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DOUBLE TOTAL DOMINATION NUMBER ON SOME CHEMICAL NANOTUBES

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ABSTRACT. Suppose G is a graph with the vertex set $V(G)$. A set $D \subseteq V(G)$ is a total k-dominating set if every vertex $v \in V(G)$ has at least k neighbours in D. The total k-domination number $\gamma_{kt}(G)$ is the size of the smallest total k-dominating set. When $k = 2$ the total 2-dominating set is referred to as a double total dominating set. In this work we compute the exact values for double total domination number on H-phenylenic nanotubes $HPH(m, n)$, $m, n \geq 2$ and H-naphtalenic nanotubes $HN(m, n)$, $n = 2k$, $m, n \geq 2$. As all vertices have a degree 2 or 3, there is no total k-domination for $k \geq 3$ for H-phenylenic and H-naphtalenic nanotubes, and the double total domination is the maximum possible.

1. INTRODUCTION

Graph dominations hold significance due to their presence in diverse applications like dominating queens, computer networks, school bus route planning, social network issues, and chemistry [2, 6, 8, 9, 13–17]. In representing chemical structures as graphs, atoms correspond to vertices and chemical bonds to edges. Owing to this resemblance, numerous physical and chemical attributes of molecules are linked to graph-theoretical constants. The total (double) domination number serves as an example of such an invariant [2–4, 6–8, 11, 14, 15].

We explore double total dominations on H-phenylenic nanotube $HPH(m, n)$, $m, n \geq 2$ and H-naphtalenic nanotube $HN(m, n)$, $n = 2k$, $m, n \geq 2$. Furthermore, we give exact values for the double total domination number on mentioned graphs.

Key words and phrases. Total domination, double total domination, hexagonal systems, molecular graph, H-phenylenic nanotube, H-naphtalenic nanotube.

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H-phenylenic $HPH(m,n)$, $m,n \geq 2$ and H-naphtalenic $HN(m,n)$, $n = 2k, m,n \geq 2$ are carbon nanotubes [16]. Carbon nanotubes are molecular cylinders used for fabrication of nanoscale devices by providing molecular probes, pipes, wires, bearings and springs. Because of their substantiality and stiffness, they have many potential applications in different technologies.

Currently, there are only a limited number of publications on total and double total domination on chemical graphs [2,6,10,12,14,15]. This work is in a close relationship with our previous papers [10,12], in which we also study double total domination, but on a hexagonal grid and pyrene network.

In addition to this introduction, the paper is structured as follows. Section 2 provides an overview of the total and double domination, dominating sets, and hexagonal systems. Section 3 provides the double total domination number γ_{2t} on H-phenylenic nanotube $HPH(m,n)$, $m,n \geq 2$. Section 4 provides the double total domination number on H-naphtalenic nanotube $HN(m,n)$, $n = 2k$, $m,n \geq 2$.

2. Preliminaries

Consider a graph G with vertex set V(G). A set $D \subset V(G)$ is a dominating set of G if every vertex y in $V(G) \setminus D$ has a neighbour in D. The domination number $\gamma(G)$ is the size of the smallest dominating set. Total domination is the stronger version of domination, where a set $D \subset V(G)$ is a total dominating set of G if every vertex y in $V(G)$ has a neighbour in D. The total domination number $\gamma_t(G)$ is the size of the smallest total dominating set.

A set $D \subseteq V(G)$ is a k-dominating set, if every vertex $v \in V(G) \setminus D$ has at least k neighbours in D. The k-domination number $\gamma_k(G)$ is the size of the smallest k-dominating set. A set $D \subseteq V(G)$ is a total k-dominating set if every vertex $v \in V(G)$ has at least k neighbours in D. In such case, it must be $k \leq \delta(G)$ where $\delta(G)$ is the minimum degree of vertices in G and $|D| \geq k+1$. The total k-domination number $\gamma_{kt}(G)$ is the size of the smallest total k-dominating set. A double total dominating set is also called the total 2-dominating set.

Each vertex in H-phenylenic nanotube and H-naphtalenic nanotube is either of degree 2 or of degree 3. As a result, there is no total k-domination for $k \geq 3$ on H-phenylenic and H-naphtalenic nanotubes.

3. Double Total Domination Number of H-phenylenic Nanotubes

H-phenylenic nanotubes $HPH(m,n)$ are molecular graphs that are covered by C_6, C_4 and C_8 [1]. We denote by $HPH(m,n)$ H-phenylenic nanotube with m hexagonal rows and n hexagonal columns. The number of vertices in H-phenylenic nanotube $HPH(m,n)$ is $6mn$. See Figure 1 and Figure 2.

Lemma 3.1. $\gamma_{2t}(HPH(2,2)) = 20$.

Proof. Since we are considering double total domination, every vertex adjacent to a vertex with degree 2 must be included in any double total dominating set.

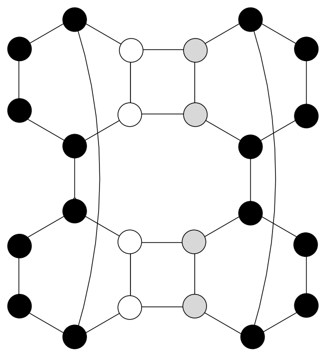

FIGURE 1. A double total dominating set in $HPH(2,2)$

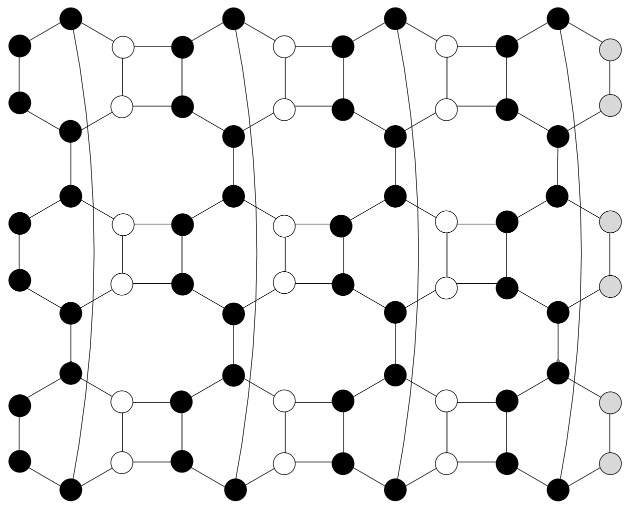

FIGURE 2. A double total dominating set in $HPH(3,4)$

Let T be double total dominating set on $HPH(2,2)$. All vertices from $HPH(2,2)$ which are not on square must be in T because they are adjacent to at least one vertex with degree 2. See Figure 1. Mentioned vertices are in black color. There is 16 such vertices on $HPH(2,2)$, 4 on each hexagonal ring.

It follows that $\gamma_{2t}(HPH(2,2)) \geq 16$. If there were only this 16 vertices in the double total dominating set T, vertices on both squares would be total dominated only once. To double total dominate vertices on one square we need at least 2 vertices at each square. See Figure 1. Additional vertices are in gray color. Thus,

$$\gamma_{2t}(HPH(2,2)) \geq 16 + 4 = 20.$$

But, it can be easily checked that 20 vertices can double total dominate all vertices on $HPH(2,2)$, hence $\gamma_{2t}(HPH(2,2)) \leq 20$. □

The following theorem is well known see [5].

Theorem 3.1. *Let $k \in \mathbb{N}$ and $G = (V, E)$ be a graph of order n with minimum degree $\delta(G) \geq k$. Then $\gamma_{kt}(G) \geq \frac{kn}{\Delta(G)}$ where $\Delta(G)$ is maximum degree.*

Theorem 3.2. *For H-phenylenic nanotube $HPH(m, n)$, $m, n \geq 2$ it holds*

$$\gamma_{2t}(HPH(m, n)) = 4mn + 2m.$$

Proof. From each hexagonal column of $HPH(m, n)$ we will take 4 vertices form each hexagon and denote these vertices with T_1. See Figure 2. Vertices belonging to T_1 are in black color. $|T_1| = 4mn$ as there are n hexagonal columns with m hexagons.

Set T_1 double total dominate all vertices on $HPH(m, n)$, except gray vertices on the last column see Figure 2. Gray vertices are total dominated only once. Also, gray vertices are adjacent to some vertex of degree 2. It follows that all of them must be in the double total dominating set. There are m rows, each containg 2 gray vertices, so we need at least $2m$ vertices to double total dominate all vertices on $HPH(m, n)$. It follows $\gamma_{2t}(HPH(m, n)) \leq 4mn + 2m$.

From Theorem 3.1. follows that $\gamma_{2t}(HPH(m, n)) \geq \frac{2 \cdot 6mn}{3} = 4mn$. But $|T_1| = 4mn$ and its vertices double total dominate all vertices except vertices from the last column. Moreover, the dominated vertices are double total dominated with only 2 vertices from T_1 which is minimal. See Figure 2. It follows that we need at least $2m$ more vertices to double total dominate remaining undominated vertices. Hence, $\gamma_{2t}(HPH(m, n)) \geq 4mn + 2m$. □

4. Double Total Domination Number of H-naphtalenic Nanotubes

H-naphtalenic nanotubes are molecular graphs that are obtained by the sequence C_6, C_6, C_4, C_6 and $C_6, \dots, C_6, C_6, C_4, C_6, C_6$ and the repeat unit C_6, C_6, C_4 [18]. See Figure 3 and Figure 4. We denote by $HN(m, n)$, $n = 2k$ H-naphtalenic nanotube with m hexagonal rows and n hexagonal columns. The number of vertices in H-naphtalenic nanotube $HPH(m, n)$ is $5mn$.

A zigzag line in HN(m, n) that does not contain vertical edges is referred to as a horizontal zigzag line The horizontal zigzag line of $HN(m, n)$ are denoted by L_i, $1 \leq i \leq 2m$. For all zigzag lines on $HN(m, n)$ it holds $|L_i| = 5n/2$. See Figure 3.

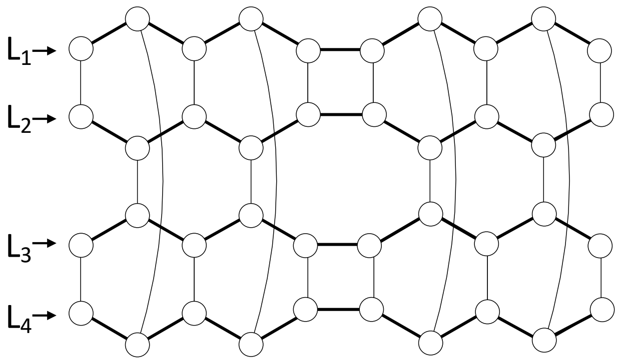

FIGURE 3. Zig-zag lines on $HN(2,4)$

Theorem 4.1. *For H-naphtalenic nanotubes $HN(m,n), n = 2k$ it holds*

$$\gamma_{2t}(HN(m,n)) = \begin{cases} 2m\left(2\left\lfloor\frac{5n}{6}\right\rfloor + 2\right), & \text{if } n \equiv 2 \bmod 3, n \equiv 1 \bmod 3, \\ 2m\left(2\left\lfloor\frac{5n}{6}\right\rfloor + 1\right), & \text{if } n \equiv 0 \bmod 3. \end{cases}$$

Proof. We will consider three cases.

(a) Case $n \equiv 2 \bmod 3, n = 2k$.

Let T_i be the subset of the double total dominating set T on L_i of $HN(m,n)$, $1 \le i \le 2m$. For each $i, 1 \le i \le 2m$, it holds

$$T_i = \left\{v_{i,1+3j}, v_{i,2+3j}, j = 0, \ldots, \left\lfloor\frac{5n}{6}\right\rfloor - 1\right\} \cup \left(i, \frac{5n}{2} - 1\right), \left(i, \frac{5n}{2}\right).$$

Then

$$|T_i| = 2\left\lfloor\frac{5n}{6}\right\rfloor + 2 \quad \text{and} \quad |T| = 2m\left(2\left\lfloor\frac{5n}{6}\right\rfloor + 2\right).$$

T double total dominates all vertices on $HN(m,n)$. See Figure 4 for the double total dominating set on $HN(3,8)$.

Thus for $n \equiv 2 \bmod 3, n = 2k$ follows

$$\gamma_{2t}(HN(m,n)) \le |T|.$$

But also, each vertex on $HN(m,n)$ is double dominated by exactly 2 vertices, which is minimal. So,

$$\gamma_{2t}(HN(m,n)) \ge |T|.$$

(b) Case Let $n \equiv 1 \bmod 3, n = 2k$.

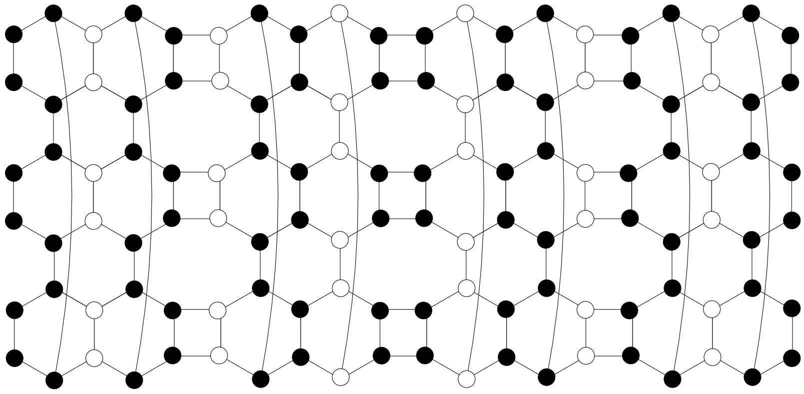

FIGURE 4. A double total dominating set in $HN(3,8)$

Again, let T_i be the subset of the double total dominating set T on the L_i of $HN(m,n)$, $1 \leq i \leq 2m$. For each $i, 1 \leq i \leq 2m$, it holds

$$T_i = \left\{ v_{i,1+3j}, v_{i,2+3j}, j = 0, \dots, \left\lfloor \frac{5n}{6} \right\rfloor - 1 \right\} \cup \left(i, \frac{5n}{2} - 1\right), \left(i, \frac{5n}{2}\right).$$

Then

$$|T_i| = 2 \left\lfloor \frac{5n}{6} \right\rfloor + 2 \quad \text{and} \quad |T| = 2m \left(2 \left\lfloor \frac{5n}{6} \right\rfloor + 2\right).$$

T double total dominates all vertices on $HN(m,n)$. See Figure 5 for the double total dominating set on $HN(2,10)$.

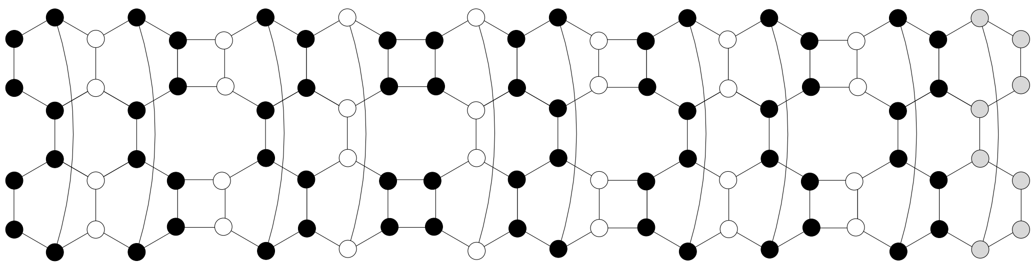

FIGURE 5. A double total dominating set in $HN(2,10)$

Hence, for $n \equiv 1 \bmod 3, n = 2k$ it follows

$$\gamma_{2t}(HN(m,n)) \leq |T|.$$

Further, note that

$$T_i \setminus \left\{ \left(i, \frac{5n}{2} - 1\right), \left(i, \frac{5n}{2}\right) \right\}, \quad 1 \leq i \leq 2m,$$

double total dominate all verices on L_i except $(i, 5n/2-1), (i, 5n/2)$, $1 \leq i \leq 2m$ and each vertex is double total dominated by two vertices, which is minimal. In order to double total dominate also $(i, 5n/2-1), (i, 5n/2)$, $1 \leq i \leq 2m$ they must be in any double total dominatig set as they are adjacent to the some vertex of degree 2.

So, $\gamma_{2t}(HN(m, n)) \geq |T|$.

(c) Case $n \equiv 0 \bmod 3, n = 2k$

Again, let T_i be the subset of the double total dominating set T on the L_i of $HN(m, n)$, $1 \leq i \leq 2m$. For each $i, 1 \leq i \leq 2m$, it holds

$$T_i = \left\{ v_{i,1+3j}, v_{i,2+3j}, j = 0, \ldots, \left\lfloor \frac{5n}{6} \right\rfloor - 1 \right\} \cup \left(i, \frac{5n}{2} \right).$$

Then

$$|T_i| = 2 \left\lfloor \frac{5n}{6} \right\rfloor + 1 \quad \text{and} \quad |T| = 2m \left(2 \left\lfloor \frac{5n}{6} \right\rfloor + 1 \right).$$

T double total dominates all vertices on $HN(m, n)$. See Figure 6 for the double total dominating set on $HN(2, 6)$.

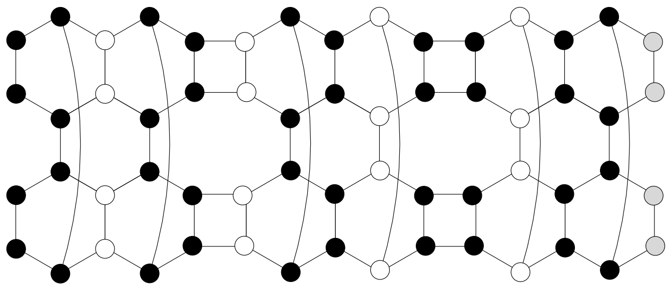

FIGURE 6. A double total dominating set in $HN(2, 6)$

Therefore, for $n \equiv 0 \bmod 3, n = 2k$ follows

$$\gamma_{2t}(HN(m, n)) \leq |T|.$$

Further note that

$$T_i \setminus \left(i, \frac{5n}{2} \right), \quad 1 \leq i \leq 2m,$$

double total dominate all vertices on L_i except $(i, 5n/2), 1 \leq i \leq 2m$ and each vertex is double total dominated by two vertices, which is minimal. In order to double total dominate also $(i, 5n/2), 1 \leq i \leq 2m$ they must be included in any double total dominating set as they are adjacent to some vertex of degree 2.

So, $\gamma_{2t}(HN(m, n)) \geq |T|$. □

5. Conclusions

We have determined the exact values for the double total domination number on the H-phenylenic nanotube $HPH(m,n)$, $m,n \geq 2$ and the H-naphtalenic nanotube $HN(m,n)$, $n = 2k$, $m,n \geq 2$. In our future work, we plan to study the total and the double total domination on some other chemical graphs.

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