




On Vulnerability of the Hexagonal Cactus Chains

Altıgen Kaktüs Zincirlerin Zedelenebilirliği Üzerine

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Abstract

Let $G = (V(G), E(G))$ be a simple molecular graph without directed and multiple edges and without loops. The vulnerability value of a graph shows the resistance of the network after the disruption of some centers or connection lines until a communication breakdown. The domination number and its variations are the most important vulnerability parameters for graphs. One of them is the average lower domination number. It is denoted by $\gamma_{av}(G)$, also is defined as: $\gamma_{av}(G) = \frac{1}{|V(G)|} \sum_{v \in V(G)} \gamma_v(G)$, where the *lower domination number*, denoted by $\gamma_v(G)$, is the minimum cardinality of a dominating set of the graph G that contains the vertex v (Henning 2004). In this paper, the average lower domination number of different hexagonal cactus chains are determined.

Keywords: Average lower domination number, Domination number, Graph vulnerability, Hexagonal cactus chains

Öz

$G = (V(G), E(G))$ yönlendirilmemiş, katlı ayrıt içermeyen ve bukleli basit bir moleküler çizge olsun. Bir çizgenin zedelenebilirliği bazı merkezlerin veya bunlar arasındaki ayrıtların zarar görmesinden sonra iletişim kesilene kadar geçen sürede çizgenin dayanıklılığını gösterir. Baskınlık sayısı ve bunun çeşitli tipleri, çizgeler için en önemli zedelenebilirlik parametreleridir. Bunlardan biride ortalama alt baskınlık sayısıdır. Bu parametre $\gamma_{av}(G)$ ile gösterilir, ve $\gamma_{av}(G) = \frac{1}{|V(G)|} \sum_{v \in V(G)} \gamma_v(G)$ şeklinde tanımlanır, buradaki $\gamma_v(G)$ değeri alt baskınlık değeridir ve G çizgesinin v tepesini içeren bir minimum elemanlı baskın kümesinin eleman sayısı olarak tanımlanır (Henning 2004). Bu çalışmada, farklı tipteki altıgen kaktüs zincirlerin ortalama alt baskınlık değerleri belirlenmiştir.

Anahtar Kelimeler: Ortalama alt baskınlık sayısı, Baskınlık sayısı, Çizge zedelenebilirliği, Altıgen kaktüs zincirler

1. Introduction

Graph theory, with its diverse applications in natural science (Chemistry, Biology) in particular is becoming an important component of the mathematics, and also it has become one of the most powerful mathematical tools in the analysis and study of the architecture of a network. The networks are important structures and appear in many different applications and settings. The study of networks has become an important area of multidisciplinary research involving computer science, mathematics, chemistry, social sciences, informatics and other theoretical and applied sciences (Frank et al. 1970, Mishkovski et al. 2011). The vulnerability value of a communication network shows the resistance of the network after the disruption of some centers or

connection lines until a communication breakdown. The vulnerability parameters are numerical parameters of a graph which are invariant under graph isomorphism. Research on the vulnerability parameters has been intensively rising recently. A vulnerability parameter is a numeric quantity from the structural graph of a molecule. The vulnerability parameters are the numerical indices based on the topology of the atoms and their bonds. Perhaps, there are more than one hundred the vulnerability parameters which enable us to characterize the physicochemical properties of most of molecules. Molecules and molecular compounds are often represented by graphs, which are identified by their vertices and edges where vertices are atom types and edges are bonds (Turacı et al. 2015). There are several types of theoretical vulnerability parameters namely as the connectivity (Frank et al. 1970), the toughness (Chvatal et al. 1973), the integrity (Barefoot et al. 1987), the domination number (Bauer et al. 1983, Haynes et al. 1998), the bondage number (Aytaç et

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al. 2011, Aytaç et al. 2013), the edge eccentric connectivity index (Turaci et al. 2015 and Aslan 2015), the residual closeness (Turaci et al. 2015). Moreover, there are many graph theoretical parameters depending upon local damage for the graphs like as the average lower independence number (Aytaç et al. 2011, Henning 2004), the average lower domination number (Aytaç 2012, Henning 2004), the average connectivity number (Beineke et al. 2002), the average lower connectivity number (Aslan 2014) and the average lower bondage number (Turaci 2016).

Let $G = (V(G), E(G))$ be a simple undirected graph of order n and size m . We begin by recalling some standard definitions that we need throughout this paper. For any vertex $v \in V(G)$, the open neighborhood of v is $N_G(v) = \{u \in V \mid uv \in E(G)\}$ and closed neighborhood of v is $N_G[v] = N_G(v) \cup \{v\}$. The degree of vertex v in G denoted by $deg_G(v)$, that is the size of its open neighborhood. The distance $d_G(u, v)$ between two vertices u and v in G is the length of a shortest path between them (Haynes et al. 1998). We shall use $\lceil x \rceil$ for the smallest integer not less than x . A set $S \subseteq V(G)$ is a dominating set if every vertex in $V(G) - S$ is adjacent to at least one vertex in S . The minimum cardinality taken over all dominating sets of G is called the domination number of G and it is denoted by $\gamma(G)$ (Haynes et al. 1998). In 2004, Henning introduced the concept of average domination and average independence (Henning 2004). The average lower domination number of a graph G , denoted by $\gamma_{av}(G)$, is defined as: $\gamma_{av}(G) = \frac{1}{|V(G)|} \sum_{v \in V(G)} \gamma_v(G)$, where the lower domination number, denoted by $\gamma_v(G)$, is the minimum cardinality of a dominating set of the graph G that contains the vertex v (Aytaç 2012 and Henning 2004). In example 1.1. readers can see finding the average lower domination number of any given graph G .

Example 1.1. Let G be a graph with 6-vertices and 7-edges as like the following graph in Figure 1. Find the average lower domination number of this graph.

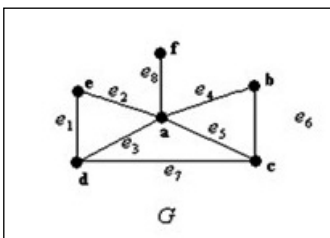


Figure 1. The graph G with 6-vertices and 7-edges.

The lower domination number of each vertex of G is as follows Table 1.

Table 1. The Lower Domination Number of Each Vertex of G

| $v \in V(G)$ | γ_v -set | $\gamma_v(G)$ |
|--------------|-----------------|---------------|
| a | {a} | 1 |
| b | {b, a} | 2 |
| c | {c, a} | 2 |
| d | {d, a} | 2 |
| e | {e, a} | 2 |
| f | {f, a} | 2 |

As a result, the average lower domination of G is $\gamma_{av}(G) = 11/6 = 1.83$, and also the domination number of G is $\gamma(G) = 1$.

If we think of a graph as modeling a network, the average lower domination number can be more sensitive for the vulnerability of graphs than the other known vulnerability measures of a graph (Aytaç 2012). We consider two connected simple graphs G and H in Figure 2, where $|V(G)| = |V(H)| = 6$ and $|E(G)| = |E(H)| = 5$. Graphs G and H have not only equal the connectivity but also equal the domination number such as $k(G) = k(H) = 1$ and $\gamma(G) = \gamma(H) = 2$. So, how can we distinguish between the graphs G and H ?

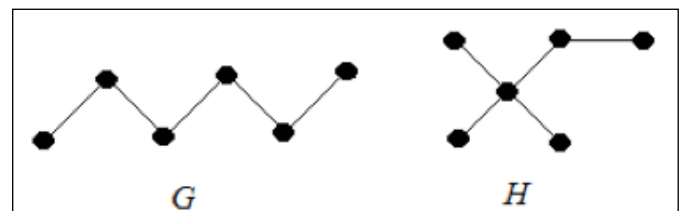


Figure 2. Graphs G and H .

When we compute the $\gamma_{av}(G)$ and $\gamma_{av}(H)$, we get $\gamma_{av}(G) = 2.66$ and $\gamma_{av}(H) = 2.5$. So, the average lower domination number may be used for distinguish between these two graphs G and H .

A cactus graph is connected graph in which no edge lies in more than one cycle. This graph was used in statistical mechanics (Uhlenbeck et al. 1956), in communication networks (Zmazek et al. 2005) and in chemistry (Zmazek et al. 2003). Hexagonal systems are considerable importance in theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbon (Qu et al. 2014).

A hexagonal cactus G is a cactus graph consisting only of cycles with 6 vertices, i.e. hexagons. If every hexagon in G has at most two cut-vertices, and every cut-vertex is shared by exactly two hexagons, we call G a hexagonal cactus chain. The number of hexagons in G is called the length of the

chain. A hexagonal cactus chain of length n , denoted by G_n , $G_n = C_1 C_2 \dots C_n$ is written. These C_i are hexagons, where $i = 1, \dots, n$. Every G_n , $n \geq 2$, has exactly two hexagons with only one cut-vertex. Such hexagons are called *terminal hexagons*. All other hexagons in a chain are called *internal hexagons* (Qu et al. 2014 and Majstorovic et al. 2012).

An internal hexagon in G_n is called an *ortho-hexagon* if its cut-vertices are adjacent, a *meta-hexagon* if the distance between its cut-vertices is 2, and a *para-hexagon* if the distance between its cut-vertices is 3. Let G_n be a hexagonal cactus chain. If all internal hexagons are ortho-hexagons in G_n , then it is called *ortho-chain*. If all internal hexagons are meta-hexagons in G_n , then it is called *meta-chain*. If all internal hexagons are para-hexagons in G_n , then it is called *para-chain*. Ortho-chain, meta-chain and para-chain are denoted by O_n , M_n and L_n , respectively (Qu et al. 2014, Majstorovic et al. 2012). In Figure 3, we display meta-chain M_4 , ortho-chain O_4 and para-chain L_4 .

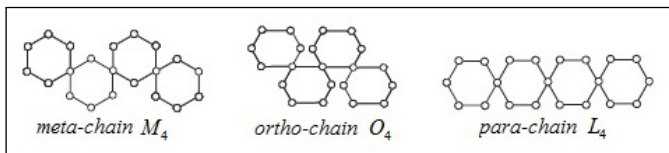


Figure 3. Meta-chain M_4 , Ortho-chain O_4 and Para-chain L_4 .

Clearly, we have

$$|V(L_4)| = |V(O_4)| = |V(M_4)| = 21 \text{ and}$$

$$|E(L_4)| = |E(O_4)| = |E(M_4)| = 24.$$

Generalization for n are as follows:

$$|V(L_n)| = |V(O_n)| = |V(M_n)| = 5n+1 \text{ and}$$

$$|E(L_n)| = |E(O_n)| = |E(M_n)| = 6n.$$

In this paper, the average lower domination number of para-chain L_n , ortho-chain O_n and meta-chain M_n are determined.

2. Basic Results

In this section well known basic results are given with regard to the domination number and the average lower domination number.

Theorem 2.1 (Haynes et al. 1998) *For a cycle graph C_n on n vertices, then $\gamma(C_n) = \lfloor \frac{n}{3} \rfloor$.*

Theorem 2.2 (Henning 2004) *For any graph G of order n with domination number γ , then $\gamma_{av}(G) \leq \gamma + 1 - \gamma/n$, with equality if and only if G has a unique γ -set.*

Theorem 2.3 (Majstorovic et al. 2012) *Let L_n be the para-chain graph of length n . Then, $\gamma(L_n) = n+1$.*

Theorem 2.4 (Majstorovic et al. 2012) *Let O_n be the ortho-chain graph of length n . Then, $\gamma(O_n) = \lfloor \frac{3n}{2} \rfloor$.*

Theorem 2.5 (Majstorovic et al. 2012) *Let M_n be the meta-chain graph of length n . Then, $\gamma(M_n) = \lfloor \frac{3n}{2} \rfloor$.*

3. The Average Lower Domination Number of Hexagonal Cactus Chains

In this section the average lower domination number of hexagonal cactus chains are calculated.

Theorem 3.1 *Let L_n be the para-chain graph of length n . Then,*

$$\gamma_{av}(L_n) = \frac{5n^2 + 10n + 1}{5n + 1}.$$

Proof. By the Theorem 2.3, we have $\gamma(L_n) = n+1$ for the *para-chain graph of length n* . This dominating set is showed the following Figure 4.

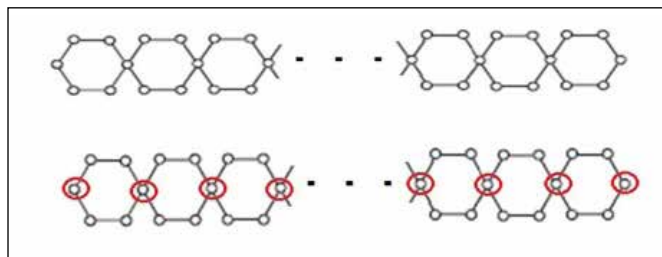


Figure 4. Para-chain L_n and dominating set of L_n .

By the definition of lower domination number of each red vertex is $\gamma_v(L_n) = n+1$. Moreover, the number of these red vertices is $n+1$. On the other hand, the lower domination number of the remaining vertices which are showed blue vertices in Figure 5 is $\gamma_v(L_n) = n+2$.

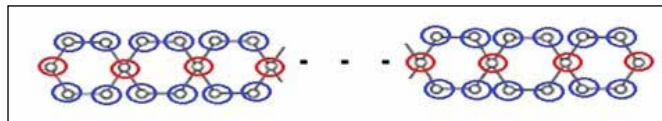


Figure 5. Para-chain L_n and characterizations of all vertices.

Clearly, the number of blue vertices is $4n$. By the definition of average lower domination number of *para-chain L_n* , this value computed as follows:

$$\begin{aligned} \gamma_{av}(L_n) &= \frac{(n+1)(n+1) + (4n)(n+2)}{5n+1} \\ &= \frac{5n^2 + 10n + 1}{5n + 1}. \end{aligned}$$

Thus, the proof is completed.

Theorem 3.2 Let M_n be the meta-chain graph of length n . Then,

$$\gamma_{av}(M_n) = \frac{33n^2 + 18n}{20n + 4}, \text{ if } n \text{ is odd};$$

$$\frac{15n^2 + 10n + 2}{10n + 2}, \text{ if } n \text{ is even}.$$

Proof. We have two cases depending on n .

Case 1. Let n be even. The dominating set of Meta-Chain graph M_n is unique (Majstorovic et al. 2012). So, we have the following result for n is even by Theorems 2.2 and 2.5.

$$\gamma_{av}(M_n) = \frac{(3n/2)(3n/2) + ((7n+2)/2)((3n+2)/2)}{5n+1}$$

$$= \frac{15n^2 + 10n + 2}{10n + 2}.$$

Case 2. Let n be odd. We have three subcases depending on the choosing the dominating set. The vertices of dominating set of Meta-Chain graph M_n are as follows:

Subcase 2.1. In this subcase red vertices must be taken the minimum dominating set of M_n , and also any two pink vertices should be taken it. These vertices are shown in Figure 6.

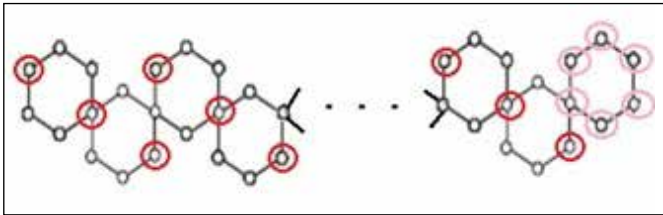


Figure 6. Para-chain M_n and characterizations of all vertices.

Subcase 2.2. This subcase is similar to the subcase 2.1. We show that these vertices which are in this subcase in Figure 7. They are showed with blue vertices and pink vertices.

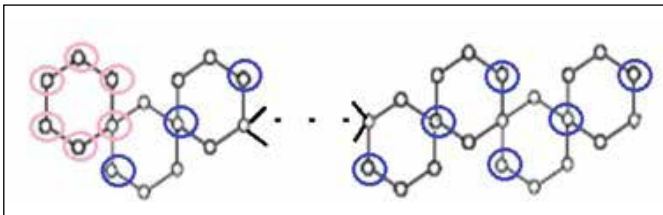


Figure 7. Para-chain M_n and characterizations of all vertices.

Subcase 2.3. The vertices which are be in this subcase is showed by yellow vertices in Figure 8.

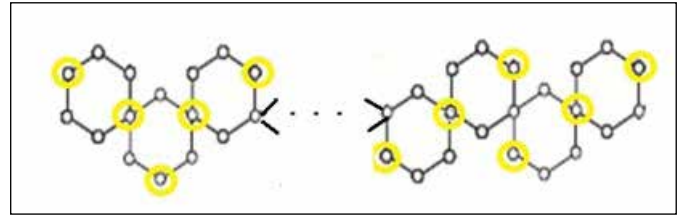


Figure 8. Para-chain M_n and characterizations of all vertices.

By Cases 1, 2 and 3, we have the following Figure 9.

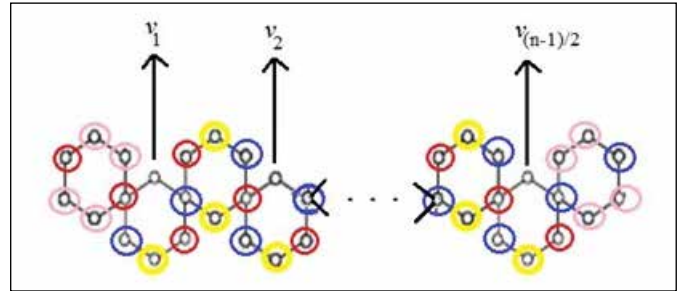


Figure 9. Para-chain M_n and characterizations of all vertices.

It is clear that the lower domination number is $(3n+1)/2$ for red, blue, yellow and pink vertices. The number of these vertices is $(9n+3)/2$. Furthermore, the lower domination number is $(3n+3)/2$ for each vertex v_k , where $k = \{1, 2, \dots, (n-1)/2\}$. The number of these vertices is $(n-1)/2$. Thus, we get

$$\gamma_{av}(M_n) = \frac{((3n+1)/2)((9n+3)/2) + ((3n+3)/2)((n-1)/2)}{5n+1}$$

$$= \frac{33n^2 + 18n}{20n + 4}.$$

Thus, the proof is completed.

Theorem 3.3 Let O_n be the ortho-chain graph of length n . Then,

$$\gamma_{av}(O_n) = \frac{15n^2 + 10n - 1}{10n + 2}, \text{ if } n \text{ is odd};$$

$$\frac{15n^2 + 10n + 2}{10n + 2}, \text{ if } n \text{ is even}.$$

Proof. We have two cases depending on n .

Case 1. Let n be even. The dominating set of O_n is unique by the Theorem 2.4. Thus, the average lower domination number of O_n can be computed as follows:

$$\gamma_{av}(O_n) = \frac{(3n/2)(3n/2) + ((7n+2)/2)((3n+2)/2)}{5n+1}$$

$$= \frac{15n^2 + 10n + 2}{10n + 2}.$$

Case 2. Let n be odd. We have three subcases depending on the choosing the dominating set. Readers can find these dominating set as like the Theorem 3.2. After the choosing the necessary vertices, we get the lower dower domination

number is $(3n+1)/2$. Furthermore, the number of these vertices is $(4n+2)$. Clearly, the lower domination is $(3n+3)/2$ for the remaining $(n-1)$ -vertices.

Thus we have,

$$\begin{aligned}\gamma_{av}(O_n) &= \frac{((3n+1)/2)(4n+2) + ((3n+3)/2)(n-1)}{5n+1} \\ &= \frac{15n^2 + 10n - 1}{10n + 2}.\end{aligned}$$

Thus, the proof is completed.

4. Conclusion

A topological representation of a molecule can be carried out molecular graph. There are several vulnerability parameters which are graph stable number calculated from a molecule that is represented by a graph. Since the hexagonal systems are the natural graph representation of benzenoid hydrocarbon, they are importance in chemistry science. In this paper we have calculated the values of the average lower domination number of hexagonal cactus chains namely para-chain L_n , ortho-chain O_n and meta-chain M_n . It is clear that the average lower domination number of Meta-Chains M_n and Ortho-Chains O_n are not equal when n is odd. It can be seen that the average lower domination number is more sensitive than the domination number for Meta-Chains M_n and Ortho-Chains O_n when n is odd.

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