# Total and double total dominations in some chemical graphs

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# Introduction

In this work, we study total and double total dominations on different chemical graphs such as hexagonal grid, pyrene network and hexabenzocoronene. We give the lower and the upper bound for total and double total domination numbers on mentioned graphs.

Pyrene networks and hexabenzocoronene are benzenoid hydrocarbons [1, 7, 2]. Benzenoid hydrocarbons and their derivates are an important class of organic compounds that have, apart from their chemical importance, big technical and farmaceutical importance as well and belong to the group of the most serious polluters of the environment. Pyrene has interesting photophysical properties and it is used to make dyes, plastics and pesticides.

# Basic definitions

### Definition

*Let $G$ be a graph with the vertex set $V(G)$. A set $D \subseteq V(G)$ is a **total dominating set** of a graph $G$ if every vertex $v \in V(G)$ has a neighbour in $D$. The **total domination number** $\gamma_t(G)$ is the cardinality of the smallest total dominating set.*

### Definition

*Let $G$ be a graph with the vertex set $V(G)$. A set $D \subseteq V(G)$ is a **total $k$-dominating set** of graph $G$ if every vertex $v \in V(G)$ has at least $k$ neighbours in $D$. The **total $k$-domination number** $\gamma_{kt}(G)$ is the cardinality of the smallest total $k$-dominating set. For $k = 2$ the total 2-dominating set is called **double total dominating set**.*

# Observed graphs

All mentioned graphs are obtained by arranging congruent regular hexagons in a plane. Each vertex in hexagonal system is either of degree 2 or of degree 3. It follows that there is no total $k$-dominating set for $k \geq 3$.

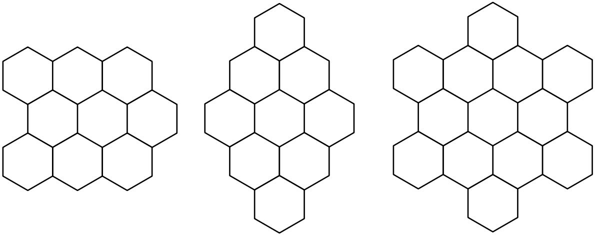

Figure 1: A hexagonal grid, pyrene network and hexabenzocoronene.

# Total domination on hexagonal grid

**Theorem 1**

*For hexagonal grid with m hexagons in a row and n hexagons ($n \geq 3$) in a column $H_{m,n}$ it holds*

$$\gamma_t(H_{m,n}) \leq \begin{cases} (n+2)\frac{2m+3}{3} - 1, & m \equiv 0(mod3) \\ (n+2)\frac{2m+4}{3} - 2, & m \equiv 1(mod3) \\ (n+2)\frac{2m+2}{3}, & m \equiv 2(mod3). \end{cases}$$

**Proposition 2**

*For hexagonal grid with m hexagons in a row and n hexagons ($n \geq 3$) in a column $H_{m,n}$ holds*

$$\gamma_t(H_{m,n}) > \frac{2nm}{3}.$$

For $n = 1, 2$ see [5, 6].

# Double total domination on hexagonal grid

**Theorem 3**

*For hexagonal grid with m hexagons in a row and n hexagons in a column $H_{m,n}$ it holds*

$$\gamma_{2t}(H_{m,n}) \leq \begin{cases} (3n+3)\lceil \frac{m}{2} \rceil + n - 1, & m, n \text{ odd} \\ n(\frac{3m}{2}+2) + 2m + 1, & m, n \text{ even} \\ (n+1)(\frac{3m}{2}+2), & m \text{ even}, n \text{ odd} \\ 3n\left(\frac{m+1}{2}\right) + 2m + n & m \text{ odd}, n \text{ even}. \end{cases}$$

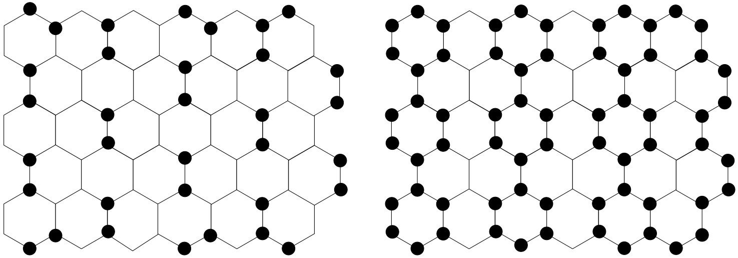

Figure 2: A total and double total dominating set on $H_{6,5}$.

# Double total domination on pyrene network I

We denote by $PY(n)$ pyrene network of dimension $n$. $PY(n)$ has $3n^2 + 4n - 1$ edges, where $n$ is the number of hexagons in the center of the graph. Pyrene network of dimension 1 has just a single hexagon.

In $PY(n)$ any zigzag line not containing vertical edges is called horizontal zigzag line. The horizontal zigzag lines of $PY(n)$ are denoted by $L_i$, $1 \leq i \leq 2n$.

$$|V(L_i)| = \begin{cases} 2i + 1, & i \leq n \\ 4n - 2i + 3, & n + 1 \leq i \leq 2n. \end{cases}$$

# Double total domination on pyrene network II

**Lemma 4**

*For pyrene network of dimension* 1 *and* 2 *it holds*

$$\gamma_{2t}(PY(1)) = 6, \quad \gamma_{2t}(PY(2)) = 14.$$

**Theorem 5**

*For pyrene network* $PY(n)$, $n \geq 3$ *it holds*

$$\gamma_{2t}(PY(n)) \leq \begin{cases} \frac{3}{2}(n+1)^2, & n \text{ odd} \\ \frac{3}{2}n(n+2)+4, & n \text{ even.} \end{cases}$$

The bounds for total domination see in [1].

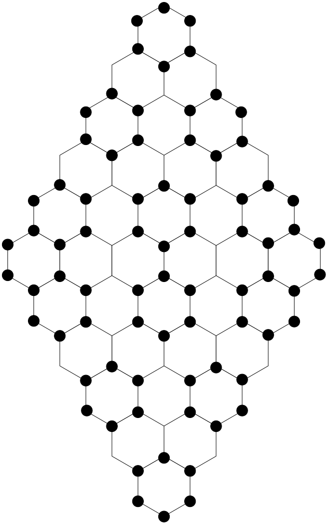

Figure 3: A double total dominating set on $PY(6)$.

# Double total domination on hexabenzocoronene I

We denote by $XC(n)$ hexabenzocoronene of dimension $n \geq 2$. This graph is also called a ring type benzenoid graph $R(n)$. $XC(n)$ has $27n^2 - 33n + 12$ edges, where $n$ is the number of rings from the center of the graph to the bottom or top.

Again, any zigzag line in $XC(n)$ not containing vertical edges is called a horizontal zigzag line. The horizontal zigzag lines of $XC(n)$ are denoted by $L_i$, $1 \leq i \leq 4n - 2$.

$$|V(L_i)| = \begin{cases} 6i - 3, & 1 \geq i \geq n \\ 6n - 3, & n + 1 \geq i \geq 3n - 2 \\ 3 + 6((4n - 2) - i), & 3n - 1 \geq i \geq 4n - 2. \end{cases}$$

# Double total domination on hexabenzocoronene II

## Lemma 6

$$\gamma_{2t}(XC(2)) = 36$$

## Theorem 7

*For hexabenzocoronene of dimension $n \geq 3$ it holds*

$$\gamma_{2t}(XC(n)) \leq \begin{cases} (n-1)(9n-3) + \frac{n}{2}(9n+10) - \frac{11}{2}, & n \text{ odd} \\ (n-1)(9n-2) + \frac{n}{2}(9n+10) - 6, & n \text{ even.} \end{cases}$$

## Theorem 8

*For hexabenzocoronene of dimension $n \geq 2$ it holds*

$$\gamma_{2t}(XC(n)) > 24n - 18.$$

The bounds for total domination see in [1].

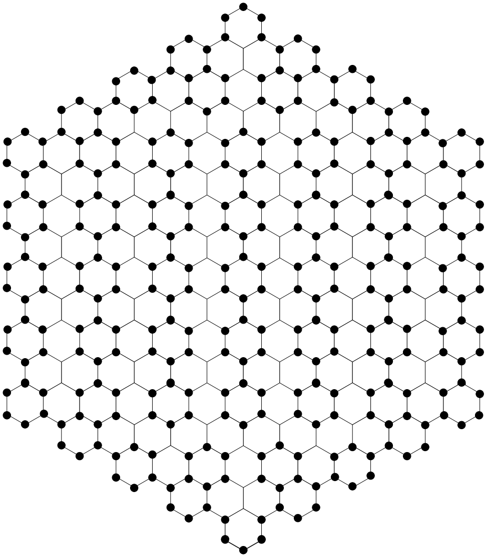

Figure 4: A double total dominating set on $XC(5)$.

For more details see [3, 4].
Thank you for your attention!

# Literature I


[1] Y. Gao, E. Zhu, Z. Shao, I. Gutman, A. Klobučar, Total domination and open packing in some chemical graphs, *J. Math. Chem.*, **56** (2018), 1481–1492.

[2] I. Gutman, Hexagonal systems: a chemistry motivated excursion to combinatorial geometry, *Teach. Math.*, **10** (2007), 1–10.

[3] A. Klobučar, A. Klobučar, Total and double total domination on hexagonal grid, *Mathematics*, **7** (2019), 1110.

[4] A. Klobučar Barišić, A. Klobučar. Double total domination number in certain chemical graphs, *AIMS Mathematics*, **7(11)** (2022), 19629-19640.

[5] S. Majstorović, A. Klobučar, Upper bound for total domination number on linear and double hexagonal chains, *International Journal of Chemical Modeling*, **3** (2011), 139–146.

[6] D. Mojdeh, M. Habibi, L. Badakhshian, Total and connected domination in chemical graphs, *Ital. J. Pure Appl. Math.*, **39** (2018), 393–401.

# Literature II

[7] D. Vukičević, A. Klobučar, k-Dominating sets on linear benzenoids and on the infinite hexagonal grid, *Croat. Chem. Acta*, **80** (2007), 187–191.