (see our construction in Fig. 3.13).

So, $|D| \leq |D| = |D_i| + |D_q| + |S| +$. Thus, $\gamma(B_{p,q}) \leq \frac{p}{2}(q+1) + \frac{p}{2} + q$, which proves the result. $\square$

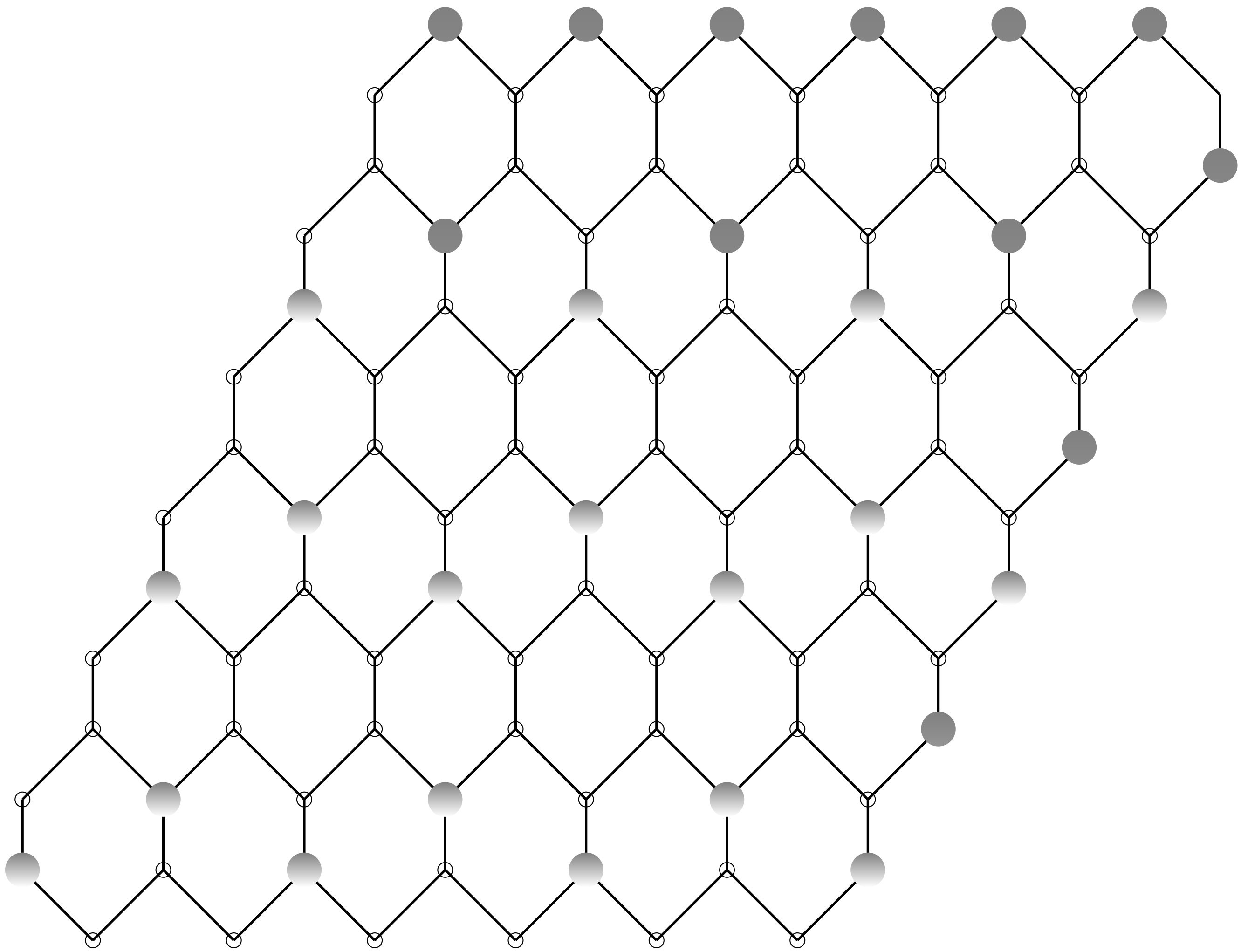

Figure 3.13: The shaded vertices are a dominating set for $B_{6,6}$; which is an example of $B_{p,q}$ for even p and q both even with $p, q \geq 4$, corresponding to the construction in the proof of Theorem 3.13. This is dominating set $\frac{6}{2}(6+1) + \frac{6}{2} + 6 = 30$ vertices. So, $\gamma(B_{6,6}) \leq 30$.

Case 6. Remaining special cases.

The cases that were not considered by the previous theorems are $B_{2,2}$, $B_{4,4}$ and $B_{4,6}$. In each case, a packing ρ which is a dominating set can be constructed. Then Theorem 2.2 guarantees the domination number is the cardinality of this set.

1. For $B_{2,2}$, see Fig.3.14. The constructed packing has 5 vertices. So $\gamma(B_{2,2}) = 5$.

2. For $B_{4,4}$, see Fig.3.15. The constructed packing has 13 vertices. So $\gamma(B_{2,2}) = 13$.

3. For $B_{4,6}$, see Fig.3.16. The constructed packing has 18 vertices. So $\gamma(B_{4,6}) = 18$.

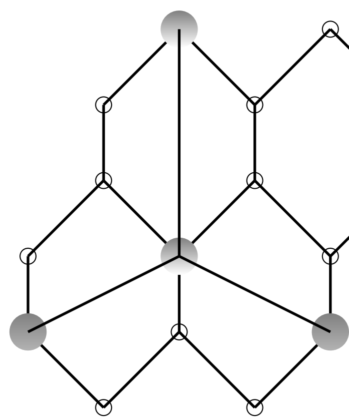

Figure 3.14: The shaded vertices are a dominating set for $B_{2,2}$; this dominating set is a packing and has 5 vertices. So, $\gamma(B_{2,2}) = 5$.

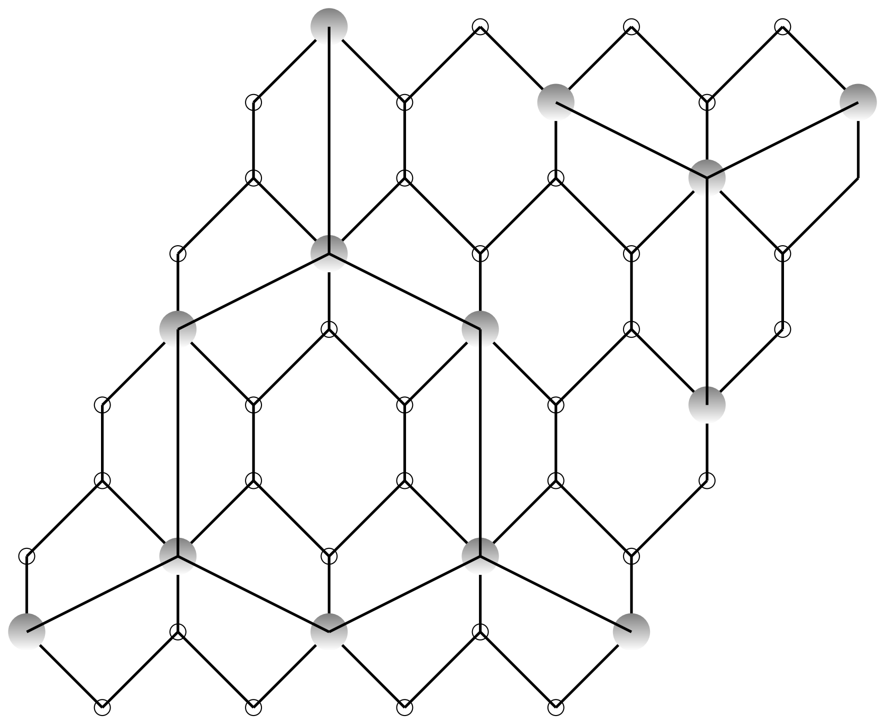

Figure 3.15: The shaded vertices are a dominating set for $B_{4,4}$; this dominating set is a packing and has 13 vertices. So, $\gamma(B_{4,4}) = 13$.

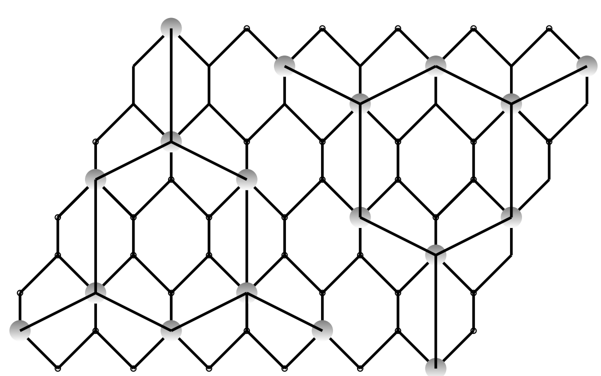

Figure 3.16: The shaded vertices are a dominating set for $B_{4,6}$; this dominating set is a packing and has 18 vertices. So, $\gamma(B_{4,6}) = 18$.

Domination Ratio

The domination ratio of a graph G is $\frac{\gamma(G)}{n(G)}$, the ratio of the domination number of G to the number of vertices of G. As mentioned above, the domination ratio of a benzenoid may correspond to chemical properties of the benzenoid.

Furthermore, for any benzenoid B the domination number is bounded such that $1 \leq \gamma(B) \leq n$. Each benzenoid type has outer vertices and inner vertices. For the *outer vertices*, the minimum degree is two, and the maximum degree is three, and the maximum and minimum degree for the *inner vertices* is always three, (see Fig. 4.1).

By Theorem 2.3 and Theorem 2.4, we know that $\frac{1}{4} \leq \frac{\gamma(B)}{n(B)} \leq \frac{1}{2}$. The lower bound is given as a function of the maximum degree Δ. We conjecture that due to the regular structure of the benzenoid that the upper bound can be given as a function of the maximum degree. We will propose an upper bound for $\gamma(B)$ in terms of the number of vertices n and the mazimum degree $\Delta(B) = 3$.

4.1 The upper bound for the linear benzenoid chains, triangulenes, and parallelogram benzenoids.

THEOREM 4.1. For any linear benzenoid chain $L(h)$, $\frac{\gamma(L(h))}{n(L(h))} \leq \frac{1}{3}$.

Proof. We already have proved that the linear benzenoid chain $L(h)$ with $h \geq 1$, has domination number $\gamma(L(h)) = h+1$. By Proposition 3.1, we proved $n(L(h)) = 4h+2$. So $\frac{\gamma(L(h))}{n(L(h))} = \frac{h+1}{4h+2}$. The reader can check that $h \geq 1$ implies $\frac{h+1}{4h+2} \leq \frac{1}{3}$, proving the claim. $\square$

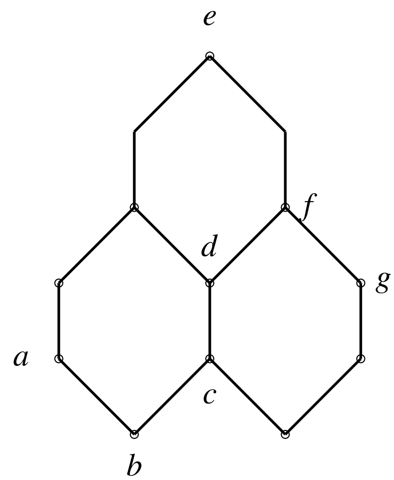

Figure 4.1: An example for the outer vertices and inner vertices in the benzenoid with three hexagons; for example, the vertices {a,b,g,e} are outer vertices with $\delta = 2$, and the vertices {c,g} are outer vertices with $\Delta = 3$. The vertex d is an inner vertex with $\Delta = 3$.

THEOREM 4.2. For even triangulene T_{2k} with $k \geq 1$, $\frac{\gamma(T_{2k})}{n(T_{2k})} \leq \frac{1}{3}$.

Proof. Let T_{2k} be any even triangulene, with $k \geq 1$. We proved from in Theorem 3.6 that $\gamma(T_{2k}) = (k+1)^2$. Also, from Proposition 3.4, we have $n(T_k) = k^2 + 4k + 1$, which follows $n(T_{2k}) = (2k)^2 + 4(2k) + 1 = 4k^2 + 8k + 1$. Hence, $\frac{\gamma(T_{2k})}{n(T_{2k})} = \frac{(k+1)^2}{4k^2+8k+1}$. Note that for $k \geq 1$, it is true that $2 \leq k^2 + 2k$. Then it follows that $3k^2 + 6k + 3 \leq 4k^2 + 8k + 1$. This implies that $3(k+1)^2 \leq 4k^2 + 8k + 1$, and $\frac{(k+1)^2}{(2k)^2+4(2k)+1} \leq \frac{1}{3}$, proving the claim. □

In this paper, we proved an approximate bound for the domination nmber of an odd triangulene since it was difficult to deduce an exact formula for $\gamma(T_{2k+1})$. Similarly, we do not have an exact formula for the domination ratio for these graphs, but we do have an approximate bound.

THEOREM 4.3. For any odd triangulene T_{2k+1}, $\frac{\gamma(T_{2k+1})}{n(T_{2k+1})} \leq \frac{1}{3}$.

Proof. From Theorem 3.7, we have shown that $\gamma(T_{2k+1}) \leq (k+1)^2 + k$. Moreover, Proposition 3.4 implies that $n(T_{2k+1}) = (2k+1)^2 + 4(2k+1) + 1 = 4k^2 + 12k + 6$. So $\frac{\gamma(T_{2k+1})}{n(T_{2k+1})} \leq$

$\frac{(k+1)^2+k}{4k^2+12k+6}$. For $k \geq 0$, the inequality $0 \leq k^2+5k+3$ is true. Then it follows that $3[(k+1)^2+k] \leq 4k^2+12k+6$, and $\frac{(k+1)^2+k}{4k^2+12k+6} \leq \frac{1}{3}$. proving the claim. $\square$

For the parallelogram benzeoid $B_{p,q}$ we covered six cases which in every case, we had $\frac{\gamma(B_{p,q})}{n(B_{p,q})} \leq \frac{1}{3}$.

Case 1. $p = 2$ **and** $q \geq 4$**.**

THEOREM 4.4. For any parallelogram benzenoids $B_{2,q}$ with $q \geq 4$ and $p = 2$, $\frac{\gamma(B_{2,q})}{n(B_{2,q})} \leq \frac{1}{3}$.

Proof. From Theorem 3.9, we have shown the bound for $B_{2,q}$ with $p = 2$ and $q \geq 4$, is $\gamma(B_{2,q}) \leq 2q$. Also, we have known $n(B_{p,q}) = 2pq+2p+2q$ for any p and q from Proposition 3.8. So we will verify that the domination number for $\gamma(B_{2,q})$ divide by the number of vertices no more than $\frac{1}{3}$. Thus, we have $\frac{\gamma(B_{2,q})}{n(B_{2,q})} \leq \frac{2q}{2(2)q+2(2)+2q}$. Since $q \geq 4$ and $p = 2$, it follows that $3(2q) \leq 2pq+2p+2q$. Thus, $\frac{2q}{2pq+2p+2q} \leq \frac{1}{3}$, so proving the claim. $\square$

Case 2. p **is even and** $q \geq 4$**.**

THEOREM 4.5. For any parallelogram benzenoids $B_{p,q}$ with p even and $q \geq 4$, $\frac{\gamma(B_{p,q})}{n(B_{p,q})} \leq \frac{1}{3}$.

Proof. As what we did in Theorem 4.4, we will show the upper bound for $B_{p,q}$ with p even and $q \geq 4$. From Theorem 3.10, and from Proposition 3.8, we know that $\gamma(B_{p,q}) \leq \frac{pq}{2}+\frac{p}{2}+q-1$ and $n(B_{p,q}) = 2(4)q+2(4)+2q$. So, $\frac{\gamma(B_{p,q})}{n(B_{p,q})} = \frac{\frac{pq}{2}+\frac{p}{2}+q-1}{2pq+2p+2q}$. It remains to show that $\frac{\frac{pq}{2}+\frac{p}{2}+q-1}{2pq+2p+2q} \leq \frac{1}{3}$. For p even, it follows that $0 \leq (p-2)q+p+6$, and that implies $3pq+3p+6q-6 \leq 4pq+4p+4q$. Hence, $\frac{\frac{pq}{2}+\frac{p}{2}+p-1}{2pq+2p+2q} \leq \frac{1}{3}$, proving for claim. $\square$

Case 3. $p = 3$ **and** q **is even.**

THEOREM 4.6. For any parallelogram benzenoids $B_{3,q}$ with q even, $\frac{\gamma(B_{3,q})}{n(B_{3,q})} \leq \frac{1}{3}$.

Proof. From Theorem 3.11, we have shown the bound for $B_{3,q}$ with $p = 3$ and q is even, is $\gamma(B_{3,q}) \leq 2q+3$. Also, we know $n(B_{p,q}) = 2pq+2p+2q$ for any p and q from Proposition

3.8. So we have $\frac{\gamma(B_{3,q})}{n(B_{3,q})} \leq \frac{2q+3}{2(3)q+2(3)+2q}$. It remains to show that $\frac{2q+3}{2(3)q+2(3)+2q} \leq \frac{1}{3}$. That is, $\frac{2q+3}{8q+6} \leq \frac{1}{3}$. This inequality is equivalent to $6q+9 \leq 8q+6$, which is true for $q \geq 1$, proving the claim.

Case 4. p **and** q **are both odd.**

THEOREM 4.7. For any parallelogram benzenoids $B_{p,q}$ with odd p and q, $\frac{\gamma(B_{p,q})}{n(B_{p,q})} \leq \frac{1}{3}$.

Proof. From Theroem 3.12 we note that the domination number for parallelogram benzenoid is $\gamma(B_{p,q}) = \frac{1}{2}(p+1)(q+1)$ p and q both odd. since the domination number for $B_{p,q}$ is an integers. From Proposition 3.8, we have $n(B_{p,q}) = 2pq+2p+2q$. So, $\frac{\gamma(B_{p,q})}{n(B_{p,q})} = \frac{(\frac{1}{2}(p+1)(q+1)}{2pq+2p+2q}$. It remains to show that $\frac{(\frac{1}{2}(p+1)(q+1)}{2pq+2p+2q} \leq \frac{1}{3}$. For $p \geq 1$ and $q \geq 1$, it follows that $3 \leq pq+p+q$. It then follows that $3(p+1)(q+1) \leq 2(2pq+2p+2q)$ and, from this, we conclude that $\frac{\frac{1}{2}(p+1)(q+1)}{2pq+2p+2q} \leq \frac{1}{3}$, proving the claim. □

Case 5. p **and** q **are both even.**

THEOREM 4.8. For any parallelogram benzenoids $B_{p,q}$ with p and q both even and $p,q \geq 6$, $\frac{\gamma(B_{p,q})}{n(B_{p,q})} \leq \frac{1}{3}$.

Proof. We have proved in Theorem 3.13, that $B_{p,q}$ with even p and q and both of them $p,q \geq 6$, has $\gamma(B_{p,q}) = \frac{p}{2}(q+1) + (\frac{p}{2} + \frac{p}{2})$. We also know, from Proposition 3.8, that $n(B_{p,q}) = 2pq+2p+2q$. So, $\frac{\gamma(B_{p,q})}{n(B_{p,q}} \leq \frac{3(pq+p)+3p+6q}{4pq+4p+4q}$. It remains to show that $\frac{\frac{p}{2}(q+1)+\frac{p}{2}+q}{2pq+2p+2q} \leq \frac{1}{3}$. For p and q both even and $p,q \geq 6$, it follows that $3 \leq pq-2p-2q$, and that implies $3(pq+p)+3p-3+6q \leq 4pq+4p+4q$. Hence, $\frac{\frac{p}{2}(q+1)+\frac{p-1}{2}+q}{2pq+2p+2q} \leq \frac{1}{3}$, proving the claim. □

Case 6. The remaining special cases: $B_{2,2}$**,** $B_{4,4}$**, and** $B_{4,6}$**.**

The cases that were not considered by the previous theorems are $B_{2,2}$, $B_{4,4}$ and $B_{4,6}$. We found that $\gamma(B_{2,2}) = 5$. Since $n(B_{2,2}) = 16$, it follows that $\frac{\gamma(B_{2,2})}{n(B_{2,2})} = \frac{5}{16} \leq \frac{1}{3}$. We also found that $\gamma(B_{4,4})) = 13$. Since $n(B_{4,4}) = 32$, it follows that $\frac{\gamma(B_{4,4})}{n(B_{4,4})} = \frac{13}{32} \leq \frac{1}{3}$. Finally, we found that $\gamma(B_{4,6}) = 18$. Since $n(B_{4,6}) = 68$, it follows that $\frac{\gamma(B_{4,6}}{n(B_{4,6})} = \frac{18}{68} \leq \frac{1}{3}$. In each case, a packing ρ which is a dominating set can be constructed. Then Theorem 2.2 guarantees the domination number is the cardinality of this set. (see Fig.3.14, Fig. 3.15, and Fig. 3.16, $\gamma(B_{2,2}) = 5$, $\gamma(B_{4,4}) = 13$ and for $\gamma(B_{4,6}) = 18$).

Thus we have show that the domination ratio for any linear chain $L(h)$, ant triangulene T_k, and any parallelogram benzenoid $B_{p,q}$ is no more than $\frac{1}{3}$.

Open Problems

We show that for any even triangulene T_{2k} the domination number is $\gamma(T_{2k}) = (k+1)^2$. For odd triangulenes, it was difficult to define an exact formula. It is hard to use the same packing that we used for the even triangulenes since we had a problem dominating the vertices in the last row for each odd triangulene.

Also, it was difficult to determine a formula for parallelogram benzenoids $B_{p,q}$ with even rows since we cannot find a packing set that dominates all the vertices in $B_{p,q}$.

We have shown that for every class of benzenoid that we have considered that the domination ratio never exceeds $\frac{1}{3}$.

CONJECTURE 5.1. For any benzenoid B, $\frac{\gamma(B)}{n(B)} \leq \frac{1}{3}$.

It is not true that for any graph G, $\frac{\gamma(G)}{n(G)} \leq \frac{1}{3}$. In our approach, the upper bound of the domination number $\gamma(B)$ for the benzenoid is basically based from Theorem 2.3 and Theroem 2.4, that $\frac{1}{4} \leq \frac{\gamma(B)}{n(B)} \leq \frac{1}{2}$ for any benzenoid B. Moreover, our results of this new relationships inequality provides an important new feature for the benzenoid domination number, which becomes possible to determain a close bound for the benzenoid domination number. So we will leave for the interested reader to check and find the exact formula for the domination number γ for the odd triangulenes and parallelogram benzenoids, and to prove the inequality for benzenoid B.

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Vita

Nisreen was born in Saudi Arabia, then she moved with her parents to the U.S.A at age of one month because her parents where studying in Arizona. Her childhood was in the U.S.A. until she went back to Saudi Arabia. She took all of her education in Jeddah, Saudi Arabia. Because Nisreen had a good recommended from her math teachers in high school, she decided to attend *Jeddah Girls College of Education-The scientific Sections*, where she majored in Mathematics and Education. After Nisreen graduated, she taught for a while in the middle school and high school as a math teacher. In 2007, she received a scholarship from her government in Kingdom of Saudi Arabia to complete her masters degree in applied mathematics in the U.S.A. She started at University of Florida in Gainesville, Florida, for one year; then she moved to Virginia Commonwealth University in Richmond, Virginia, to start her masters degree in applied mathematics.

In real life, Nisreen likes to spend her time with her parents and there brothers and sisters. Also, she likes to do are painting, reading, swimming, and bicycle racing. However, in the U.S.A. she is mostly busy with her studying, but during the weekend she spends time with her friends. Nisreen has had a wonderful chance to visit many states in the U.S.A., and have many new experinces. Nisreen has learned much from her family who thought her to be struggler, active and provident lady.