UPPER BOUND FOR TOTAL DOMINATION NUMBER ON LINEAR AND DOUBLE HEXAGONAL CHAINS

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ABSTRACT: For any graph G by $V(G)$ and $E(G)$ we denote the vertex-set and the edge-set of G, respectively. For graph G subset D of the vertex-set of G is called a total dominating set if every vertex $v \in V(G)$ is adjacent to at least one vertex of D. The total domination number $\gamma_t(G)$ is the cardinality of the smallest total dominating set.

In this paper we examine total dominations on linear and double hexagonal chains and determine upper bound for total domination numbers for such graphs.

KEY WORDS: *total dominating set, total dominating number, linear hexagonal chain, double hexagonal chain*

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1. INTRODUCTION

Let G be connected graph with vertex-set $V(G)$ and the edge-set $E(G)$. Subset D of the vertex-set of G is called a dominating set if every vertex $v \in V \setminus D$ is adjacent to at least one vertex in D. The domination number $\gamma(G)$ is the cardinality of the smallest dominating set.

Set D is a total dominating set if every vertex $v \in V$ is adjacent to at least one vertex of D. The total domination number $\gamma_t(G)$ is the cardinality of the smallest total dominating set.

Hexagonal systems are geometric objects obtained by arranging mutually congruent regular hexagons in the plane. They are of considerable importance in theoretical chemistry because they are natural graph representation of benzenoid hydrocarbons [3]. Each vertex in hexagonal system is either of degree two or of degree three. Vertex shared by three hexagons is called an internal vertex of the respective hexagonal system. We call hexagonal system catacondensed if it does not posses internal vertices, otherwise we call it pericondensed.

A hexagonal chain is a catacondensed hexagonal system in which every hexagon is adjacent to at most two hexagons. Linear hexagonal chain is hexagonal chain which is a graph representation of linear polyacene. The linear hexagonal chain with h hexagons will be denoted with $B(h)$. A double hexagonal chain consists of 2 condensed identical hexagonal chains.

Since chemical stuctures are conveniently represented by graphs, where atoms correspond to vertices and chemical bounds correspond to edges, many physical and chemical properties of molecules are well correlated with graph theoretical invariants.

One very important graph theoretical invariant is total domination number [2]. In [2] total domination was investigated on the Cartesian products of two paths and many interesting results were obtained.

In this paper we deal with total domination on linear hexagonal chain, and on double hexagonal chain $B(2h)$ that is consisted of 2 identical linear hexagonal chains with h hexagons. As result we give an upper bound for total domination number in such chains.

2. UPPER BOUND FOR TOTAL DOMINATION ON LINEAR HEXAGONAL CHAINS

For isomorphic graphs the total dominating number is equal. Therefore, each hexagon will be represented with its isomorphic graph that is illustrated in Figure 1.

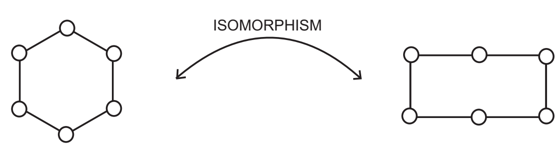


Figure 1

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

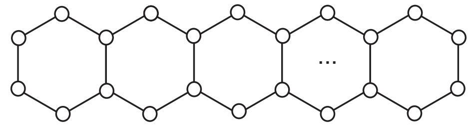


Figure 2

The above structure is isomorphic with the one illustrated in Figure 3. In such structure each vertex is denoted by (i, j), $i = 1, 2$, $j = 1, \ldots, 2h + 1$.

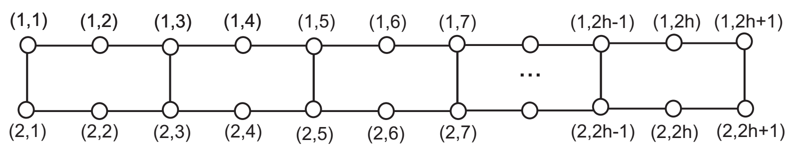


Figure 3

Theorem 2.1. Let $B(h)$ be the linear hexagonal chain with h hexagons. Then

$$\gamma_t(B(h)) \leq 2h + 2. \tag{1}$$

Proof. From Figure 4 it follows that the total dominating set of $B(h)$ is

$$D = \{(1, k), (2, k) \quad | \quad k = 1, \ldots, 2h + 1, \quad k \quad \text{odd}\},$$

so $\gamma_t(B(h)) \leq |D| = 2h + 2$.

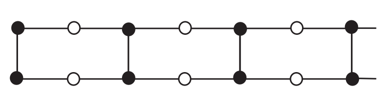
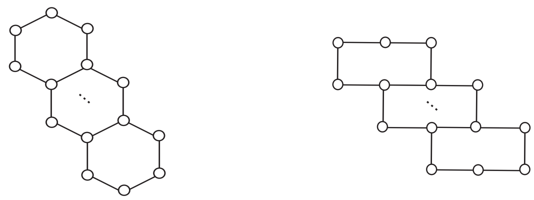


Figure 4

Remark 2.2. Theorem 2.1 also holds for a hexagonal systems and its isomorphic graphs represented in Figure 5a and Figure 5b, respectively. It is easy to find isomorphism beteween these structures and $B(h)$.



a) b)

Figure 5

3. UPPER BOUND FOR TOTAL DOMINATION ON DOUBLE HEXAGONAL CHAINS

Let $B(2h)$ be the double hexagonal chain with h hexagons on each linear chain. See Figure 6.

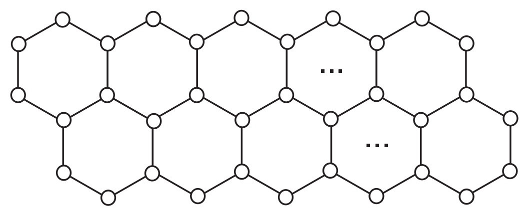


Figure 6

Again, we will determine the upper bound for total domination number on its isomorphic graph:

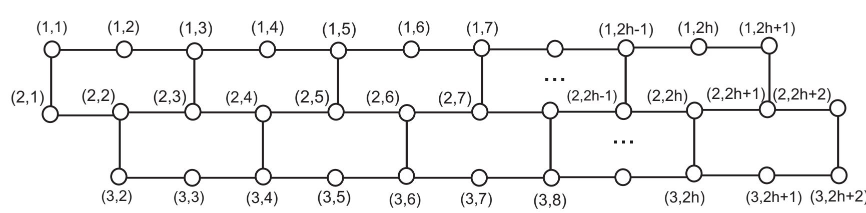


Figure 7

Lemma 3.1 $\gamma_t(B(2 \cdot 3)) \leq 10.$

Proof: Let us consider set $D_0 = \{(1,3),(1,4),(1,7),(2,1),(2,2),(2,4),(2,7),(3,4),(3,7),(3,8)\}$. This is the total dominating set for $B(2\cdot 3)$, so $\gamma_t(B(2\cdot 3)) \le 10$.

Theorem 3.2 Let $B(2h)$ be the double hexagonal chain. Then

$$\gamma_t(B(2h)) \le \begin{cases} \dfrac{5h}{2}+2, & \text{if } h \equiv 0(\mathrm{mod})4 \\ 10\left\lfloor \dfrac{h}{4} \right\rfloor + 6, & \text{if } h \equiv 1(\mathrm{mod})4 \\ 10\left\lfloor \dfrac{h}{4} \right\rfloor + 8, & \text{if } h \equiv 2(\mathrm{mod})4 \\ 10\left\lceil \dfrac{h}{4} \right\rceil, & \text{if } h \equiv 3(\mathrm{mod})4 \end{cases}$$

Proof: We consider the set

$$\begin{aligned} D = \ & \Big\{(1,3+8k),(1,4+8k),(1,7+8k),(2,1+8k),(2,2+8k),(2,4+8k),(2,7+8k), \\ & (3,4+8k),(3,7+8k),(3,8+8k) \quad | \quad k=0,1,\ldots,\left\lfloor \frac{h}{4} \right\rfloor\Big\}. \end{aligned}$$

Then, we consider blocks $B(2\cdot 3)_k$, $k = 0,1,2,\ldots,\left\lfloor \dfrac{h-3}{4} \right\rfloor$, $h \ge 3$. See Figure 10. We will denote $B(2\cdot 3)_k$ with C_k. Blocks C_k and C_{k+1} have no common vertices nor common edges. For each block C_k we have total dominating set

$$\begin{aligned} D_k = \ & \Big\{(1,3+8k),(1,4+8k),(1,7+8k),(2,1+8k),(2,2+8k),(2,4+8k),(2,7+8k), \\ & (3,4+8k),(3,7+8k),(3,8+8k)\Big\} \end{aligned}$$

and

$$\gamma_t(C_k) \le |D_k| = 10, \quad k = 0,1,2,\ldots,\left\lfloor \frac{h-3}{4} \right\rfloor.$$

Notice that for $k=0$ we have total dominating set D_0 from Lemma 3.1.

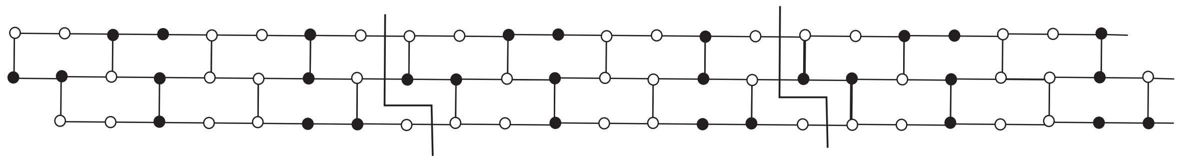


Figure 10

a) Let us consider first $h \equiv 3(\mathrm{mod}4)$. Then D is total dominating set and we have

$$\gamma_t(B(2h)) \leq |D| = 10\Big(\Big\lfloor\frac{h}{4}\Big\rfloor + 1\Big) = 10\Big\lceil\frac{h}{4}\Big\rceil.$$

If we add 4 hexagons to $B(2 \cdot 3)$, then the structure that is not totally dominated by the set D_0 is $B(2 \cdot 1)$, and from Theorem 2.1 and Remark 2.2 it follows $\gamma_t(B(2 \cdot 1)) \leq 6$. From this, we conclude $\gamma_t(B(2 \cdot 5)) \leq 10 + 6 = 16$, and the total dominating set is $S_0 = D_0 \cup \{(2,9),(2,10),(1,10),(1,11),(2,12),(3,12)\}$.
By adding 6 hexagons to $B(2 \cdot 3)$, we can see that the structure which is not totally dominated by D_0 is $B(2 \cdot 2)$. For this structure we can easily see that the set $\{(1,3),(1,4),(2,1),(2,2),(2,4),(3,4),(3,5),(3,6)\}$ is total dominating set, so $\gamma_t(B(2 \cdot 2)) \leq 8$. Now we conclude $\gamma_t(B(2 \cdot 6) = 10 + 8 = 18$. We choose the total dominating set $S_1 = (S_0 \setminus \{(1,10)\}) \cup \{(1,12),(2,14),(3,14)\}$.
By the same procedure we conclude that $\gamma_t(B(2 \cdot 7)) \leq 10 + 10 = 20$, and the total dominating set is $S_2 = (S_1 \setminus (2,14),(3,14)) \cup \{(1,15),(2,15),(3,15),(3,16)\}$.

If $h = 11$ we have the same situation as above: we start with $B(2 \cdot 7)$ and then we add hexagons, step by step. By induction on $h = 3((\mathrm{mod}4)$, we conclude that

$\gamma_t(B(2h)) \leq |D| = 10\left\lceil \frac{h}{4} \right\rceil.$

b) If $h \equiv 0(\text{mod})4$, it is easy to see that the total dominating set is

$$D \cup \{(2, 2h+1), (2, 2h+2)\}$$

and

$$\gamma_t(B(2h)) \leq 10\left\lfloor \frac{h}{4} \right\rfloor + 2.$$

c) If $h \equiv 1(\text{mod})4$, then the total dominating set is

$$D \cup \{(2, 2h+1), (2, 2h+2), (1, 2h+2), (1, 2h+3), (2, 2h+4), (3, 2h+4)\}$$

and $\gamma_t(B(2h)) \leq 10\left\lfloor \frac{h}{4} \right\rfloor + 6.$

d) If $h \equiv 2(\text{mod})4$, then the total dominating set is

$$D\cup\{(2, 2h+1), (2, 2h+2), (1, 2h+2), (1, 2h+3), (2, 2h+4), (3, 2h+4), (2, 2h+6), (3, 2h+6)\}$$

and $\gamma_t(B(2h)) \leq 10\left\lfloor \frac{h}{4} \right\rfloor + 8.$

Remark 3.8. Theorem 3.7 also holds for a hexagonal systems and its isomorphic graphs represented in Figure 11a and Figure 11b, and also for structures represented in Figure 11c and 11d, respectively. It is easy to find isomorphism beteween all these structures and $B(2h)$.

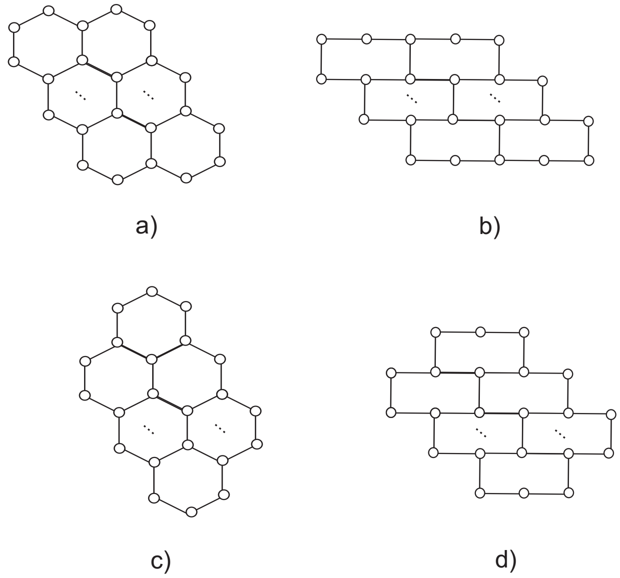


Figure 11

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