DOMINATION ON CACTUS CHAINS OF PENTAGONS

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Abstract

Introduction/purpose: A graph as a mathematical object occupies a special place in science. Graph theory is increasingly used in many spheres of business and scientific fields. This paper analyzes pentagonal cactus chains, a special type of graphs composed of pentagonal cycles in which two adjacent cycles have only one node in common. The aim of the research is to determine the dominant set and the dominance number on ortho and meta pentagonal cactus chains.

Methods: When the corresponding destinations are treated as graph nodes and the connections between them as branches in the graph, the complete structure of the graph is obtained, to which the laws of graph theory are applied. The vertices of the pentagon are treated as nodes of the graph and the sides as branches in the graph. By applying mathematical methods, the dominance was determined on one pentagon, then on two pentagons with a common node, and then on ortho and meta pentagonal cactus chains.

Results: The research has shown that the dominance number on the ortho chain O_h of the length h ≥ 2 is equal to the value of the expression $\left\lceil \frac{3h}{2} \right\rceil$ while on the meta chain M_h it is equal to the value of the expression h+1, which was proven in this paper.

Conclusion: The results show that the dominant sets and the dominance numbers on ortho and meta pentagonal cactus chains are determined and explicitly expressed by mathematical expressions. They also point to the possibility of their application in the fields of science as well as in the spheres of business in which these structures appear.

Keywords: graph, pentagonal cactus-chain, dominant set, dominance number.

Introduction

Mathematical apparatus and mathematical methods are used in almost all fields of science, both natural (Ghergu & Radulescu, 2011; Veličković et al, 2020) and social (Vladimirovich & Vasilyevich-Chernyaev, 2021). A graph as a mathematical object occupies a special place in science (Bakhshesh, 2022; Hajian & Rad, 2021; Hernández Mira et al, 2021). It is used in medicine, genetics, chemistry, etc. All structural formulas of covalently bound compounds are graphs. Chemical elements are represented by graphs where atoms are vertices and chemical bonds are lines in the graph (Balaban, 1985). A graphical representation of chemical structures provides a visual insight into molecular bonds and chemical properties of molecules. The QSPR study has shown that many of chemical properties of molecules are closely related to theoretical graphical invariants called molecular descriptors (Mihalić & Trinajstić, 1992). The theoretical graphical invariant is also the dominance number, which is the simplest variant of the k-dominance number that is used many times in mathematics (Zmazek & Žerovnik, 2003).

A graph is usually denoted by *G*, a set of its vertices (nodes) by *V(G)* and a set of its branches (lines) by *E(G).*

A set *D* that is a subset of the set *V(G)* is called a *k*-dominant set in the graph *G* if for each vertex outside the set *D* there is at least one vertex in the set *D* such that the distance between them is less than or equal to *k*. The number of elements of the smallest *k*-dominant set is called the *k*-dominance number and is denoted by γ_k. If *k* = 1, the 1-dominance number is called the dominance number and is denoted by γ and the 1-dominant set is called the dominant set.

A cactus graph is a connected graph in which no line (branch) is in more than one cycle. The study of cactus graphs began in the middle of the 20th century. In his work (Husimi, 1950) Husimi uses these graphs in studies of cluster integrals. Riddell (Riddell, 1951) uses them in the theory of condensation. They were later used in the theory of electrical and communication networks (Zmazek & Zerovnik, 2005) as well as in chemistry (Sharma et al, 1997; Gupta et al, 2001; Gupta et al, 2002).

It is known that many chemical compounds have a pentagonal shape in their configuration. Among them are cycloalkanes, which are very common compounds in the nature. The five-membered and six-membered cycloalkanes, cyclopentane (Figure 1) and cyclohexane, which contain 5 and 6 ring carbon atoms, respectively, are very stable and their structures appear in many biological molecules.

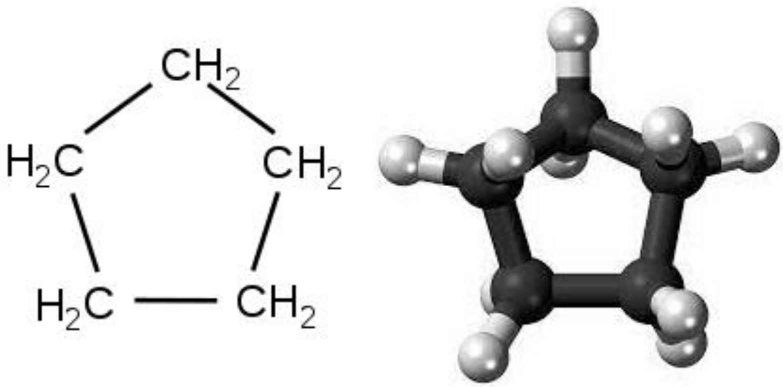


Figure 1– Cyclopentane
Рис. 1 – Циклопентан
Слика 1 – Циклопентан

Their ring structures are also included in the composition of steroids. A large number of steroids are synthesized in laboratories and used in the treatment of cancer, arthritis, various allergies and other diseases (Balaban & Zeljković, 2021). Pentagonal forms in combination with hexagonal forms are present in many compounds, among which are heterocyclic compounds: morphine, benzofuran, dibenzothiophene and others.

In this paper, we analyze the k-dominance of pentagonal cactus chains. Hexagonal cactus chains were investigated in papers (Farrell, 1987; Vukičević & Klobučar, 2007). Afterwards, the papers (Majstorovic et al, 2012; Klobučar & Klobučar, 2019) determined the dominance number on a uniform hexagonal cactus chain, the dominance number on an arbitrary hexagonal network, and the total and double total dominance number on a hexagonal network. The K-dominance on rhomboidal cactus chains (Carević et al, 2020) as well as on the icosahedral-hexagonal network (Carević, 2021) was also investigated.

Pentagonal cactus-chains

The pentagonal cactus-chain *G* is a graph consisting of a cycle with 5 vertices. A vertex that is common to two or three pentagons is called a cut-vertex. If each pentagon in the graph *G* has at most 2 cut-vertices and each cut-vertex is divided between exactly 2 pentagons, the graph *G* is called a pentagonal cactus-chain.

With G_h we will denote a pentagonal cactus-chain of the length h and G_h= $P^1P^2 \dots P^h$ where P^i are successive pentagons in the chain (Figure 2).

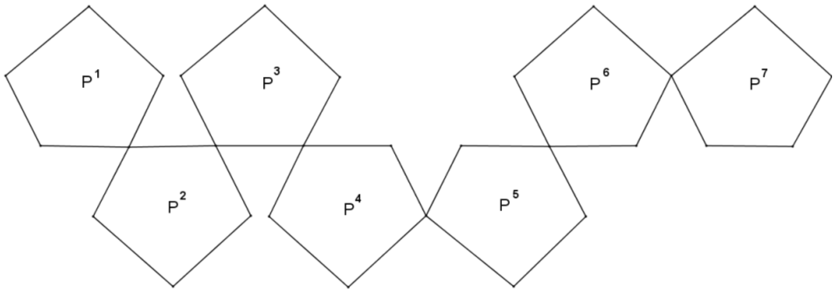


Figure 2 – Pentagonal cactus-chain of the length 7
Рис. 2 – Пятиугольная кактус-цепочка длиной 7
Слика 2 – Петоугаони кактус-ланац дужине 7

Denote by *x* and *y* the vertices in the graph *G* and by *d(x, y)* the distance between them, where the distance between two vertices is equal to the number of branches located from one vertex to another. Denote by p_i the minimum distance between the pentagons P^i and P^{i+2}:

p_i = *min*$\{d(x,y): x\epsilon P^i \wedge y\epsilon P^{i+2}, i = 1, 2, \ldots, h-2\}$

Then p_i is the distance between the pentagons P^i and P^{i+2}.

With the exception of the first and last pentagons in the cactus chain, which have one cut-vertex, all other pentagons have two cut-vertices, and they are called inner pentagons.

In the pentagonal cactus chain G_h, we distinguish between ortho and meta inner pentagons. An inner pentagon is called an ortho pentagon if its cut-vertices are adjacent, and a meta pentagon if the distance between its cut-vertices is d = 2.

A pentagonal cactus chain is uniform if all its inner pentagons are of the same type. A chain G_h is called an ortho-chain, and is denoted by O_h if all its inner pentagons are ortho-pentagons (Figure 3).

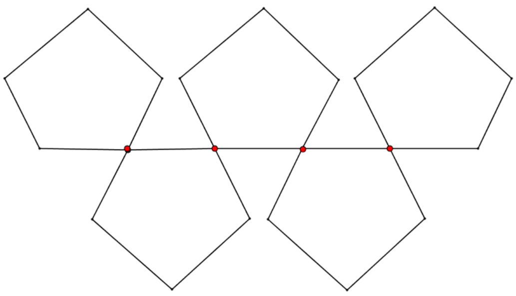


Figure 3 – Ortho cactus-chain O_5
Рис. 3 – Орто-кактус-цепочка O_5
Слика 3 – Орто кактус-ланац O_5

Analogously, a chain G_h is called a meta-chain, and is denoted by M_h if all its inner pentagons are meta-pentagons (Figure 4).

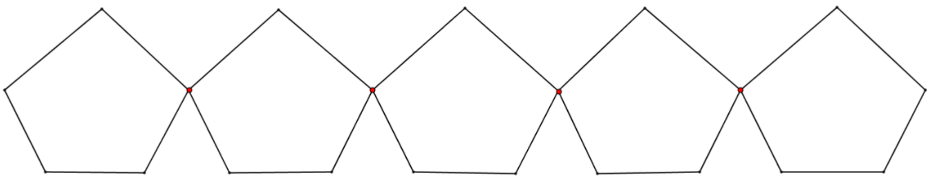


Figure 4 – Meta cactus-chain M_5
Рис. 4 – Мета кактус-цепочка M_5
Слика 4 – Мета кактус-ланац M_5

To determine the dominant set on the uniform pentagonal cactus chains O_h and M_h, it will be necessary to point out certain vertices in the cactus chain. That is why it is necessary to mark them. In the ortho pentagon P^i the cut-vertices are adjacent and we will denote them by V_i and V_{i+1}. The other vertices in P^i it will be denoted by x_1^i, x_2^iandx_3^i (Figure 5):

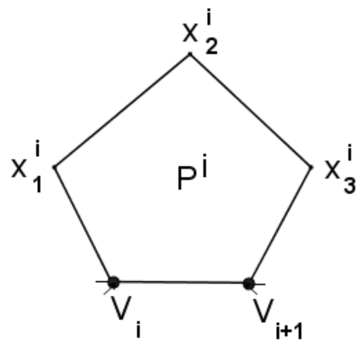


Figure 5 – Marking vertices in the ortho pentagon
Рис. 5 – Обозначение вершин в ортогональном пятиугольнике
Слика 5 – Означавање чворова у орто петоуглу

In the meta pentagon P^i the cut-vertices are at a distance d = 2 and we will denote them by V_{2i-1} and V_{2i+1}. With V_{2i}we will denote the vertex to which it applies *d(*V_{2i-1}, V_{2i}*)* = *d(*V_{2i}, V_{2i+1}*)* = 1. The other two nodes in the pentagon P^i will be denoted x_1^iandx_2^i (Figure 6):

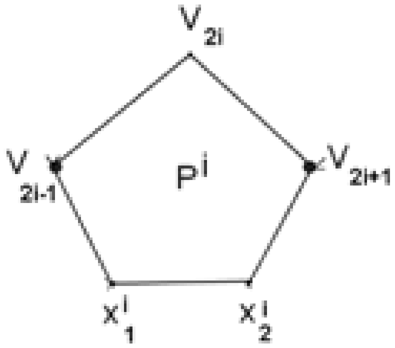


Figure 6 – Marking vertices in the meta pentagon
Рис. 6 – Обозначение вершин в мета-пятиугольнике
Слика 6 – Означавање чворова у мета петоуглу

Research results

In this section, we consider 1-dominance on ortho and meta pentagonal cactus chains. We will first consider the dominance of one pentagon and two adjacent pentagons in the ortho and meta chain of cacti.

Lemma 3.1. The dominance number for the pentagon is γ = 2.

Proof: Let us denote the vertices of the pentagon by x_1, x_2, x_3, x_4, x_5 (Figure 7):

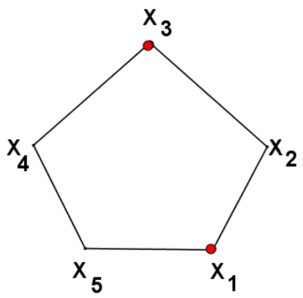


Figure 7 – Dominant set on a pentagon
Рис. 7 – Доминирующее множество на пятиугольнике
Слика 7 – Доминантни скуп на петоуглу

One pentagon vertex dominates two adjacent vertices. Let us take the vertex x_1. It dominates the vertices x_2 and x_5. As the pentagon has 5 vertices, domination over the other two vertices x_3 and x_4 is necessary. We conclude that one of the remaining two vertices must belong to the dominant set on the pentagon. Let it be the vertex x_3. Thus, the set *D* = $\{x_1, x_3\}$ is the dominant set for a given pentagon but it is not the only dominant set whose cardinality is equal to 2. They are also sets that contain any two non-adjacent pentagon vertices. Let us prove that any of the mentioned two-membered sets is the minimum dominant set on the pentagon. Assuming that there is a dominant set of less cardinality *D'*, it would have to contain only one vertex and one vertex cannot dominate the remaining 4 vertices of the pentagon. Thus, the minimum dominant set on a pentagon is a two-membered set, so the dominance number for the pentagon is γ = 2.

Lemma 3.2. The dominance number for two pentagons with one cut-vertex is γ = 3.

Proof: Let us denote the vertices of two pentagons by one common vertex with x_1, x_2, . . . , x_9 (Figure 8):

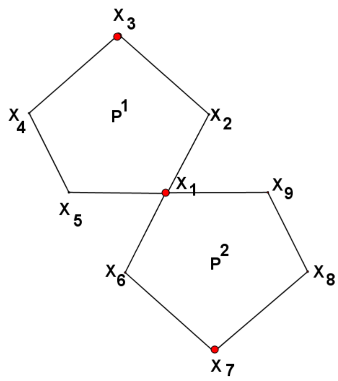


Figure 8 – Dominant set for two pentagons with a cut-vertex
Рис. 8 – Доминирующее множество для двух пятиугольников с пересекающейся вершиной
Слика 8 – Доминантни скуп за два петоугла са пресеченим чвором

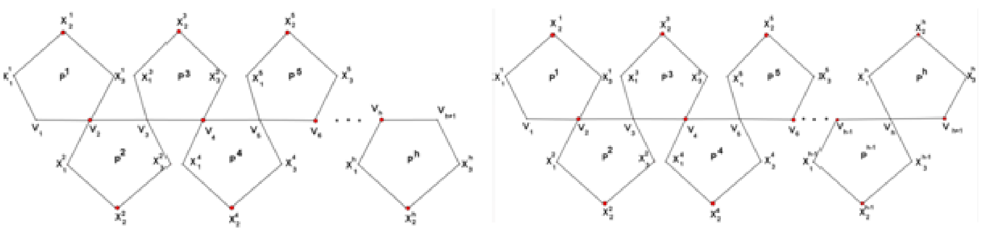
Let x_1 be the cut-vertex of the given pentagons P^1 and P^2.Based on Lemma 3.1. the pentagon P^1 excluding the vertex x_1 must have another dominant vertex that is not adjacent to the vertex x_1.Let it be the vertex x_3. Also by applying Lemma 3.1. the pentagon P^2 excluding the vertex x_1 must have another dominant vertex that is not adjacent to the vertex x_1. Let it be the vertex x_7. Thus the nodes x_1, x_3 and x_7 dominate over the nodes x_2, x_4, x_5, x_6, x_8 andx_9 so the dominant set for the pentagons P^1P^2 is the set D = $\{x_1, x_3, x_7\}$. Analogous to the consideration in Lemma 3.1. the set D is not the only three-membered set that is dominant on P^1P^2but there is no dominant set of less cardinality. Suppose that there is a dominant set D' whose cardinality is equal to 2. Let D' contain one vertex from each pentagon, for example D' = {x_1,x_3}.The vertices x_1 and x_3 would then dominate over the remaining 7 vertices in P^1P^2 and this is impossible.The vertex x_1 as a common vertex for both pentagons dominates over two neighboring vertices in both pentagons, so it dominates over 4 vertices in P^1P^2.The vertex x_3, or any other vertex not adjacent to the vertex x_1 dominates two adjacent vertices.So, the total sum of vertices covered by dominance is 4 + 2 = 6 and that is less than 7.Thus, 2 vertices cannot dominate the remaining 7 vertices in P^1P^2. We conclude that the minimum dominant set for P^1P^2 is a three-membered set and γ = 3.

Let us consider the dominance on pentagonal ortho and meta cactus chains of arbitrary length.

Theorem 3.1. $\gamma(O_h)$ = $\left\lceil\frac{3h}{2}\right\rceil$ for each *h*≥ 2 ∧*h* **ϵ** *N*.

Proof: We observe a pentagonal ortho cactus-chain O_h = P^1P^2... P^h(Figure 9) and a set:

D_{O_h} = { x_2^i, *i* = 1, *h*} ∪ { V_{2i}, *i* = 1, $\left\lfloor\frac{h}{2}\right\rfloor$}



$9_A 9_B$

Figure 9 – Minimum dominant set for O_h
Рис. 9 – Минимально доминирующее множество для O_h
Слика 9 – Минимални доминантни скуп за O_h

Let us prove that D_{O_h} is the dominant set of minimum cardinality for a pentagonal ortho cactus-chain O_h= P^1P^2… P^h.

Let us divide the ortho-chain O_h into subchains $P^{2i-1}P^{2i}$, *i* = 1, 2, ... , $\left\lfloor\frac{h}{2}\right\rfloor$ (Figure 10) and the last pentagon P^h if h is an odd number.

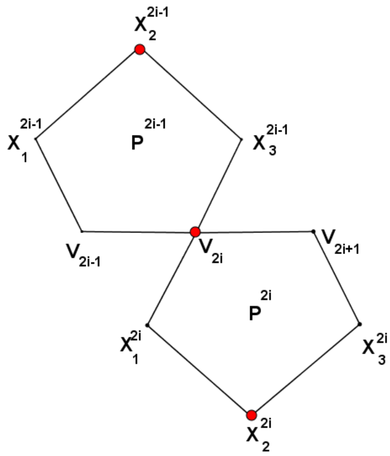


Figure 10 – Subchain of the ortho-chain O_h
Рис. 10 – Подцепочка орто-цепочки O_h
Слика 10 – Подланац орто ланца O_h

Based on Lemma 3.2. the set $A_i = \{x_2^{2i-1}, x_2^{2i}, V_{2i}\}$ for *i = 1, 2, ... ,* $\left\lfloor\frac{h}{2}\right\rfloor$ is the dominant set of minimum cardinality for the subchain $P^{2i-1}P^{2i}$. An ortho-chain of the length *h* for *h = 2k, k ϵ N* is composed of $\frac{h}{2}$ subchains $P^{2i-1}P^{2i}$, *i = 1, 2, ... ,* $\frac{h}{2}$ (Figure 9_{A}), so the set

$$D_1 = \bigcup_{i=1}^{k} A_i, \quad \text{for } k = \frac{h}{2}$$

is a dominant set for the ortho-chain O_h. Therefore, it is

$$\gamma(O_h) \leq card(D_1) = \frac{h}{2} \cdot 3 = \frac{3h}{2}$$

where we have marked the cardinality of the set D_1 with $card(D_1)$.
If *h* is an odd number (Figure 9_{B}), then the set

$$D_2 = \bigcup_{i=1}^{k} A_i \cup \{x_2^h, V_{h+1}\}, \text{ for } k = \left\lfloor\frac{h}{2}\right\rfloor$$

is a dominant set for the ortho-chain O_h and then is

$$\gamma(\mathrm{O_h}) \leq card(D_2) = \left\lfloor\frac{h}{2}\right\rfloor \cdot 3 + 2 = \left\lceil\frac{3h}{2}\right\rceil.$$

Note that the set D_1 for $k = \frac{h}{2}$ if *h* an even number is equal to the following expression:

$$D_1 = \bigcup_{i=1}^{k} A_i = \bigcup_{i=1}^{k} \{x_2^{2i-1}, x_2^{2i}, V_{2i}\} =$$
$$= \{x_2^1, x_2^2, V_2\} \cup \{x_2^3, x_2^4, V_4\} \cup \ldots \cup \{x_2^{h-1}, x_2^h, V_h\} =$$
$$= \{x_2^i,\ i = 1, 2, \ldots, h\} \cup \{V_{2i}, i = 1, 2, \ldots, \frac{h}{2}\}$$

Also for $k = \lfloor \frac{h}{2} \rfloor$ and h is an odd number, the set D_2 is equal to the following expression:

$D_2 = \bigcup_{i=1}^{k} A_i \cup \{x_2^h, V_{h+1}\} =$
$= \bigcup_{i=1}^{k} \{ x_2^{2i-1}, x_2^{2i}, V_{2i}\} \cup \{x_2^h, V_{h+1}\} =$
$= \{ x_2^1, x_2^2, V_2\} \cup \{ x_2^3, x_2^4, V_4\} \cup \ldots \cup \{ x_2^{h-1}, x_2^h, V_h\} \cup \{x_2^h, V_{h+1}\} =$
$= \{ x_2^i,\ i = 1, 2, \ldots, h\} \cup \{V_{2i}, i = 1, 2, \ldots, \lceil \frac{h}{2} \rceil\}$

In case h is an even number, $\frac{h}{2} = \lceil \frac{h}{2} \rceil$ then we conclude that it is $D_1 = D_2$.

So, the set $D_{O_h} = \{ x_2^i,\ i = 1, h\} \cup \{ V_{2i},\ i = 1, \lceil \frac{h}{2} \rceil\}$ is the dominant set for the ortho-chain O_h when h is even or odd number.

Also, in the case where h is an even number, $\frac{3h}{2} = \lceil \frac{3h}{2} \rceil$. So, $\gamma(\mathrm{O_h}) \leq \lceil \frac{3h}{2} \rceil$ when h is even or odd number. Prove that the set D_{O_h} is the dominant set of minimal cardinality. Each subchain $P^{2i-1}P^{2i}$ contains 3 dominant nodes based on Lemma 3.2. Based on this, we conclude that each dominant set on the chain O_h contains more than 3 or exactly 3 dominant nodes in each subchain $P^{2i-1}P^{2i}$ and more than 2 or exactly 2 dominant nodes in the last pentagon if h is an odd number, based on Lemma 3.1. So, we conclude that it is $\gamma(\mathrm{O_h}) \geq \frac{h}{2} \cdot 3$ in case h is an even number, and $\gamma(\mathrm{O_h}) \geq \frac{h}{2} \cdot 3 + 2$ in case h is an odd number. When we combine both cases, we get that $\gamma(\mathrm{O_h}) \geq \lceil \frac{3h}{2} \rceil$.

It follows from $\gamma(O_h) \leq \lceil \frac{3h}{2} \rceil$ and $\gamma(O_h) \geq \lceil \frac{3h}{2} \rceil$ that it is $\gamma(O_h) = \lceil \frac{3h}{2} \rceil$.

Corollary 3.1. $D_{O_h} \subset D_{O_{h+1}}$ for each $h \geq 2 \wedge h \in N$.

Theorem 3.2. $\gamma(M_h) = h + 1$ for each $h \geq 2 \wedge h \in N$.

Proof: We observe a pentagonal meta cactus-chain $M_h = P^1 P^2 \ldots P^h$ (Figure 11) and set:

$D_{M_h} = \{ V_{2i-1},\ i = 1, h + 1\}$

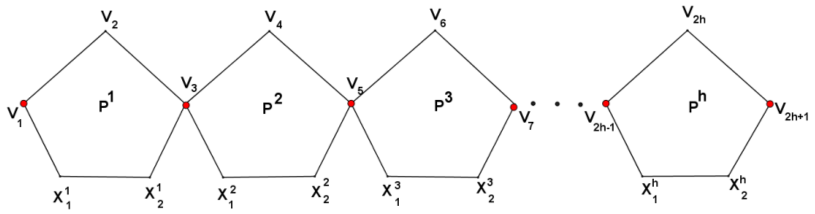


Figure 11 – Minimum dominant set for M_h
Рис. 11 – Минимально доминирующее множество для M_h
Слика 11 – Минимални доминантни скуп за M_h

Let us prove that D_{M_h} is the dominant set of minimum cardinality for a pentagonal meta cactus-chain $M_h= P^1P^2... P^h$. Based on Lemma 3.1. each pentagon has a dominant set made up of two non-adjacent vertices. Thus, the set $\{ V_{2i-1}, V_{2i+1}\}$ is dominant for the pentagon P^i for each i = 1, h. By merging the dominant sets of all pentagons in the chain, we get a set that is dominant for the whole chain. But, each pentagon P^i has a common vertex with the pentagon P^{i+1} for each i = 1, h – 1. Common vertices should not be repeated in the dominant set. So, the set

$$D_{M_h} = \bigcup_{i=1}^{h}\{ V_{2i-1}, V_{2i+1}\} \setminus \bigcup_{i=1}^{h-1}\{ V_{2i+1}\}$$

is the dominant set for the meta-chain M_h.

Note that it is

$$\bigcup_{i=1}^{h}\{ V_{2i-1}, V_{2i+1}\} \setminus \bigcup_{i=1}^{h-1}\{ V_{2i+1}\} =$$
$$\{\{V_1,V_3\} \cup \{V_3,V_5\} \cup \{V_5,V_7\} \cup ... \cup \{V_{2h-1},V_{2h+1}\}\} \setminus \{V_3,V_5,V_7,...,V_{2h-1}\} =$$
$$\{V_1,V_3,V_5,...,V_{2h-1},V_{2h+1}\} = \{ V_{2i-1},\ i = 1, h + 1\}$$

Thus, the set $D_{M_h}= \{ V_{2i-1},\ i = 1, h + 1\}$ is the dominant set for the meta-chain M_h for each h$\in$N and h ≥2. Let us prove that D_{M_h} is the dominant set of minimal cardinality. Suppose that there is a set S of less cardinality that is dominant on the meta-chain M_h. The set S would then have one node less than the set D_{M_h}. Let it be a vertex V_{2i+1} for any i = 1, h. Then the pentagon P^i would have only one dominant node V_{2i-1}. Based on Lemma 3.1. that is not possible. We conclude that D_{M_h} is the minimum dominant set for M_h so it is $\gamma(M_h) = h + 1$.

Corollary 3.2. $D_{M_h} \subset D_{M_{h+1}}$ for each $h \geq 2 \wedge h \in N$.

Conclusion

In this paper, we have shown the arrangement of vertices in dominant sets on uniform ortho and meta pentagonal cactus chains that appear in molecule structures of numerous compounds. We also proved that the dominance number for a pentagonal ortho-chain of the length h is equal to the value of the expression $\left\lceil\frac{3h}{2}\right\rceil$ while for a pentagonal meta-chain it is equal to h + 1.

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ДОМИНИРОВАНИЕ НА ПЯТИУГОЛЬНЫХ КАКТУС-ЦЕПЯХ

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РУБРИКА ГРНТИ: 27.45.17 Теория графов,
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ВИД СТАТЬИ: оригинальная научная статья

Резюме:

Введение/цель: Граф как математический объект занимает особое место в науке. Теория графов все чаще используется во многих видах деятельности и различных научных областях. В данной статье анализируются пятиугольные кактус-цепочки, как особый вид графов, состоящих из пятиугольных циклов, в которых два соседних цикла имеют только один общий узел. Цель исследования заключалась в определении доминирующего множества и доминируещего числа в орто- и мета-пятиугольных куктус-цепочках.

Методы: Когда соответствующие положения рассматриваются как узлы графа, а связи между ними − как ветви графа, получается полная структура графа, к которой применяются законы теории графов. Вершины пятиугольника рассматриваются как узлы графа, а стороны − как ветви графа. С помощью математических методов, было определено доминирование на одном пятиугольнике, затем на двух пятиугольниках с общим узлом, а затем на орто- и мета-пятиугольных кактус-цепочек.

Результаты: Исследование показало, что число доминирования на орто-цепи O_h *с длиной* $h \geq 2$ *равно значению выражения* $\left\lceil \frac{3h}{2} \right\rceil$*, в то время как на мета-цепи* M_h *оно равно значению выражения h+1, что и следовалось доказать в данной статье.*

Выводы: Результаты исследования показали, что доминирующие множества и числа доминирования в орто- и мета-пятиугольных кактус-цепочках определяются и эксплицитно исчисляются математическими выражениями. Они также указывают на возможность их применения как в области науки, так и в сферах бизнеса, в которых присутствуют эти структуры.

Ключевые слова: граф, пятиугольная кактус-цепочка, доминирующее множество, число доминирования.

ДОМИНАЦИЈА НА ПЕТОУГАОНИМ КАКТУС-ЛАНЦИМА

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ВРСТА ЧЛАНКА: оригинални научни рад

Сажетак:

Увод/циљ: Граф као математички објекат заузима посебно место у науци. Теорија графова налази све већу примену у многобројним *сферама пословања, као и научним областима. У овом раду анализирани су петоугаони кактус-ланци који представљају посебну врсту графа састављеног од петоугаоних циклуса у којима два суседна циклуса имају заједнички само један чвор. Циљ истраживања јесте одређивање доминантног скупа и доминацијског броја на орто и мета петоугаоним кактус-ланцима.*

Методе: Када се одговарајућа одредишта третирају као чворови графа, а везе међу њима као гране у графу, добија се потпуна структура графа на коју се примењују законитости теорије графова. Темена петоугла су третирана као чворови графа, а странице као гране у графу. Применом математичких метода одређена је доминација на једном петоуглу, затим на два петоугла са заједничким чвором, а након тога на орто и мета петоугаоним кактус-ланцима.

Резултати: Истраживања су показала да је доминацијски број на орто ланцу O_h *дужине* $h \geq 2$ *једнак вредности израза* $\left\lceil \frac{3h}{2} \right\rceil$, *док је на мета ланцу* M_h *једнак вредности израза* $h + 1$, *што је доказано у раду.*

Закључак: Резултати показују да су доминантни скупови и доминацијски бројеви на орто и мета петоугаоним кактус-ланцима одређени и експлицитно исказани математичким изразима. Такође, упућују на могућност њихове примене у областима науке, као и у сферама пословања у којима се појављују ове структуре.

Кључне речи: граф, петоугаони кактус-ланац, доминантни скуп, доминацијски број.

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