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Research article

k-domination and total k-domination numbers in catacondensed hexagonal systems

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Abstract: In this paper we study the k-domination and total k-domination numbers of catacondensed hexagonal systems. More precisely, we give the value of the total domination number, we find upper and lower bounds for the 2-domination number and the total 2-domination number, characterizing the catacondensed hexagonal systems which attain these bounds, and we give the value of the 3-domination number for any catacondensed hexagonal system with a given number of hexagons. These results complete the study of k-domination and total k-domination of catacondensed hexagonal systems for all possible values of k.

Keywords: domination; k-domination; hexagonal systems; catacondensed hexagonal systems

1. Introduction

Let $G = (V, E)$ be a simple graph. For a positive integer k, a set $S \subseteq V$ is a *k-dominating set* of G if every vertex in $V \setminus S$ is adjacent to at least k vertices of S. The minimum cardinality among all k-dominating sets is called the *k-domination number*, and it is denoted as $\gamma_k(G)$. This invariant was introduced by Fing and Jacobson [1], and has been studied by many researchers [2–9]. A set $S \subseteq V$ is a *total k-dominating set* of G if every vertex in V is adjacent to at least k vertices of S. The *total k-domination number* is the minimum cardinality among all total k-dominating sets, denoted as $\gamma_{kt}(G)$. We refer to [10–13] for more details on this definition. When $k = 1$ in the previous definitions, we recover the extensively studied *domination number* $\gamma(G)$ and *total domination number* $\gamma_t(G)$ of G [14, 15]. For recent results in domination number of graphs we refer to [16–19].

Molecular structures are represented by (molecular) graphs, where the atoms correspond to the vertices and the chemical bonds correspond to the edges. Perhaps one of the most important molecular graphs are the hexagonal systems, graph representation of benzenoid hydrocarbons which have innumerable applications in chemistry [20]. In QSAR and QSPR studies, a topological index (or molecular descriptor) is a numerical parameter associated to the molecular graph, which correlates well with many physical and chemical properties of the molecules [21–24]. One such descriptor is the domination number. The connection between the domination number and the RNA structure given in [25], motivated many researchers to use domination based parameters to study chemical graphs [26–32].

In recent years there has been much interest in the study of the domination number and the total domination number of hexagonal systems [26, 27, 30, 31, 33–37]. In this paper we go one step further and study the 2-domination and the total 2-domination of a significant class of hexagonal systems, the so-called catacondensed hexagonal systems. Specifically, we find upper and lower bounds for γ_2 and γ_{2t} over the set of catacondensed hexagonal systems, and characterize those which attain the bounds. Also, we give the value of the total domination number and the 3-domination number for any catacondensed hexagonal system with a given number of hexagons.

Recall that a *hexagonal system* is a finite connected plane graph without cut vertices, in which all interior regions are mutually congruent regular hexagons. A hexagonal system is said to be *simple* if it can be embedded into the regular hexagonal lattice in the plane without overlapping of its vertices. Hexagonal systems that are not simple are called *jammed*. They are of great importance for theoretical chemistry because they are natural graph representations of benzenoid hydrocarbons. We refer to [20] for more details on the hexagonal systems. A *hexagonal chain* (abbreviated as HC) is a hexagonal system with the properties that (a) it has no vertex belonging to three hexagons, and (b) it has no hexagon with more than two adjacent hexagons (Figure 1, both figures on the left). A *catacondensed*

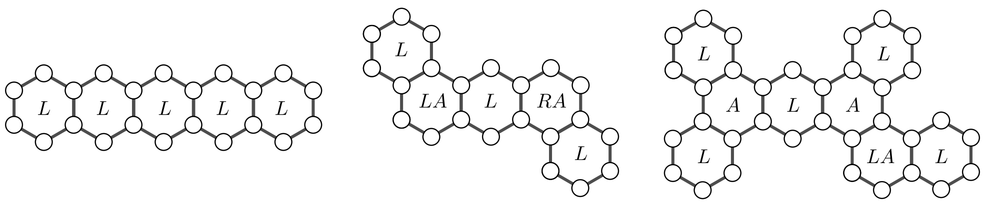

Figure 1. A linear HC, a general HC and a CHS.

hexagonal system (abbreviated as CHS) is a hexagonal system which has no vertex belonging to three hexagons (Figure 1, the figure on the right). It is clear that a hexagonal chain is a particular case of a catacondensed hexagonal system. We will say that a hexagon in a CHS is a *linear* hexagon L if it has exactly two non-adjacent vertices with degree 2. We will say that a hexagon is an *angular* hexagon (LA or RA, see Figure 1) if it has exactly two adjacent vertices with degree 2. A hexagon in a CHS is a *leaf* if it is adjacent to only one hexagon, and a hexagon in a CHS is a *branching* hexagon A if it is adjacent to three hexagons. An *inner branch* in a CHS is a consecutive sequence $A_1 - T_1 - T_2 - \cdots - T_k - A_2$ of adjacent hexagons such that A_1 and A_2 are the only branching hexagons in that sequence. Two consecutive branching hexagons is also considered an inner branch. An *outer branch* in a CHS is a consecutive sequence $T - T_1 - T_2 - \cdots - T_k - A$ of adjacent hexagons such that T is a leaf and A is the only branching hexagon in that sequence. We denote by $\mathcal{HC}$ or $\mathcal{CHS}$ the set of all hexagonal chains or catacondensed hexagonal systems, respectively. If we want to indicate the number of hexagons h or the number of branching hexagons a_3, we will write $\mathcal{CHS}(h)$ or $\mathcal{CHS}(h, a_3)$.

In this work we study the k-domination and total k-domination numbers of catacondensed hexagonal systems. Since the maximum degree of a CHS is 3, and taking into account that the domination number was studied in two previous works [26,27], we focus here on the remaining cases; the total domination number, the 2-domination number, the total 2-domination number and the 3-domination number of a catacondensed hexagonal system.

We show here some operations we will continuously use to get the results. Given $H \in \mathcal{CHS}$ and a set of vertices $S \subseteq V(H)$, we denote by $H - S$ the subgraph of H obtained by removing the vertices in S and all the edges incident to those vertices. Given a hexagonal leaf T of H whose vertices are $\{v_i\}_{i=1}^6$, such that $\deg(v_1) = \deg(v_6) = 3$, we define $H \ominus T = H - \{v_i\}_{i=2}^4$ (see Figure 2).

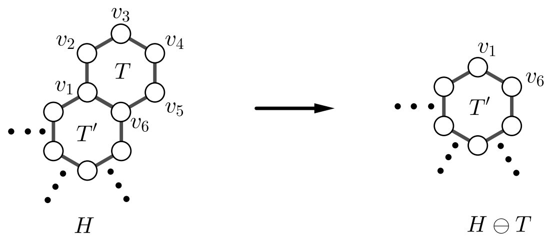

Figure 2. The graph $H \ominus T$.

On the other hand, if T_i is a hexagon in H adjacent to exactly two hexagons T_{i-1} and T_{i+1}, and we denote $V(T_i) = \{v_j^i\}_{j=1}^6$, then we define $H \ominus T_i$ in the following way:

(1) If $v_3^i, v_4^i \in V(T_{i-1})$ and $v_1^i, v_6^i \in V(T_{i+1})$ (see Figure 3 on the left), then $v_3^i = v_1^{i-1}$ and $v_4^i = v_6^{i-1}$, and we denote by $H \ominus T_i$ the catacondensed hexagonal system such that $V(H \ominus T_i) = V(H - \{v_j^i\}_{j=2}^5)$ and $E(H \ominus T_i) = E(H - \{v_j^i\}_{j=2}^5) \cup \{v_5^{i-1}v_6^i, v_2^{i-1}v_1^i\}$ (see Figure 3 on the right).

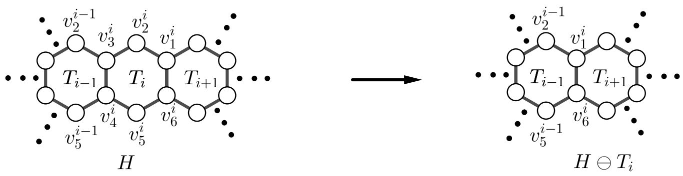

Figure 3. The graph $H \ominus T_i$.

(2) If $v_4^i, v_5^i \in V(T_{i-1})$ and $v_1^i, v_6^i \in V(T_{i+1})$ (see Figure 4 on the left), then $v_4^i = v_1^{i-1}$ and $v_5^i = v_6^{i-1}$, and we denote by $H \ominus T_i$ the catacondensed hexagonal system such that $V(H \ominus T_i) = V(H - \{v_j^i\}_{j=2}^5)$ and $E(H \ominus T_i) = E(H - \{v_j^i\}_{j=2}^5) \cup \{v_5^{i-1}v_6^i, v_2^{i-1}v_1^i\}$ (see Figure 4 on the right).

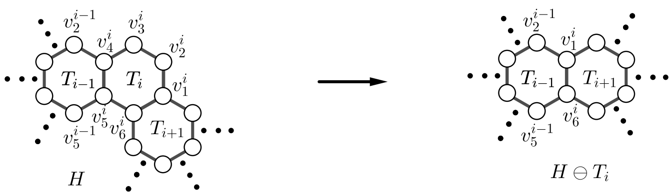

Figure 4. The graph $H \ominus T_i$.

(3) If $v_2^i, v_3^i \in V(T_{i-1})$ and $v_1^i, v_6^i \in V(T_{i+1})$ (see Figure 5 on the left), then $v_2^i = v_1^{i-1}$ and $v_3^i = v_6^{i-1}$, and we denote by $H \ominus T_i$ the catacondensed hexagonal system such that $V(H \ominus T_i) = V(H - \{v_j^i\}_{j=2}^5)$ and $E(H \ominus T_i) = E(H - \{v_j^i\}_{j=2}^5) \cup \{v_5^{i-1}v_6^i, v_2^{i-1}v_1^i\}$ (see Figure 5 on the right).

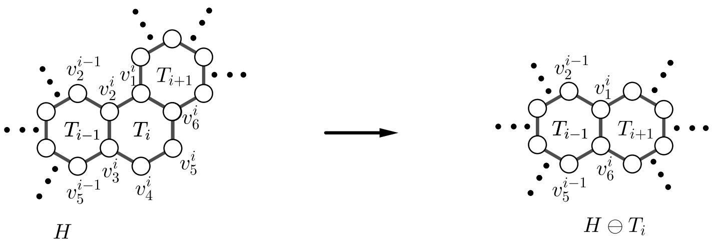

Figure 5. The graph $H \ominus T_i$.

2. Total domination number in catacondensed hexagonal systems

In this section we give the value of the total domination number for any catacondensed hexagonal systems with a given number of hexagons. For that, we will use the following well known result for cycles with n vertices.

Proposition 2.1. *For any cycle C_n with n vertices*

$$\gamma_t(C_n) = \begin{cases} \frac{n}{2} + 1 & \text{if} \quad n \equiv 2 \ (mod\ 4) \\ \left\lceil \frac{n}{2} \right\rceil & \text{otherwise.} \end{cases}.$$

Theorem 2.2. *If $H \in \mathcal{CHS}(h)$, then $\gamma_t(H) = 2(h+1)$.*

Proof. We prove the result by induction on the number of hexagons h. The result can be easily checked when $h = 1$, so we suppose that $\gamma_t(H') = 2h$ for any $H' \in \mathcal{CHS}(h-1)$ and we take $H \in \mathcal{CHS}(h)$. Since every catacondensed hexagonal system has a Hamiltonian cycle, by Proposition 2.1 we have that $\gamma_t(H) \le \gamma_t(C_{4h+2}) = 2(h+1)$. Now, we take a minimum total dominating set D of H and we consider a hexagonal leaf T in H, whose vertices are named as in Figure 6. If we suppose that $v_3 \notin D$, then

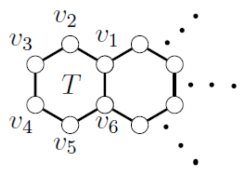

Figure 6. A leaf T of H.

$v_1, v_5 \in D$ and we can study two cases. If $v_2 \notin D$, then $v_4 \in D$ and $D' = D \setminus \{v_4, v_5\}$ is a total dominating set in $H' = H \ominus T$. Therefore, $\gamma_t(H') = 2h \le |D'| = |D| - 2 = \gamma_t(H) - 2$, that is, $\gamma_t(H) \ge 2(h+1)$. If $v_2 \in D$, since v_5 must be dominated, we have that $|\{v_4, v_6\} \cap D| = 1$, then $D' = (D \setminus \{v_2, v_4, v_5, v_6\}) \cup \{v_6\}$ is a total dominating set in H' with cardinality $|D| - 2$. Therefore, $\gamma_t(H') = 2h \le |D'| = |D| - 2 = \gamma_t(H) - 2$, that is, $\gamma_t(H) \ge 2(h+1)$. Finally, we suppose that $v_3 \in D$ and, by symmetry, that $v_4 \in D$. Moreover, we can assume that $v_2, v_5 \notin D$, then $D' = D \setminus \{v_3, v_4\}$ is a dominating set in H' and we get the result.

3. 2-domination number in catacondensed hexagonal systems

In this section we present a lower and an upper bound for the 2-domination number of any catacondensed hexagonal system with a given number of hexagons. As we did in Section 2, since any catacondensed hexagonal system has a Hamiltonian cycle, we get the following upper bound.

Proposition 3.1. *If $H \in \mathcal{CHS}(h)$, then $\gamma_2(H) \leq 2h + 1$.*

Proof. It is well known that $\gamma_2(C_n) = \left\lceil \frac{n}{2} \right\rceil$ for a cycle C_n with n vertices, then, since H has a Hamiltonian cycle with $4h + 2$ vertices, we have that

$$\gamma_2(H) \leq \gamma_2(C_{4h+2}) = 2h + 1.$$

Next, we will give a characterization for all catacondensed hexagonal systems attaining that upper bound. More precisely, we will prove that a catacondensed hexagonal system attains that upper bound if and only if the number of angular hexagons in all its inner branches is an odd number. For that, we will need the following lemmas.

Lemma 3.2. *If H is a CHS, then there exists a minimum 2-dominating set such that it does not contain two adjacent vertices with degree 2.*

Proof. The result is trivial if H has only one hexagon. Let D be a minimum 2-dominating set of H and let $u_1, u_2 \in D$ be two adjacent vertices such that $\deg(u_1) = 2 = \deg(u_2)$. We name by u_3, u_4, u_5, u_6 the remaining consecutive vertices in the same hexagon, where u_1 is adjacent to u_6 and u_2 is adjacent to u_3, so we know that $u_3, u_6 \notin D$. If u_6 (or u_3) has degree 3, then $D' = (D \setminus \{u_1\}) \cup \{u_6\}$ (or $D' = (D \setminus \{u_2\}) \cup \{u_3\}$) is also a 2-dominating set. If $\deg(u_3) = \deg(u_6) = 2$, since $u_6 \notin D$ and $deg(u_5) = 3$, the set $D' = (D \setminus \{u_1\}) \cup \{u_6\}$ is also a 2-dominating set.

Lemma 3.3. *If H is a CHS and T is a leaf in H with consecutive vertices $\{v_1, v_2, \dots, v_6\}$, then there exists a minimum 2-dominating set D such that $\{v_i\}_{i=1}^6 \cap D = \{v_1, v_3, v_5\}$ or $\{v_i\}_{i=1}^6 \cap D = \{v_2, v_4, v_6\}$.*

Proof. If $\deg(v_1) = 3 = \deg(v_6)$ and D is a minimum 2-dominating set of H given by Lemma 3.2, then $\{v_1, v_3, v_5\} \subseteq D$ or $\{v_2, v_4, v_6\} \subseteq D$. If we suppose, for instance, that $\{v_1, v_3, v_5\} \subseteq D$ and $v_6 \in D$, if $w \in N(v_6) \setminus \{v_1, v_5\}$, we have that $D' = (D \setminus \{v_6\}) \cup \{w\}$ is a minimum 2-dominating set.

For any catacondensed hexagonal system H we will denote by $\mathcal{D}_2(H)$ the set of minimum 2-dominating sets in H satisfying Lemmas 3.2 and 3.3.

Lemma 3.4. *Let H be a CHS with a leaf T non adjacent to a branching hexagon, then*

$$\gamma_2(H) = \gamma_2(H \ominus T) + 2.$$

Proof. We suppose that T_1 is the adjacent hexagon to T, and that $v_1, v_2 \dots, v_6$ and $v_1, u_2, u_3, u_4, u_5, v_6$ are the consecutive vertices of T and T_1, respectively. If $D_1 \in \mathcal{D}_2(H \ominus T)$, then $v_1 \in D_1$ or $v_6 \in D_1$. For instance, if $v_1 \in D_1$, then $D_1 \cup \{v_3, v_5\}$ is a 2-dominating set in H, therefore, $\gamma_2(H) \leq \gamma_2(H \ominus T) + 2$. If $D \in \mathcal{D}_2(H)$ and, for instance, $v_1, v_3, v_5 \in D$, we can have the three situations showed in Figure 7. In cases (a) and (b) we have that $u_5 \in D$, then $D_1 = D \setminus \{v_3, v_5\}$ is a 2-dominating set in $H \ominus T$,

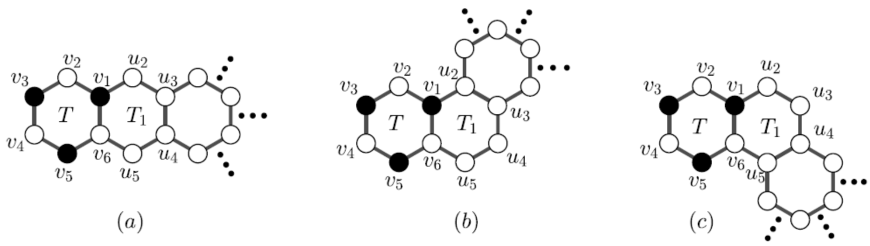

Figure 7. Three possibilities for T_1.

that is, $\gamma_2(H \ominus T) \leq \gamma_2(H) - 2$. The same happens in case (c) if $u_5 \in D$. Thus, we suppose case (c) such that $u_5 \notin D$. In such a case, $u_4 \in D$ and there exists w such that $w \in \{u_2, u_3\} \cap D$. If we take $D_1 = (D \setminus \{v_1, v_3, v_5, w\}) \cup \{u_2, v_6\}$, we obtain a 2-dominating set in $H \ominus T$ and, consequently, $\gamma_2(H \ominus T) \leq \gamma_2(H) - 2$.

In Figure 8 we can see that Lemma 3.4 is not true if T is adjacent to a branching hexagon.

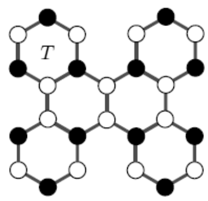

Figure 8. $\gamma_2(H) = 12$ and $\gamma_2(H \ominus T) = 11$.

Lemma 3.5. *Let H be a CHS and let $T_1 - T_2 - T_3$ be three consecutive hexagons in H such that T_2 is a linear hexagon and T_1 and T_3 are not branching hexagons. Then,*

$$\gamma_2(H) = \gamma_2(H \ominus T_2) + 2.$$

Proof. We name the vertices in T_1, T_2 and T_3 as shown in Figure 9. If D is a minimum 2-dominating

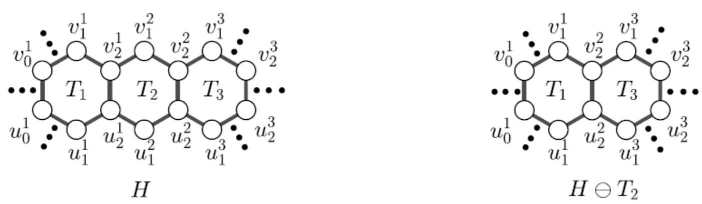

Figure 9. Vertices in T_1, T_2 and T_3.

set in H, the possibilities for vertices in $V(T_2) \cap D$ could be supposed to be, by symmetry, the ones shown in black in Figure 10.

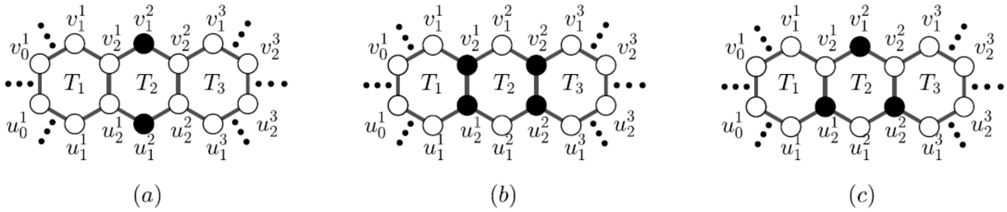

Figure 10. Vertices in T_1, T_2 and T_3.

In cases (a) and (b), $D \setminus \{u_1^2, v_1^2\}$ and $D \setminus \{u_2^1, v_2^1\}$ are 2-dominating sets in $H \ominus T_2$, respectively. In case (c), if $D \setminus \{u_2^1, v_1^2\}$ is not a 2-dominating set in $H \ominus T_2$, then $v_1^1, v_1^3 \notin D$. Since T_1 and T_3 are not branching hexagons, we have the situation showed in Figure 11, where $\{u_0^1, u_1^1\} \cap D \neq \emptyset$ and $\{u_1^3, u_2^3\} \cap D \neq \emptyset$. Without loss of generality, we can assume that $u_1^1, u_1^3 \in D$. In such a case, $D' = (D \setminus \{u_2^1, u_2^2, v_1^2\}) \cup \{v_2^2\}$ is a 2-dominating set in $H \ominus T_2$.

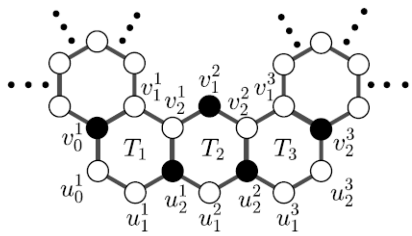

Figure 11. Vertices in T_1, T_2 and T_3.

Finally, if D' is a minimum 2-dominating set in $H \ominus T_2$ we have three different cases. If $D' \cap \{v_2^2, u_2^2\} = \{v_2^2, u_2^2\}$, then $D = D' \cup \{v_2^1, u_2^1\}$ is a 2-dominating set in H. If $D' \cap \{v_2^2, u_2^2\} = \{u_2^2\}$, then $D = D' \cup \{v_1^2, u_2^1\}$ is a 2-dominating set in H. If $D' \cap \{v_2^2, u_2^2\} = \emptyset$, then $D = D' \cup \{v_1^2, u_1^2\}$ is a 2-dominating set in H. Therefore, $\gamma_2(H) \leq \gamma_2(H \ominus T_2) + 2$.

Lemma 3.6. *Let H be a CHS and let A be a branching hexagon in H. If T is a linear hexagon adjacent to A and there exists a minimum 2-dominating set D such that $D \cap V(T) \cap V(A) = \emptyset$, then*

$$\gamma_2(H) = \gamma_2(H \ominus T) + 2.$$

Proof. If we name the vertices as in the Figure 12, then $v_1, v_3, u_1, u_3 \in D$, so $D \setminus \{v_3, u_3\}$ is a 2-dominating set in $H \ominus T$. To prove that $\gamma_2(H) \leq \gamma_2(H \ominus T) + 2$ we can do the same we did in the last part of the proof of Lemma 3.5 with vertices v_4, u_4 instead of v_2^2, u_2^2.

Notice that any branching hexagon adjacent to two leaves and to a linear hexagon, satisfies the condition needed in Lemma 3.6.

Lemma 3.7. *Let H be a CHS and let A be a branching hexagon in H adjacent to two leaf hexagons T and T'. If $D \in \mathcal{D}_2(H)$ satisfies $|D \cap V(A)| \geq 3$, then*

$$\gamma_2(H) = \gamma_2(H \ominus T) + 2.$$

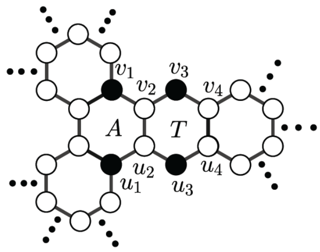

Figure 12. Black vertices must belong to D.

Proof. If D' is a minimum 2-dominating set in $H \ominus T$, it is clear that it contains a vertex in $V(A) \cap V(T)$, so $\gamma_2(H) \leq \gamma_2(H \ominus T) + 2$. If $D \in \mathcal{D}_2(H)$ satisfies $|D \cap V(A)| \geq 3$, by Lemma 3.3, without loss of generality, and moving the vertices in D if it were necessary, we can assume that D contains the black vertices shown in Figure 13. Then, $\gamma_2(H \ominus T) \leq \gamma_2(H) - 2$.

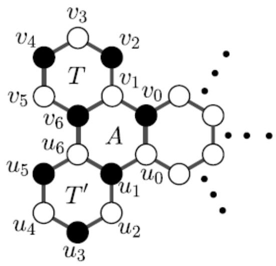

Figure 13. Black vertices belong to D.

Proposition 3.8. *If $H \in \mathcal{CHS}(h, 0)$ or $H \in \mathcal{CHS}(h, 1)$, then $\gamma_2(H) = 2h + 1$.*

Proof. If $H \in \mathcal{CHS}(h, 0)$, we can apply Lemma 3.4 recursively to get the result. For $H \in \mathcal{CHS}(4, 1)$, it can be checked that $\gamma_2(H) = 9$, and, if $H \in \mathcal{CHS}(h, 1)$ with $h \geq 5$ we can apply Lemma 3.4 to any leaf non adjacent to a branching hexagon.

In Figure 8 was shown that this result might not be true for $H \in \mathcal{CHS}(h, a_3)$ with $a_3 \geq 2$, in other words, when H has inner branches.

Theorem 3.9. *For any $H \in \mathcal{CHS}(h)$, $\gamma_2(H) = 2h + 1$ if and only if every inner branch in H has an odd number of angular hexagons.*

Proof. By absurdum, we suppose that there exists $H \in \mathcal{CHS}(h, a_3)$ such that all its inner branches have an odd number of angular hexagons and $\gamma_2(H) \leq 2h$. We take that catacondensed hexagonal system H with the minimum number of hexagons and, if there is more than one, the one with the minimum number of branching hexagons. As a consequence, $a_3 \geq 2$, H does not have two adjacent branching hexagons and H does not satisfy the conditions given in Lemmas 3.4–3.7. If T and T' are two leaves adjacent to a branching hexagon A and T_1 is the other hexagon adjacent to A, we know that, for any $D \in \mathcal{D}_2(H)$ we have $|V(A) \cap D| = 2$, $V(A) \cap V(T_1) \cap D = \emptyset$ and T_1 is not a linear hexagon. Without loss of generality, we can assume that T_1 is a *RA* hexagon. We consider the inner branch

$A - T_1 - T_2 - \cdots - T_k - A'$ in H. If $k \geq 3$, by Lemma 3.5, $T_1, T_2, \ldots, T_{k-1}$ are angular hexagons. For instance, we suppose that T_1 and T_2 are *RA* and *LA* hexagons, respectively (the case is similar when both are *RA* hexagons), as shown in Figure 14 on the left. By Lemmas 3.3 and 3.7 we know that there

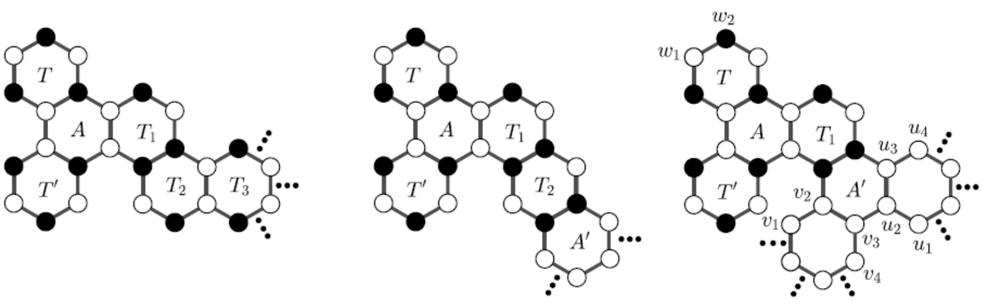

Figure 14. Black vertices belong to D.

exists $D \in \mathcal{D}_2(H)$ which contains the black vertices shown in that figure. Therefore, every branch in $H' = (H \ominus T_1) \ominus T_2$ has an odd number of angular hexagons, $D \setminus (V(T_1) \cup V(T_2))$ is a 2-dominating set in H' and $\gamma_2(H') \leq \gamma_2(H) - 4 \leq 2(h-2)$, a contradiction. If $k = 2$, then we have the situation shown in the center of Figure 14, and we get the same contradiction with $H' = H \ominus T_2$. If $k = 1$, then we have the situation shown in Figure 14 on the right. If v_2 or u_3 belongs to D, we can move some vertices in D to get $D' \in \mathcal{D}_2(H)$ satisfying the condition given in Lemma 3.7. Then, $v_2, u_3 \notin D$ and $v_3 \in D$ or $u_2 \in D$. If $v_3 \in D$, then we consider $H' \in \mathcal{CHS}(h, a_3 - 1)$ such that $V(H') = V(H)$ and $E(H') = (E(H) \setminus \{v_1v_2, v_3v_4\}) \cup \{v_4w_2, v_1w_1\}$. It is easy to check that D is a 2-dominating set in H', then, since all the inner branches of H' have an odd number of angular hexagons, we get a contradiction with the minimality of the number of branching hexagons. If $u_2 \in D$, then we consider $H' \in \mathcal{CHS}(h, a_3 - 1)$ such that $V(H') = V(H)$ and $E(H') = (E(H) \setminus \{u_1u_2, u_3u_4\}) \cup \{u_1w_2, u_4w_1\}$ to get the same contradiction.

Now, let us see that, if $\gamma_2(H) = 2h + 1$, then every inner branch in H has an odd number of angular hexagons. By absurdum, if we suppose that H has a inner branch $A_1 - T_1 - \cdots - T_{r-2} - A_2$ with an even number of angular hexagons and we denote the vertices in the Hamiltonian cycle $v_1, v_2, \ldots, v_{4r+2}$ as shown in Figure 15, we denote by l, a_r and a_l the number of linear hexagons, right angular hexagons

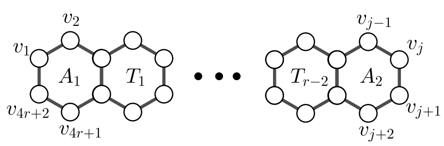

Figure 15. Inner branch with an even number of angular hexagons.

and left angular hexagons in this hexagonal chain, respectively, by P_u the path $v_1 - v_2 - \cdots - v_j$ and by P_l the path $v_{j+1} - v_{j+2} - \cdots - v_{4r+2}$, we have that

$$\begin{aligned} j &= 2l + 3a_r + a_l + 5 = 2l + 2a_r + (a_r + a_l) + 5 \\ 4r + 2 - j &= 2l + a_r + 3a_l + 5 = 2l + 2a_l + (a_r + a_l) + 5. \end{aligned}$$

Therefore, since $a_r + a_l$ is an even number, then $j = 2r_1 + 5, 4r + 2 - j = 2r_2 + 5$ and $r_1 + r_2 = 2r$. We will build a 2-dominating set D in H such that $|D| \leq 2h$. Firstly, we take the set

$$D' = \{v_2, v_4, \ldots, v_{j-3}, v_{j-1}, v_{j+2}, v_{j+4}, \ldots, v_{4r-1}, v_{4r+1}\},$$

whose cardinality is $2r$, and we start with $D = D'$. Secondly, we include vertices in D in the following way. If there is a hexagon in H, different from $A_1, A_2, T_1, \ldots, T_{r-2}$, with consecutive vertices $u_1, u_2, \ldots, u_6$ such that u_1 is already in D, we include u_3, u_5 in D. If we do this process with all the hexagons in H, we get a final set D such that it is a 2-dominating set with cardinality equal to $2h$, a contradiction.

Next, we give a lower bound for the 2-domination number using the number of hexagons and the number of branching hexagons.

Theorem 3.10. *If $H \in \mathcal{CHS}(h, a_3)$, then*

$$2h + 1 - \left\lfloor \frac{a_3}{2} \right\rfloor \leq \gamma_2(H).$$

Proof. By Proposition 3.8 we can assume that $a_3 \geq 2$. By absurdum, we suppose that there exists $H \in \mathcal{CHS}(h, a_3)$ such that $\gamma_2(H) \leq 2h - \left\lfloor \frac{a_3}{2} \right\rfloor$, and we take H, satisfying this inequality, with the minimum number of hexagons. Therefore, H and $D \in \mathcal{D}_2(H)$ cannot satisfy the conditions given in Lemmas 3.4–3.7. If A is a branching hexagon adjacent to two leaves T and T', and to another hexagon T_1, then T_1 is a branching hexagon or an angular hexagon, and, without loss of generality, we can assume that we have one of the two situations shown in Figure 16, where black vertices belong to D. If we denote $H' = H \ominus T \ominus T' \ominus A$ and $D' = D \setminus (V(T) \cup V(T') \cup V(A))$, and we consider the case when

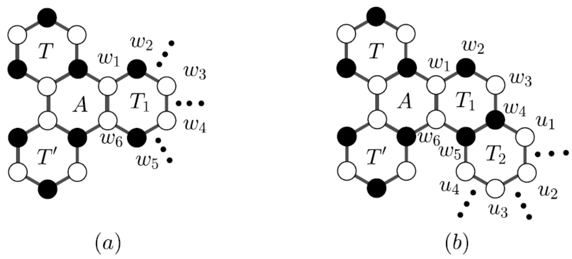

Figure 16. Two possible situations when A is a branching hexagon adjacent to two leaves.

T_1 is a branching hexagon, then $D' \cup \{w_1\}$ is a 2-dominating set in H' and

$$\gamma_2(H') \leq |D' \cup \{w_1\}| = \gamma_2(H) - 5 \leq 2h - \left\lfloor \frac{a_3}{2} \right\rfloor - 5 = 2(h-3) - \left\lfloor \frac{a_3 - 2}{2} \right\rfloor,$$

a contradiction. If T_1 is an angular hexagon and $u_1 \in D$, then $D' = (D \setminus \{w_2, w_4\}) \cup \{w_1, w_3\}$ is a minimum 2-dominating set and, by Lemma 3.7, we get a contradiction. The same happens if $u_4 \in D$. Since $u_1, u_4 \notin D$, we know that $u_2 \in D$ or $u_3 \in D$. If T_2 is a branching hexagon, we can see that $D' \setminus \{w_2\}$ is a 2-dominating set in $H' \ominus T_1$ and

$$\gamma_2(H' \ominus T_1) \leq |D' \setminus \{w_2\}| = \gamma_2(H) - 7 \leq 2h - \left\lfloor \frac{a_3}{2} \right\rfloor - 7 = 2(h-4) - \left\lfloor \frac{a_3 - 2}{2} \right\rfloor,$$

a contradiction. If T_2 is a linear hexagon, then we know that $u_2, u_3 \in D$ and, by Lemma 3.5, we can assume that T_2 is adjacent to a branching hexagon, consequently, $D' \setminus \{w_2, w_4, w_5\}$ is a 2-dominating set in $H' \ominus T_1 \ominus T_2$ and

$$\begin{aligned}\gamma_2(H' \ominus T_1 \ominus T_2) &\leq |D' \setminus \{w_2, w_4, w_5\}| = \gamma_2(H) - 9 \leq 2h - \left\lfloor \frac{a_3}{2} \right\rfloor - 9 \\ &= 2(h-5) - \left\lfloor \frac{a_3 - 2}{2} \right\rfloor,\end{aligned}$$

a contradiction.

Finally, if T_2 is also an angular hexagon, as we did in the proof of Theorem 3.9 with Figure 14 on the left, $D \setminus (V(T_1) \cup V(T_2))$ is a 2-dominating set in $H \ominus T_1 \ominus T_2$ and

$$\begin{aligned}\gamma_2(H \ominus T_1 \ominus T_2) &\leq |D \setminus (V(T_1) \cup V(T_2))| = \gamma_2(H) - 4 \leq 2h - \left\lfloor \frac{a_3}{2} \right\rfloor - 4 \\ &= 2(h-2) - \left\lfloor \frac{a_3}{2} \right\rfloor,\end{aligned}$$

a contradiction.

Proposition 3.11. *For any $h \geq 6$ and any a_3 such that $2 \leq a_3 \leq \frac{2(h-1)}{5}$, there exists $H \in \mathcal{CHS}(h, a_3)$ such that $\gamma_2(H) = 2h + 1 - \left\lfloor \frac{a_3}{2} \right\rfloor$.*

Proof. We prove the result studying different cases. *Case 1.* We suppose that a_3 is an even number and $h = \frac{5a_3}{2} + 1$. We consider $G \in \mathcal{CHS}(6, 2)$ and $H \in \mathcal{CHS}(5, 1)$ shown in Figure 17. If $a_3 = 2$, then G satisfies the equality required. If $a_3 \geq 4$, we consider four consecutive vertices v_1, v_2, v_3, v_4

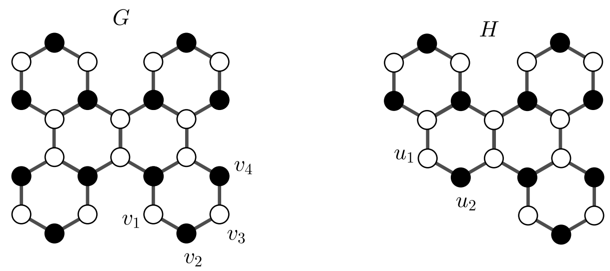

Figure 17. Two CHS used in the proof of Proposition 3.11.

with degree 2 in a leaf hexagon of G and G_1 the CHS such that $V(G_1) = (V(G) \setminus \{v_2, v_3\}) \cup V(H)$ and $E(G_1) = (E(G) \setminus \{v_1v_2, v_2v_3, v_3v_4\}) \cup E(H) \cup \{v_1u_2, v_4u_1\}$. If $a_3 = 4$, then G_1 satisfies the equality required, if not, we continue this process, it means, we take four vertices v_1, v_2, v_3, v_4 with degree 2 in a leaf hexagon of G_1 and we take another CHS like H in Figure 17, then we construct G_2 as the CHS such that $V(G_2) = (V(G_1) \setminus \{v_2, v_3\}) \cup V(H)$ and $E(G_2) = (E(G_1) \setminus \{v_1v_2, v_2v_3, v_3v_4\}) \cup E(H) \cup \{v_1u_2, v_4u_1\}$. If $a_3 = 2 + 2k$, in k steps we obtain G_k satisfying all the requirements.

Case 2. We suppose that a_3 is an even number and $h > \frac{5a_3}{2} + 1$. Then we call $h' = \frac{5a_3}{2} + 1 = h - j$ and apply Case 1 to obtain G'_k such that $\gamma_2(G'_k) = 2h' + 1 - \left\lfloor \frac{a_3}{2} \right\rfloor$. If we attach a linear chain with j hexagons to any leaf of G'_k, we obtain a new $H \in \mathcal{CHS}(h, a_3)$ satisfying the equality.

Case 3. We suppose that a_3 is an odd number. If we apply Case 1 and 2 to $a'_3 = a_3 - 1$ and any $h' \geq \frac{5a'_3}{2} + 1$, we obtain $G'_k \in \mathcal{CHS}(h', a'_3)$ such that $\gamma_2(G'_k) = 2h' + 1 - \left\lfloor \frac{a'_3}{2} \right\rfloor$. Finally, if we take any leaf

T of G'_k and we attach two new hexagons to this leaf in such a way that, in the obtained catacondensed hexagonal system H, the hexagon T is now a branching hexagon, then we need four extra vertices to 2-dominate H, therefore

$$\gamma_2(H) \leq \gamma_2(G'_k) + 4 = 2h' + 1 - \left\lfloor \frac{a'_3}{2} \right\rfloor + 4 = 2(h' + 2) + 1 - \left\lfloor \frac{a_3}{2} \right\rfloor,$$

and this can be obtain for every $h = h' + 2 \geq \frac{5a'_3}{2} + 1 + 2 = \frac{5a_3+1}{2}$, in particular, for any $h \geq \frac{5a_3}{2} + 1$.

It is easy to check that, for any $H \in \mathcal{CHS}(h, a_3)$, it is satisfied $a_3 \leq \frac{h-2}{2}$, so the inequality $2h + 1 - \left\lfloor \frac{h-2}{4} \right\rfloor \leq \gamma_2(H)$ is immediately obtained. Next, let us see that we can improve this lower bound. For that, we will need the following lemmas.

Lemma 3.12. *If $H \in \mathcal{CHS}(h, a_3)$ does not have three consecutive branching hexagons, then* $a_3 \leq \frac{2(h-1)}{5}$.

Proof. The result is trivial if $a_3 = 2$, so we suppose that $a_3 \geq 3$. Let $T_1 - T_2 - \cdots - T_k - A_1$ and $T_{k+1} - T_{k+2} - \cdots - T_{k+j} - A_1$ two outer branches in H. We build a partition of the hexagons in H in the following way:

(1) If there is an inner branch $A_1 - T_{k+j+1} - \cdots - T_{k+j+i} - A_2$, then we take $M_1 = \{T_1, T_2, \ldots, T_{k+j+i}, A_1\}$.

(2) If A_1 is adjacent to another branching hexagon A_2, then we take $A_1, A_2, T_1, T_2, \ldots, T_{k+j}$ in M_1 and, for any inner branch $A_2 - T'_1 \cdots - T'_l - A_3$ or outer branch $A_2 - T'_1 \cdots - T'_l$, we take $T'_1, \ldots, T'_l$ in M_1.

(3) For every $p \geq 2$, we take M_p in the following way. Let $T \in \bigcup_{s=1}^{p-1} M_s$ be a hexagon adjacent to a branching hexagon $A'_1 \notin \bigcup_{s=1}^{p-1} M_s$, then we distinguish two cases.

(3.a) If A'_1 is not adjacent to another branching hexagon, then we take A'_1 in M_p and, for any inner branch $A'_1 - T'_1 \cdots - T'_l - A'_2$ or outer branch $A'_1 - T'_1 \cdots - T'_l$, we take $T'_1, \ldots, T'_l$ in M_p.

(3.b) If A'_1 is adjacent to another branching hexagon A'_2, then we take A'_1 and A'_2 in M_p and, for any inner branch $A'_i - T'_1 \cdots - T'_k - A'_3$ ($T'_1 \neq T$ if $i = 1$) or outer branch $A'_i - T'_1 \cdots - T'_k$ ($i = 1, 2$), we take $T'_1, \ldots, T'_k$ in M_p.

With this partition, if we name $h(M_p)$ and $a_3(M_p)$ the number of hexagons and the number of branching hexagons in M_p, respectively, we have

$$\begin{aligned} a_3 &= a_3(M_1) + \sum_{p\geq 2} a_3(M_p) \leq \frac{2(h(M_1) - 1)}{5} + \sum_{p\geq 2} \frac{2h(M_p)}{5} \\ &= \frac{2}{5}\left(\sum_{p\geq 1} h(M_p) - 1\right) = \frac{2(h-1)}{5}. \end{aligned}$$

Lemma 3.13. *Let $H \in \mathcal{CHS}$ and let D be a 2-dominating set in H. If T_1, T_2 and T_3 are three consecutive hexagons in H such that T_2 is an angular hexagon in the hexagonal chain $H' \equiv T_1 - T_2 - T_3$, then there exists $i \in \{1, 2, 3\}$ such that $|D \cap V(T_i)| \geq 3$.*

Proof. Firstly, there are not three consecutive vertices in $V(H')$ such that none of them belongs to D, so $|D \cap V(T_i)| \geq 2$ for $i \in \{1,2,3\}$. Secondly, if $|D \cap V(T_i)| = 2$, then the distance between these two vertices is three. Therefore, an easy verification shows that there exists $i \in \{1,2,3\}$ such that $|D \cap V(T_i)| \geq 3$.

Theorem 3.14. *If $H \in \mathcal{CHS}(h)$, then*

$$2h + 1 - \left\lfloor \frac{h-1}{5} \right\rfloor \leq \gamma_2(H).$$

Proof. By absurdum, we suppose that there exists $H \in \mathcal{CHS}(h)$ such that $\gamma_2(H) \leq 2h - \left\lfloor \frac{h-1}{5} \right\rfloor$, and we take H, satisfying this inequality, with the minimum number of hexagons. So, by Lemma 3.4, we know that every leaf hexagon is adjacent to a branching hexagon. Moreover, we take H with the minimum number of branching hexagons.

If D is a minimum 2-dominating set in H and there exists a branching hexagon A such that $|D \cap V(A)| \geq 3$, then there exist three consecutive vertices $u_1, u_2, u_3 \in V(A)$ such that $u_1, u_3 \in D$, $u_2 \notin D$ and the edge u_1u_2 belongs to another hexagon T. We take any leaf T' in H with consecutive vertices $w_1, w_2, \ldots, w_6$, and we suppose that $\deg(w_2) = \deg(w_3) = \deg(w_4) = \deg(v_5) = 2$, $w_3 \in D$ and $w_4 \notin D$. If $u_1, u_2, v_3, v_4, v_5, v_6$ are the consecutive vertices in T, and we consider the catacondensed hexagonal system H' such that $V(H') = V(H)$ and $E(H') = (E(H) \setminus \{u_2v_3, u_1v_6\}) \cup \{v_6w_3, v_3w_4\}$, we have that D is also a 2-dominating set in H', so $\gamma_2(H') \leq \gamma_2(H) \leq 2h - \left\lfloor \frac{h-1}{5} \right\rfloor$, but H' has less branching hexagons, which is a contradiction.

Finally, since $2h+1-\left\lfloor \frac{a_3}{2} \right\rfloor \leq \gamma_2(H) \leq 2h - \left\lfloor \frac{h-1}{5} \right\rfloor$, we deduce that $\left\lfloor \frac{h-1}{5} \right\rfloor + 1 \leq \left\lfloor \frac{a_3}{2} \right\rfloor$ and, consequently, $a_3 > \frac{2(h-1)}{5}$. By Lemma 3.12, there exists a branching hexagon A_2 adjacent to another two branching hexagons A_1 and A_3 and, by Lemma 3.13 there exists $i \in \{1,2,3\}$ such that $|D \cap V(A_i)| \geq 3$. Therefore, we get again the contradiction.

4. Total 2-domination number in catacondensed hexagonal systems

In this section we show a lower and an upper bound for the total 2-domination number of a catacondensed hexagonal system, and we characterize the ones attaining the bounds. Given $H \in \mathcal{CHS}$, we denote by $s_2(H)$ the number of sequences $X - L - L - \cdots - L - Y$ in H such that the number of linear hexagons L is zero or an even number, and X and Y are not linear hexagons. We need the following two results, which appear in [10], to get the bounds for the total 2-domination number.

Lemma 4.1. *Let G be a graph with minimum degree 2 and let D be a total 2-dominating set in G. Then $N(v)$ is contained in D for every vertex v such that $deg(v) = 2$.*

Proposition 4.2. *Let G be a graph with order n and maximum degree Δ. If $A = \{v \in V(G) : deg(v) = \Delta\}$, then $\gamma_{2t}(G) \geq \frac{2n-|A|}{\Delta-1}$.*

Theorem 4.3. *Let $H \in \mathcal{CHS}(h)$. Then,*

$$3(h+1) \leq \gamma_{2t}(H) \leq 3(h+1) + s_2(H).$$

Proof. If $H \in \mathcal{CHS}(h)$, then the maximum degree is $\Delta = 3$ and the number of vertices with degree 3 is equal to $2(h-1)$, consequently, the lower bound is directly obtained by Proposition 4.2.

Now, we construct a total 2-dominating set D in the following way. For any sequence $X - L_1 - L_2 - \cdots - L_{2k} - Y$ such that X and Y are the only non-linear hexagons, we take $V(X) \cup V(L_2) \cup V(L_4) \cup \cdots \cup V(L_{2k}) \cup V(Y) \subseteq D$. Therefore, for the $2k + 1$ hexagons $L_1 - L_2 - \cdots - L_{2k} - Y$ we have left $2k$ vertices outside D. For any sequence $X - L_1 - L_2 - \cdots - L_{2k+1} - Y$ such that X and Y are the only non-linear hexagons, we take $V(X) \cup V(L_2) \cup V(L_4) \cup \cdots \cup V(L_{2k}) \cup V(Y) \subseteq D$, Therefore, for the $2k + 2$ hexagons $L_1 - L_2 - \cdots - L_{2k+1} - Y$ we have left $2k + 2$ vertices outside D. It is clear that D is a total 2-dominating set and $|D| = 4h + 2 - (h - 1 - s_2(H)) = 3h + 3 + s_2(H)$.

There are many catacondensed hexagonal systems attaining the upper bound, for instance, H_1 and H_2 shown in Figure 18.

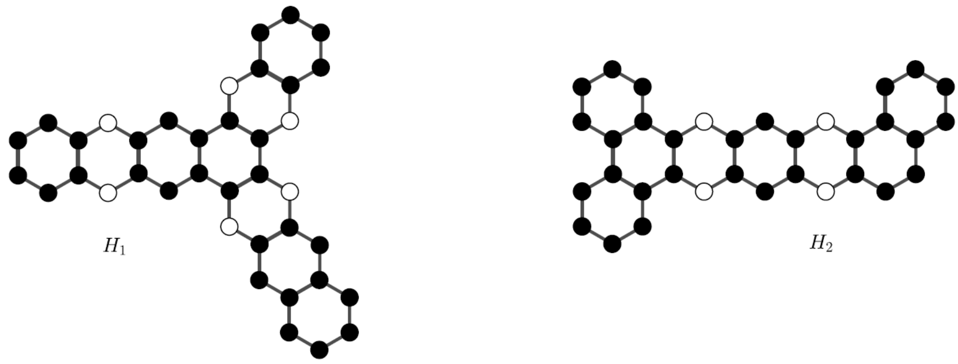

Figure 18. Two CHS such that $\gamma_{2t}(H_1) = 3(9 + 1) + 2, s_2(H_1) = 2, \gamma_{2t}(H_2) = 3(8 + 1) + 3, s_2(H_2) = 3$.

In the following theorem we characterize all catacondensed hexagonal systems attaining the lower bound in Theorem 4.3.

Theorem 4.4. *If $H \in \mathcal{CHS}(h)$, $\gamma_{2t}(H) = 3(h + 1)$ if and only if $s_2(H) = 0$.*

Proof. By Theorem 4.3 we only need to prove that, if $\gamma_{2t}(H) = 3(h + 1)$, then $s_2(H) = 0$. This result is true when $h \leq 3$. By induction, we suppose that it is true for every $H' \in \mathcal{CHS}(h')$, when $h' < h$, and let us prove the result for $H \in \mathcal{CHS}(h)$. Let $H \in \mathcal{CHS}(h)$ such that $\gamma_{2t}(H) = 3(h + 1)$ and let D be a minimum total 2-dominating set in H. We group the vertices of H in the following way. We name by $T_1, T_2, \ldots, T_h$ the hexagons in H, such that T_1 is a leaf and T_2 is adjacent to T_1. If $v_1, v_2, \ldots, v_6$ are the consecutive vertices in T_1 such that $\deg(v_1) = \deg(v_6) = 3$, then we define $V_4(T_1) = \{v_1, v_2, v_5, v_6\}$. Next, if $V(T_k) \cap V(T_j) \neq \emptyset$ and $V_4(T_j)$ has been already defined, then $V_4(T_k) = V(T_k) \setminus (V(T_k) \cap V(T_j))$. It is clear that $V(H) = \{v_3, v_4\} \cup \left(\bigcup_{k=1}^{h} V_4(T_k)\right)$.

Firstly, we suppose that there exists a linear hexagon T_k in H such that $|D \cap V_4(T_k)| = 2$. In such a case, if v and v' are the two vertices in $V_4(T_k)$ with degree equal to 2, then they do not belong to D. We denote by T_{k-1} and T_{k+1} the two hexagons adjacent to T_k and we consider the two catacondensed hexagonal systems $H_1 \in \mathcal{CHS}(h_1)$ and $H_2 \in \mathcal{CHS}(h_2)$ in $H - \{v, v'\}$. Then, we have that $D_1 = D \cap V(H_1)$ and $D_2 = D \cap V(H_2)$ are total 2-dominating sets in H_1 and H_2, respectively. Moreover, $3(h_1 + h_2 + 2) = 3(h + 1) = |D| = |D_1| + |D_2| \geq 3(h_1 + 1) + 3(h_2 + 1)$, then $|D_1| = 3(h_1 + 1)$ and $|D_2| = 3(h_2 + 1)$. Therefore, by induction hypothesis we know that $s_2(H_1) = 0 = s_2(H_2)$. If T_{k-1} and T_{k+1} are angular hexagons or branching hexagons in H, then $s_2(H) = 0$. If T_{k-1} is an angular or branching hexagon in H and T_{k+1} is a linear hexagon in H, since the number of linear hexagons in the hexagonal chain $T_{k+1} - T_{k+2} - \cdots - T_{k+r}$ is an odd number, the number of linear hexagons in the hexagonal chain $T_{k-1} - T_k - T_{k+1} - T_{k+2} - \cdots - T_{k+r}$ is also an odd number. If T_{k-1} and T_{k+1} are linear hexagons in H, since the number of linear hexagons in the hexagonal chains $T_{k-r'} - \cdots - T_{k-2} - T_{k-1}$ and $T_{k+1} - T_{k+2} - \cdots - T_{k+r}$ is an odd number in both cases, the number of linear hexagons in the hexagonal chain $T_{k-r'} - T_{k-1} - T_k - T_{k+1} - T_{k+2} - \cdots - T_{k+r}$ is also an odd number. Consequently, $s_2(H) = 0$.

Finally, we suppose that $|D \cap V_4(T_k)| \geq 3$ for any linear hexagon T_k. Since $|D \cap V_4(T_k)| \geq 3$ for every angular hexagon T_k and $|D \cap V_4(T_k)| \geq 2$ for any branching hexagon T_k, if we denote by l the number of linear hexagons, by a_3 the number of branching hexagons, and by a the number of angular hexagons, using also that the number of leaves is equal to $a_3 + 2$, we conclude that

$$\begin{aligned} |D| &= 2 + \left| \bigcup_{k=1}^{h} D \cap V_4(T_k) \right| \geq 2 + 4(a_3 + 2) + 2a_3 + 3l + 3a \\ &= 6a_3 + 3l + 3a + 10 > 3(2a_3 + 2 + l + a + 1) = 3(h + 1), \end{aligned}$$

which is a contradiction.

As we saw in Figure 18, there are many catancondensed hexagonal systems attaining the upper bound given in Theorem 4.3, so we characterize now the ones attaining that upper bound when $s_2(H)$ is as big as possible, that is, when $s_2(H) = h - 1$. A hexagonal chain such that its consecutive (from left to right) hexagons are $L - LA - RA - LA - RA \cdots - LA - RA - L$ or $L - LA - RA - LA - RA \cdots - RA - LA - L$ is called *zigzag*.

Proposition 4.5. *If $H \in \mathcal{CHS}(h)$, $\gamma_{2t}(H) = 4h + 2$ if and only if H is a zigzag or $H \in \mathcal{CHS}(4, 1)$.*

Proof. If H is a zigzag or $H \in \mathcal{CHS}(4, 1)$, every vertex has a neighbor with degree 2, so every vertex must be in the total 2-dominating set. If $\gamma_{2t}(H) = 4h + 2$, then every vertex must have a neighbor with degree two. Let v_1 be any vertex and let v_2 be a vertex adjacent to v_1, such that $\deg(v_2) = 2$ and both belong to the hexagon T with consecutive vertices $v_1, v_2, \ldots, v_6$. If $\deg(v_1) = 3$, then $\deg(v_3) = 2$, so T is an angular hexagon or a leaf, that is, every vertex belongs to a leaf or to an angular hexagon. If H contains two consecutive angular hexagons of the same type or and angular hexagon adjacent to a branching hexagon, there is a vertex such that all its neighbors have degree equal to 3. Therefore, H is a zigzag or $H \in \mathcal{CHS}(4, 1)$.

5. Final conclusions

In any catacondensed hexagonal system (with more than one hexagon) the maximum degree is equal to three, so all possible cases for the k-domination number and total k-domination number are when $1 \leq k \leq 3$, except for the total 3-domination number, which does not make sense. Since the domination number was studied in two previous papers [26,27], the whole study of these two parameters will finish after giving the next result about the 3-domination number.

Theorem 5.1. *If $H \in \mathcal{CHS}(h)$, then $\gamma_3(H) = 3(h + 1)$.*

Proof. If D is 3-dominating set, then every vertex with degree 2 must belong to D, and there are $2h + 4$ vertices with degree equal to 2. Moreover, in any edge sharing two hexagons must have a vertex of D, therefore, $|D| \geq 2h + 4 + h - 1 = 3(h + 1)$. Now, if we consider a set of vertices A such that it contains exactly one vertex in any edge sharing two hexagons, and such that every two vertices in A are at a distance bigger than or equal to 2, then $D = V(H) \setminus A$ is a 3-dominating set with cardinality $3(h+1)$.

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Conflict of interest

The authors declare there is no conflict of interest.

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