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K-dominating Sets on Linear Benzenoids and on the Infinite Hexagonal Grid*

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The paper presents the results referring to the *k*-dominating numbers on the linear benzenoid chain (for each $k \geq 1$) and perfect *k*-dominating sets on an infinite hexagonal grid.

INTRODUCTION

We will first give some mathematical definitions.

For any graph G we denote the vertex-set and the edge-set of G by V(G) and E(G), respectively. A subset D of V(G) is called a *k*-dominating set, if for every vertex *y* not in D, there is at least one vertex *x* in D, such that the distance between them $(d(x, y)) \leq k$. For convenience, we also say that D *k*-dominates G.

The *k*-domination number γ_k is the cardinality of the smallest *k*-dominating set. The l-domination number γ is also called a domination number.

A set S perfectly *k*-dominates a hexagonal grid if for each *v* vertex there is exactly one vertex $u \in$ S, such that $d(u,v) \leq k$. The set of vertices *k*-dominated by *u* will be denoted by $D_k(u)$.

Dominating sets appear to have their origins in the game of chess, where the goal is to cover or dominate various squares of a chessboard by certain chess pieces. The problem of determining domination numbers of graphs first emerged in 1862 in the paper of de Jaenisch.[1]

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. Domination as a theoretical area in graph theory was formalized by Berge[2] in 1958 and Ore[3] in 1962.

Two edges in graph G are independent if they are not adjacent in G. A set of pairwise independent edges of G is called a matching in G, while a matching of maximum cardinality is a maximum matching in G. The number of edges in a maximal matching of G is β_1.

If we have a graph G without isolated vertices, with *n* vertices, then he following holds: $\gamma(G) \leq \min\{\beta_1(G), n-\beta_1(G)\}$. It follows that from the domination number we can say something about a lower bound on the maximal matching.

* Dedicated to Professor Haruo Hosoya in happy celebration of his 70th birthday.

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Chemical structures are conveniently represented by graphs, where atoms correspond to vertices and chemical bonds correspond to edges.[4,5] However, this representation does not only provide a visual insight into molecular structures, but inherits many useful information about chemical properties of molecules. It has been shown in QSAR and QSPR studies that many physical and chemical properties of molecules are well correlated with graph theoretical invariants termed topological indices or molecular descriptors.[6]

One of such graph theoretical invariants is the domination number.[7] It has been shown that this number discriminates well between even the slightest changes in trees and hence it is very suitable for analyses of the RNA structures.[8] From the above said it follows that the domination number is just the simplest variant of *k*-domination numbers well known in mathematics.[9]

In this paper, we analyze *k*-domination of two well known chemical structures: graphite and chain benzenoids. Usage of topological indices for the analyses of graphite samples has already shown to be useful[10] and there is quite a substantial amount of literature covering the connection between benzenoids and topological indices (see, for instance, Ref. 11 and references therein). In some papers,[12,13] *k*-domination was investigated on the Cartesian product of two paths, which is equivalent to a rectangular square grid.

K-DOMINATING SETS ON THE LINEAR BENZENOID

Let B(h) be a linear benzenoid chain with h hexagons represented by the following figure:

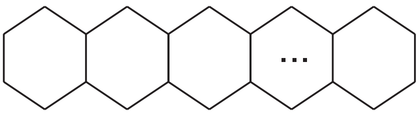

Figure 1. Linear benzenoid chain.

Since the domination number of graphs is equal for isomorphic graphs, we shall represent B(h) with the following figure and introduce the following coordinates:

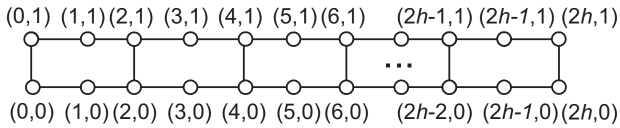

Figure 2. Coordinate system.

Denote by a γ_k the k-domination number of B(h).

$$\textit{Theorem.} - \gamma_k(h) = \begin{cases} \left\lceil \frac{h+1}{k} \right\rceil, & k \neq 2 \\ \left\lceil \frac{h+2}{k} \right\rceil, & k = 2 \end{cases}$$

Proof: First, assume that $k = 1$. Note that the set $P_h = \left\{ \left(2x, \frac{1+(-1)^{x+1}}{2} \right) : x = 0, \ldots, h \right\}$ is a 1-dominating set of B(h). Hence, $\gamma_1(h) \leq h + 1$. On the other hand, each vertex in B(h) can 1-dominate at most 4 vertices. Hence, $\gamma_1(\mathrm{h}) \geq \left\lceil \frac{4h+2}{4} \right\rceil = h + 1$. Hence, indeed $\gamma_1(h) = h + 1$.

Now, assume that $k = 2$. If $h = 1,2$, the claim is obvious. Hence, suppose that $h \geq 3$. Note that set (1) is a 2-dominating set of B(h) and it has $\left\lceil \frac{h+2}{2} \right\rceil$ elements. It remains to prove that $\gamma_2(\mathrm{h}) \geq \left\lceil \frac{h+2}{2} \right\rceil$. We prove a somewhat more general claim. Let B(h) be observed as a subgraph of $G = P_\infty \times P_2$ as illustrated in Figure 3.

We prove that there is no subset S of G with less than $\left\lceil \frac{h+2}{2} \right\rceil$ elements, such that it dominates B(h). The claim is proved by induction on h. If $h = 1,2$, the claim is trivial. Suppose that $h \geq 3$. Suppose that there are two vertices of S in the left-most hexagon. They cannot 2-dominate any vertices form the fourth hexagon on. Hence, the smallest 2-dominating set (by an inductive hypothesis) has $2 + \left\lceil \frac{(h-3)+2}{2} \right\rceil \geq \left\lceil \frac{h+2}{2} \right\rceil$ elements. On the other

$$Q_h = \begin{cases} \left\{ \left(4x, \frac{1+(-1)^{x+1}}{2} \right) : x = 0, \ldots h/2 \right\}, & h \text{ is even} \\ \left\{ \left(4x, \frac{1+(-1)^{x+1}}{2} \right) : x = 0, \ldots \lfloor h/2 \rfloor \right\} \cup \left\{ \left(2h, \frac{1+(-1)^{\lfloor h/2 \rfloor}}{2} \right) \right\}, & h \text{ is odd} \end{cases} \qquad (1)$$

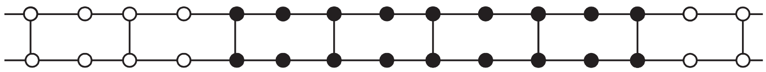

Figure 3. Infinite benzenoid chain.

hand, suppose that S has only one vertex in the first hexagon. That vertex 2-dominates both corners. Hence, it cannot 2-dominate any vertex from the third hexagon on. Hence, S has at least 1 + $\left\lceil \frac{(h-2)+2}{2} \right\rceil = \left\lceil \frac{h+2}{2} \right\rceil$ elements. This proves the claim.

It remains to assume that $k \geq 3$. Note:

$$S_z = \left\{ \left(2kx - k - 1, \frac{1+(-1)^{x+1}}{2} \right) : x = 1,\dots,z \right\}.$$

$$S_{z,h} = \begin{cases} S_z, & 2kz-k-1 \leq h \\ S_z \setminus \left\{ \left(2kz-k-1, \frac{1+(-1)^{z+1}}{2} \right) \right\} \cup \left\{ \left(h+1, \frac{1+(-1)^{z+1}}{2} \right) \right\}, & 2kz-k-1 > h \end{cases}$$

Set $S_{z,h}$ is a k-dominating set of B(h) when z is the smallest number, such that $2kz - k - 1 \geq 2h - (k - 1)$, *i.e.*, when $z = \left\lceil \frac{2h+2}{2k} \right\rceil$ (then all vertices on B(h) are k-dominated and $S_{z,h}$ is a subset of vertices of B(h)).

Examples for $k = 5$ and $h = 9$; for $k = 3$ and $h = 9$; for $k = 4$ and $h = 9$ are given below:

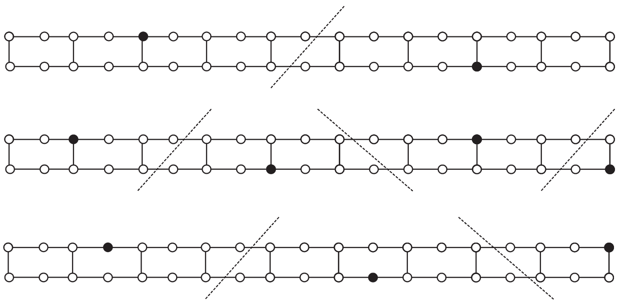

Figure 4. Examples for: $k = 5$ and $h = 9$; for $k = 3$ and $h = 9$; for $k = 4$ and $h = 9$.

Thus, we have constructed a k-dominating set with $\left\lceil \frac{2h+2}{2k} \right\rceil = \left\lceil \frac{h+1}{k} \right\rceil$ elements. Now, let us prove that there is no smaller k-dominating set. Suppose in contrast that S is a smaller domination set. Note that each vertex can k-dominate at most $4k$ vertices. Also note that the vertex that k-dominates one of the corner elements can k-dominate only $4k - 1$ elements. We have $(|S| - 1) \cdot 4k + 1 \cdot (4k - 1) \geq 4h + 2$, *i.e.*, $|S| \geq \left\lceil \frac{4h+3}{4k} \right\rceil = \left\lceil \frac{h+\frac{3}{4}}{k} \right\rceil$. Since $h + \frac{3}{4}$ and $h + 1$ are between the same two integers (both larger than a smaller value), values of $\left\lceil \frac{h+1}{k} \right\rceil$ and $\left\lceil \frac{h+\frac{3}{4}}{k} \right\rceil$ are equal.

PERFECT *K*-DOMINATING SET ON THE INFINITE HEXAGONAL GRID

Let us observe the subsets of an infinite hexagonal grid. We shall see that perfect k-domination does not appear very often. More precisely:

Theorem 1. – There is a set S that perfectly k-dominates the hexagonal grid if and only if $k = 1$.

Proof: It can be easily seen that the set S represented in the figure below by black squares and circles perfectly 1-dominates the hexagonal grid:

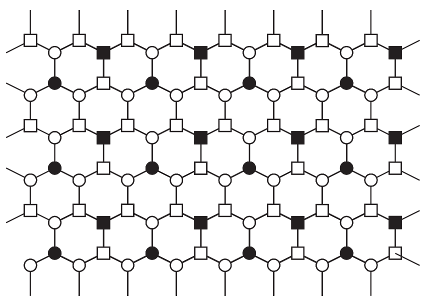

Figure 5. 1-Domination of the hexagonal grid.

Let us introduce a coordinate system as in the following figure:

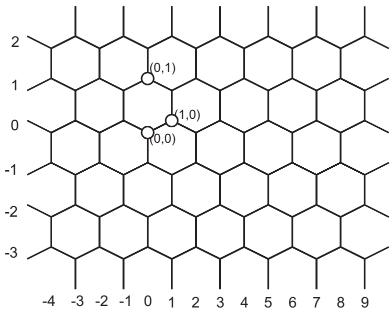

Figure 6. Coordinate system on the hexagonal grid.

Now, let us prove that there is no perfect k-domination for $k \geq 2$. Suppose in contrast that the set S which perfectly k-dominates the hexagonal grid exists. Without loss of generality, we may assume that $s_0 \in$ S, where:

$$s_0 = (0,0), \text{ if } k \bmod 4 = 0, \text{ or } 2$$
$$s_0 = (0,-1), \text{ if } k \bmod 4 = 1, \text{ or } 3.$$

One can easily see that:

$$(-\lfloor k/2 \rfloor, \lfloor k/2 \rfloor)...(-\lfloor k/2 \rfloor+2, \lfloor k/2 \rfloor),...,$$
$$(\lfloor k/2 \rfloor-2, \lfloor k/2 \rfloor),(\lfloor k/2 \rfloor, \lfloor k/2 \rfloor) \in \mathrm{D}_k(s_0),$$

$$(-\lfloor k/2 \rfloor+1, \lfloor k/2 \rfloor),(-\lfloor k/2 \rfloor+3, \lfloor k/2 \rfloor),...,$$
$$(\lfloor k/2 \rfloor-3, \lfloor k/2 \rfloor),(\lfloor k/2 \rfloor-1, \lfloor k/2 \rfloor) \notin \mathrm{D}_k(s_0).$$

It can be easily seen that:

Claim A. – Vertex $s' \in$ S that k-dominates $(i, \lfloor k/2 \rfloor)$, $i \in \{-\lfloor k/2 \rfloor + 1, -\lfloor k/2 \rfloor + 3, ..., \lfloor k/2 \rfloor - 3, \lfloor k/2 \rfloor - 1\}$ has a y – coordinate equal to k.

Proof: Just note that s' does not dominate $(i-1, \lfloor k/2 \rfloor)$ and $(i+1, \lfloor k/2 \rfloor)$. (And this is then perfect k-domination.) ■

Moreover, it can be seen that vertex s' from the last claim is an element of the set $\{(i - \lfloor k/2 \rfloor, k), (i - \lfloor k/2 \rfloor + 2, k), ..., (i + \lfloor k/2 \rfloor, k)\}$.

(Because the distance between such vertex s' and vertices

$$(-\lfloor k/2 \rfloor+1, \lfloor k/2 \rfloor),(-\lfloor k/2 \rfloor+3, \lfloor k/2 \rfloor),...,$$
$$(\lfloor k/2 \rfloor-3, \lfloor k/2 \rfloor),(\lfloor k/2 \rfloor-1, \lfloor k/2 \rfloor) \notin \mathrm{D}_k(s_0)$$

is $\leq k$, and such s' is not k-dominated by s_0 and k-dominates at most other undominated vertices.)

Claim B. – Vertices

$$(-\lfloor k/2 \rfloor+1, \lfloor k/2 \rfloor),(-\lfloor k/2 \rfloor+3, \lfloor k/2 \rfloor),...,$$
$$(\lfloor k/2 \rfloor-3, \lfloor k/2 \rfloor),(\lfloor k/2 \rfloor-1, \lfloor k/2 \rfloor)$$

are k-dominated by the same vertex s.

Proof: Suppose the contrary. Let s_1 and s_2 be two domination vertices that k-dominate the above vertices. From the discussion above, follows set (2):

but then both of these vertices dominate $(0, k)$, which is a contradiction. ■

It can be easily seen that the best »covering« is if $s \in \{(-1, k), (1, k)\}$. Because of the symmetry, we may assume that $s = (-1, k)$. For $k = 4, 5, 6$, we have the situations represented in the following figures:

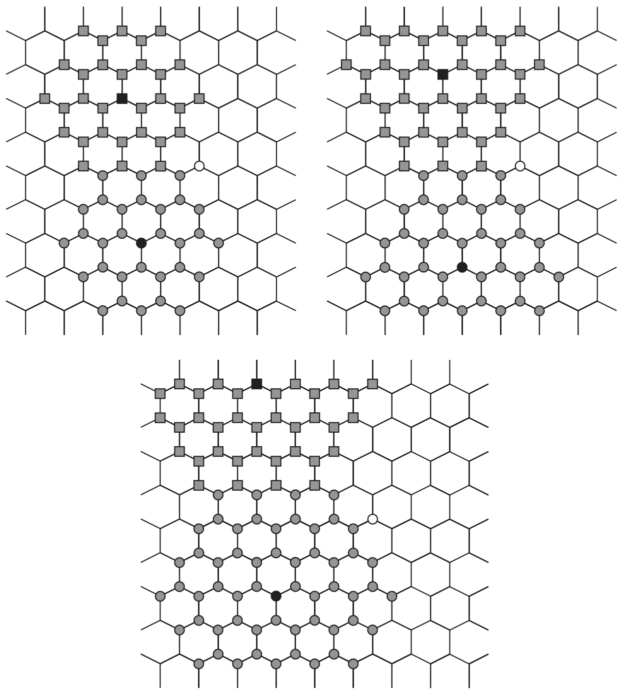

Figure 7. Hexagonal grids and dominated vertices for k = 4, 5, 6.

In Figure 7, vertex (0, 0) is denoted by a black circle; vertices dominated by it by gray circles; vertex s by a gray square; vertices dominated by it by gray squares; and vertex $(\lfloor k/2 \rfloor + 1, \lfloor k/2 \rfloor)$ by a white circle.

The only vertex that can k-dominate $(\lfloor k/2 \rfloor + 1, \lfloor k/2 \rfloor)$, without k-dominating any vertex already k-dominated by (0,0) and s, is $s' = (k + \lfloor k/2 \rfloor + 1, \lfloor k/2 \rfloor)$. For $k = 4, 5, 6$, we have the situations represented in the Figure 8. Vertex s' is represented by a black rhomb; vertices k-dominated by it by gray rhombs; and vertex $(\lfloor k/2 \rfloor + 1, \lfloor k/2 \rfloor + 1)$ by a white square.

Note that vertex $(\lfloor k/2 \rfloor, \lfloor k/2 \rfloor + 1)$ is k-dominated by s and that vertices $(\lfloor k/2 \rfloor + 2, \lfloor k/2 \rfloor + 1)$ and $(\lfloor k/2 \rfloor + 1, \lfloor k/2 \rfloor)$ are k-dominated by s'. Note that no

$$s_1, s_2 \in \left\{ \begin{array}{l} ((-\lfloor k/2 \rfloor+1)-\lfloor k/2 \rfloor, k),((-\lfloor k/2 \rfloor+1)-\lfloor k/2 \rfloor+2, k),...,((-\lfloor k/2 \rfloor+1)+\lfloor k/2 \rfloor, k), \\ ...,((\lfloor k/2 \rfloor-1)-\lfloor k/2 \rfloor, k),...,(\lfloor k/2 \rfloor-1)+\lfloor k/2 \rfloor, k) \end{array} \right\} = \quad (2)$$

$$= \{(-2 \cdot \lfloor k/2 \rfloor+1, k),(-2 \cdot \lfloor k/2 \rfloor+2, k),...,(2 \cdot \lfloor k/2 \rfloor-1, k)\},$$

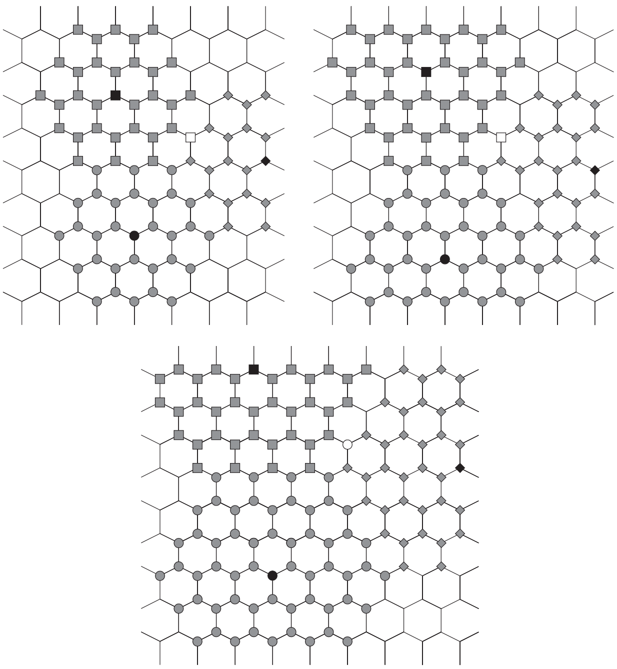

Figure 8. Hexagonal grids and dominated vertices for $k = 4,5,6$.

vertex can k-dominate $(\lfloor k/2 \rfloor + 1, \lfloor k/2 \rfloor + 1)$ without dominating at least one of its neighbors. Since vertex $(\lfloor k/2 \rfloor + 1, \lfloor k/2 \rfloor + 1)$ is not k-dominated by either s or s' , it is not k-dominated at all. This is a contradiction. ■

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SAŽETAK

K-dominacijski skupovi na linearnim benzenoidima i beskonačnoj heksagonalnoj mreži

Damir Vukičević i Antoaneta Klobučar

U ovom se radu iznose rezultati koji se odnose na k-dominacijske brojeve na linearnim lančastim benzenoidima i perfektne k-dominacijske skupove na beskonačnoj heksagonalnoj mreži.