TOTAL AND CONNECTED DOMINATION IN CHEMICAL GRAPHS

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Abstract. For a given graph G a subset D of the vertex-set $V(G)$ 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. Also D is called a connected dominating set if every vertex $v \in V(G) - D$ is adjacent to at least one vertex in D and the induced subgraph $\langle D \rangle$ is connected. The connected domination number $\gamma_c(G)$ is the minimum cardinality taken over all connected dominating sets of G. In this paper, we determine the domination number, the total domination number and the connected domination number for some chemical graphs.

Keywords: Total domination number, connected domination number, bondage number, hexagonal chains, pyrene.

1. Introduction

Domination in graph theory is a natural model form any location problems in operations research. Domination has many other applications in dominating queens problem, school bus routing problem, computer communication network problems, social network theory [5]. Also chemical structures are conveniently represented by graphs, where atoms correspond to vertices and chemical bonds correspond to edges. This representation inherits many useful information about chemical properties of molecules. Also it has been shown in QSAR and QSPR studies that many physical and chemical properties of molecules are well correlated with graph theoretical invariants that are termed topological indices or molecular descriptors.

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Let G be a graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. By the neighborhood of a vertex v of G we mean the set $N_G(v) = N(v) = \{u \in V(G) : uv \in E(G)\}$. The degree of a vertex v, denoted by $d_G(v)$, is the cardinality of its neighborhood. A subset $D \subseteq V(G)$ is a dominating set of G if every vertex of $V(G) - D$ has a neighbor in D. The domination number of G, denoted by $\gamma(G)$, is the minimum cardinality of a dominating set of G. For a comprehensive survey of domination in graphs, see [4, 5, 11, 12]. A subset $D \subseteq V(G)$ is a total dominating set, abbreviated TDS, of G if every vertex of G has a neighbor in D. The total domination number of G, denoted by $\gamma_t(G)$ and introduced by Cockayne, Dawes, and Hedetniemi [1].

A set $D \subseteq V(G)$ is called a connected dominating set if every vertex $v \in V(G)-D$ is adjacent to at least one vertex in D and the induced subgraph $\langle D \rangle$ is connected. The connected domination number $\gamma_c(G)$ is the minimum cardinality taken over all connected domination sets of G, see [6]. The cardinality of smallest dominating set D such that $\langle D \rangle$ has no edges is the independent domination number. The independent domination number of G, denoted by $\gamma_i(G)$.

The bondage number $b(G)$, to be the minimum number of edges whose removal increases the domination number.

In [9, 13] authors computed some domination number for Linear and double hexagonal chain. Here we continue this progress by computing the domination number, total domination number and connected domination number for some hexagonal chains. We shall need the following theorems [5].

Theorem 1.1. *Let D be a dominating set with the property that if every vertex $v_i \in V(G)$ is dominated by exactly one vertex of D, then D is minimum dominating set.*

Total domination number is easily calculated for cycles and paths, [7].

Theorem 1.2. *The total domination number of a cycle C_n or a path P_n on $n \geq 3$ vertices is given by:*

$$\gamma_t(C_n) = \gamma_t(P_n) = \begin{cases} \frac{n}{2}, & \text{if } n \equiv 0 \pmod 4 \\ \frac{n+2}{2}, & \text{if } n \equiv 2 \pmod 4 \\ \frac{n+1}{2}, & \text{otherwise.} \end{cases}$$

Hexagonal chains are important for theoretical chemistry because they are natural graph representations of benzenoid hydrocarbons, a great deal of investigation in mathematical chemistry has been developed to hexagonal chains [2, 3].

A hexagonal system is a connected plane graph without cut-vertices in which all inner faces are hexagons (and all hexagons are faces), such that two hexagons are either disjoint or have exactly one common edge, and no three hexagons share a common edge. Hexagonal systems are geometric objects obtained by arranging mutually congruent regular hexagons in the plane.

We call hexagonal system catacondensed if it does not possess 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.

Hexagons sharing a common edge are said to be adjacent or neighboring. Two hexagons of a hexagonal system may have either two common vertices (if they are adjacent) or none (if they are not adjacent). A vertex of a hexagonal system belongs to at most three hexagons.

A vertex shared by three hexagons is called an internal vertex the respective hexagonal system. A hexagonal chain with n hexagons, $n \geq 2$, possesses two terminal hexagons and $n-2$ hexagons that have two neighbors.

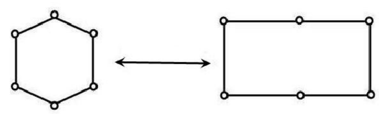

Figure 1: Isomorphism Graphs.

We have same domination number for two isomorphism graphs. Therefore, each hexagon will be represented with its isomorphic graph are shown in Figure 1.

In what follows for the sake of brevity a hexagonal chain with n hexagons will be referred to as dimension n. G_n is the hexagonal chain with n hexagons represented by Figure 2. All hexagonal chains with n hexagons have $4n+2$ vertices and $5n+1$ edges. Spiral chain is a kind of hexagonal chain that be shown with S_n (Figure 5).

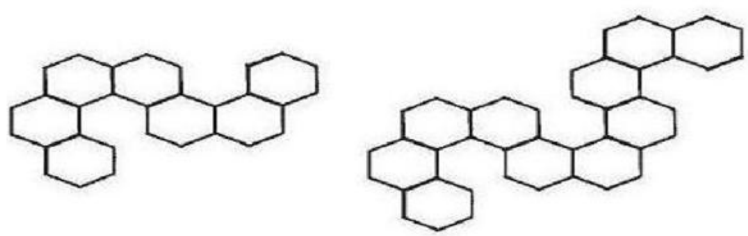

Figure 2: Hexagonal chain with 7 and 10 hexagons.

Pyrene is a typical polycyclic aromatic hydrocarbon (PAH). It has interesting photo physical properties, such as long excited state lifetime, high quantum yield of fluorescence.

Pyrene exhibits sensitive behavior, with the relative intensity of emission bands that depends on the solvent polarity. Pyrene is used to make dyes, plastics and pesticides. In order to study domination number in pyrene, it is necessary to introduce its topological properties. Let α_0 be the center line perpendicular

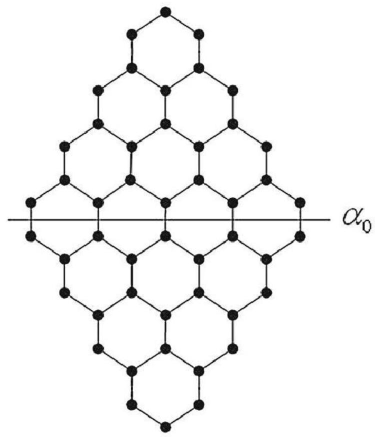

Figure 3: A Pyrene $PY(4)$

to the vertical edge direction of hexagon of $PY(n)$ as shown in Figure 3. The number of vertices and edges of $PY(n)$ are $2n^2+4n$ and $3n^2+4n-1$ respectively.

2. Main results

In this section, we compute domination number, total domination and connected domination for G_n.

Theorem 2.1. *Let G_n be a Hexagonal chain with dimension n.*
Then we have:

$$\gamma(G_n) = n + \lfloor \frac{n}{6} \rfloor + 1,$$

$$\gamma_i(G_n) = n + \lfloor \frac{n}{6} \rfloor + 1.$$

Proof. From Figure 4, we can see that G_n has exactly n cycles, C_1, C_2, $C_3, ..., C_n$. Let D be any minimum dominating set of G_n. For computing $\gamma(G_n)$, it is enough to calculate $|D|$. To do this, we must choose $u, v \in D$ in first row, by Figure 4, and consider two cases for other vertices $w \in D$.

Case 1. If k is odd then for $3k-2 \leq i \leq 3k+1$, we have vertices $w \in D$ that be common vertex between C_i and C_{i+1} in second row.

Case 2. If k is even then we choose one vertex from cycles C_{3k-1} ,C_{3k} and C_{3k+1}.

Now, we consider above cases and compute measure of dominating set D:

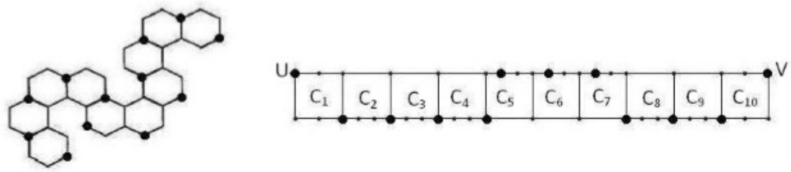

Figure 4: Dominating set of G_{10}.

1. If $n = 6k$, then we need to choose $\frac{2n}{3}$ common vertices (Case 1) and $\lfloor\frac{n}{6}\rfloor + \frac{n}{3} - 1$ internal vertices (Case 2) and so we have:

$$|D| = 2 + \frac{2n}{3} + (\lfloor\frac{n}{6}\rfloor + \frac{n}{3} - 1) = n + \lfloor\frac{n}{6}\rfloor + 1.$$

2. If $n = 6k+1, k \geq 1$, then number of vertices that dominated G_n:

$$|D| = 2 + \frac{2(n-1)}{3} + (\lfloor\frac{n}{6}\rfloor + \frac{n-1}{3}) = n + \lfloor\frac{n}{6}\rfloor + 1.$$

3. If $n = 6k+2, k \geq 1$, then we can compute domination number as follow:

$$|D| = 2 + (\frac{2(n-2)}{3} + 1) + (\lfloor\frac{n}{6}\rfloor + \frac{n-2}{3}) = n + \lfloor\frac{n}{6}\rfloor + 1.$$

4. If $n = 6k+3, k \geq 1$, then we have :

$$|D| = 2 + (\frac{2(n-3)}{3} + 2) + (\lfloor\frac{n}{6}\rfloor + \frac{n-3}{3}) = n + \lfloor\frac{n}{6}\rfloor + 1.$$

5. If $n = 6k+4, k \geq 1$, then number of vertices that dominated G_n:

$$|D| = 2 + (\frac{2(n-4)}{3} + 3) + (\lfloor\frac{n}{6}\rfloor + \frac{n-4}{3}) = n + \lfloor\frac{n}{6}\rfloor + 1.$$

6. If $n = 6k+5, k \geq 1$, then we have:

$$|D| = 2 + (\frac{2(n-5)}{3} + 4) + (\lfloor\frac{n}{6}\rfloor + \frac{n-5}{3}) = n + \lfloor\frac{n}{6}\rfloor + 1.$$

Therefore domination number G_n for any n is given by:

$$\gamma(G_n) = n + \lfloor\frac{n}{6}\rfloor + 1.$$

We consider $\langle D\rangle$, that D is dominating set of G_n, it is easy to see the subgraph generated by D is an empty graph. So, by considering the fact that $\gamma(G_n) \leq \gamma_i(G_n)$, we have

$$\gamma_i(G_n) = n + \lfloor\frac{n}{6}\rfloor + 1.$$

The proof is completed. □

Lemma 2.2. *Let G_n be a Hexagonal chain with dimension n. Then we have:*

$$\gamma_t(G_n) = 2n + 2,$$

$$\gamma_c(G_n) = 2n + 2.$$

Proof. Let G be the graph Figure 4, it is easy to see that G is isomorphism to the hexagonal chain, so $\gamma(G) = \gamma(G_n)$. It is sufficient to show that $\gamma_t(G_n) = \gamma_c(G_n) = 2n + 2$.

We can separate G_n to $n - 1$ paths with length four and note that Lemma 1.2, we have $\gamma_t(P_4) = 2$.

Therefore we can compute $\gamma_t(G_n)$. $\gamma_t(G_n) = 4 + 2(n - 1) = 2n + 2$.

Obviously, for connected domination of G_n we have $\gamma_c(G_n) \geq \gamma_t(G_n)$. So this set

$$D = \{(1, 2), (1, 3), ..., (1, n + 2), (2, 2), (2, 3), (2, 6), ..., (2, 3(n - 1)), (2, 2n + 2)\}$$

is a connected domination. In one side $|D| = \gamma_t(G_n)$ and so $\gamma_c(G_n) = 2n+2$. □

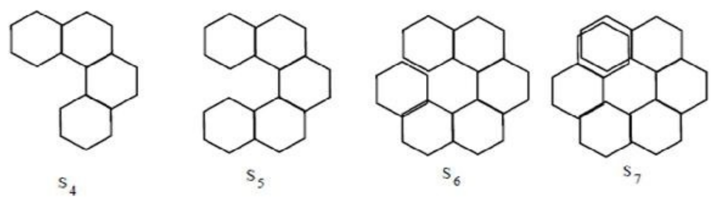

Figure 5: Spiral chain with 4,5,6, and 7 hexagons.

Theorem 2.3. *If G is a hexagonal chain with dimension n, then $b(G_n) = 1$.*

Proof. Since all the saturated vertices form a minimum dominating set of G by Theorem 2.1. Removal of an edge which is adjacent to saturated vertices, increases the domination number to $n + \lfloor \frac{n}{6} \rfloor + 2$. □

Lemma 2.4. *Let S_n be a spiral chain hexagonal with n hexagons shown in Figure 5, then $\gamma(S_n) = n + 1$.*

Proof. We consider spiral chain hexagonal, that have $4n$+2 vertices and isomorphism graph with S_n is shown in Figure 6, also we determine point of dominating set in Figure 6, the dominating set of S_n is:

$$D = \{(2, 1), (2, n + 3), (1, 3), (1, 6), ..., (1, 2n)\}.$$

So we conclude $\gamma(S_n) = n + 1$. □

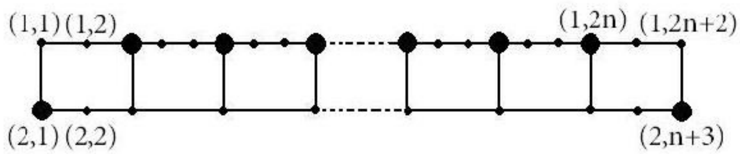

Figure 6: Dominating set of S_n

Lemma 2.5. *Let S_n be a spiral chain with dimension n, then we have:*

$$\gamma_t(S_n) = 2n + 2, \qquad \gamma_c(S_n) = 2n + 2.$$

Proof. We can use the same sketch proof of Lemma 2.3 and determine γ_t and γ_c for spiral chain hexagonal S_n. □

In [10] authors calculated domination number of $PY(n)$ as follow:

$$\gamma(PY(n)) = \begin{cases} (\frac{2n^2+4n}{4}) + 1, & \text{if } n \text{ is even} \\ \lceil \frac{2n^2+4n}{4} \rceil, & \text{if } n \text{ is odd.} \end{cases}$$

Here we compute the total domination and the connected domination number of pyrene.

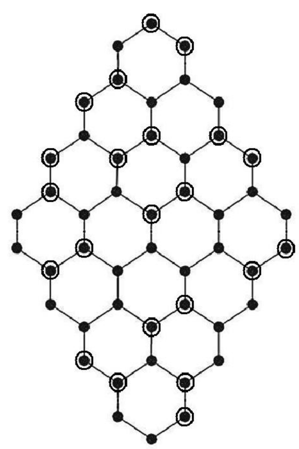

Figure 7: Total dominating set of $PY(4)$

Theorem 2.6. *Let G be a pyrene of dimension n. Then we have:*

$$\gamma_t(G) = n(n + 1) + 2, \quad \gamma_c(G) = n(n + 3) + 2.$$

Proof. It is easy to see that $\gamma(G) \leq \gamma_t(G) \leq 2\gamma(G)$, therefore we have: $\frac{1}{2}n^2 + n \leq \gamma_t(G) \leq n^2 + 2n$ also in Figure 7 is shown vertices of total dominating set, so that $\gamma_t(G) = n^2 + n + 2$. Since any nontrivial connected dominating set is also a total dominating set, $\gamma(G) \leq \gamma_t(G) \leq \gamma_c(G)$ for any connected graph G with $\Delta(G) < n - 1$. So $\gamma_c(G) \geq n^2 + n + 2$,by the same sketch from Lemma 2.2, we can compute $\gamma_c(G)$, so we have $\gamma_c(G) = n^2 + 3n + 2$. □

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