

Dominance number on cyclooctane chains

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DOI: <https://doi.org/10.5937/vojtehg72-48272>

FIELD: materials and chemical technologies, mathematics
ARTICLE TYPE: original scientific paper

Abstract:

Introduction/purpose: Chemical structures are conveniently represented by graphs where atoms are nodes (vertices) and chemical bonds are branches (lines) in the graph. A graphical representation of a molecule provides a lot of useful information about the chemical properties of the molecule. It is known that numerous physical and chemical properties of molecules are highly correlated with theoretical invariants of graphs, which we call topological indices. One such theoretical invariant is the dominance number. The aim of this research is to determine the k -dominance number for cyclooctane chains COC_n^1 , COC_n^2 , COC_n^3 and COC_n^4 , for $k \in \{1,2,3\}$, $n \in \mathbb{N}$.

Methods: The cyclooctane chain is a chain of octagons connected by a single line. The vertices of the octagon are treated as nodes of the graph, and the sides and the line connecting them, as branches in the graph. Using mathematical methods, k -dominance was determined on one octagon, $k \in \{1,2,3\}$. Then, by representing the cyclooctane chains COC_n^1 , COC_n^2 , COC_n^3 and COC_n^4 , in a convenient, isomorphic way, we determined their k -dominance number, $k \in \{1,2,3\}$.

Results: Determining k -dominance, $k \in \{1,2,3\}$, for 4 cyclooctane chains COC_n^1 , COC_n^2 , COC_n^3 and COC_n^4 , we obtained 12 different formulas to calculate their k -dominance number. All formulas are composed of several alternative algebraic expressions, the selection of which is conditioned by the divisibility of the number n by the number 2, 3 or 4, depending on the type of cyclooctane chain and k -dominance to be determined. The results of the research are fully presented in the paper through mathematically proven theorems and graphical representations.

Conclusion: The results show that the k -dominance numbers, $k \in \{1,2,3\}$, on cyclooctane chains COC_n^1 , COC_n^2 , COC_n^3 and COC_n^4 , are determined and explicitly expressed by mathematical expressions. They also indicate the possibility of their application in molecular graphs of cyclooctane rings, in computational chemistry, chemical and biological industry.

Key words: cyclooctane, cyclooctane chain, dominance number.

Introduction

Graph theory occupies an important place in many fields of science. Among them are chemistry and biology. Chemical structures are conveniently represented by graphs, where atoms are nodes (vertices) in the graph and chemical bonds are lines (branches) in the graph (Trinajstić, 1992). Graphical representation of molecules provides a wealth of useful information about the chemical properties of molecules (Gupta et al, 2001, 2022). It has been shown that numerous physical and chemical properties of molecules are highly correlated with theoretical invariants of graphs, which we call topological indices or molecular descriptors (Todeschini & Consonni, 2000). Topological indices are extremely useful in calculating the physicochemical characteristics of large chemical structures, which are otherwise difficult to calculate for large networks (Baig et al, 2018).

One of the latest concepts that represents a combination of chemistry, mathematics and informatics is chemical informatics (Ahmed et al, 2021). In computational chemistry, cyclooctane chains are an imperative class of cycloalkanes, which has led to the investigation of their structural characteristics with basic graph parameters (Raza et al, 2023). The authors of the mentioned paper derived the mathematical expected values of topological descriptors of cyclooctane. They also performed a comparative analysis for different descriptors and pointed to special classes of cyclooctane chains with exact values.

In the paper (Raza & Imran, 2021), the expected values of some molecular descriptors in a random cyclooctane chain were investigated. The authors of the paper (Wei et al, 2018) determined the exact formulas for the expected value of the Wiener index in a random cyclooctane chain. Research was also carried out on the expected values of three types of Kirchhoff indices (Liu et al, 2021), Gutman and Schultz indices (Liu et al, 2023) in the cyclooctane chain. In the previous period, other research studies were also carried out on cyclooctanes and cyclooctane chains (Bharadwaj, 2000).

It is known that the dominance number is one of the theoretical invariants of graphs (Vukičević & Klobučar, 2007). In the previous period, dominance research was carried out on various graphs. Cactus graphs, as a special type of connected graphs in which no branch is found in more than one cycle, have been investigated in numerous works. Dominance on rhomboidal cactus chains (Carević et al, 2020), pentagonal (Carević, 2022), hexagonal (Majstorović et al, 2012, 2016) was investigated. Research was also carried out on linear benzenoids (Vukičević &

Klobučar, 2007), hexagonal network (Klobučar & Klobučar, 2019), and icosahedral hexagonal network (Carević, 2021).

In this paper, we deal with k -dominance on cyclooctane chains COC_n^1 , COC_n^2 , COC_n^3 and COC_n^4 , for $k \in \{1, 2, 3\}$.

Cyclooctane chains

A cyclooctane chain is a chain of octagons in which each node is in only one octagon. The octagons are connected to each other by a line that joins two nodes from two adjacent octagons, thus forming a cyclooctane chain (Figure 1).

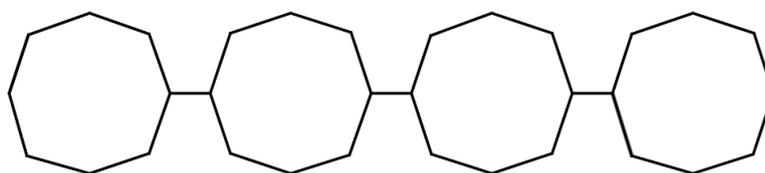


Figure 1 – Cyclooctane chain length 4

The nodes in the octagon joined by the connecting line are called cut (intersected) nodes. The minimum distance between two cut nodes in one octagon is denoted by p . In the cyclooctane chain in Figure 1, the distance between two cut nodes in each octagon is $p = 4$. We denote the cyclooctane chain of the length n formed in this way by COC_n^4 , where the length of the chain n is determined by the number of octagons in the chain. The minimum distance between two cut nodes can be $p = 3$ (Figure 2); it can also be $p = 2$ (Figure 3) or $p = 1$ (Figure 4), whereby we denote the corresponding cyclooctane chains, respectively, with COC_n^3 , COC_n^2 and COC_n^1 .

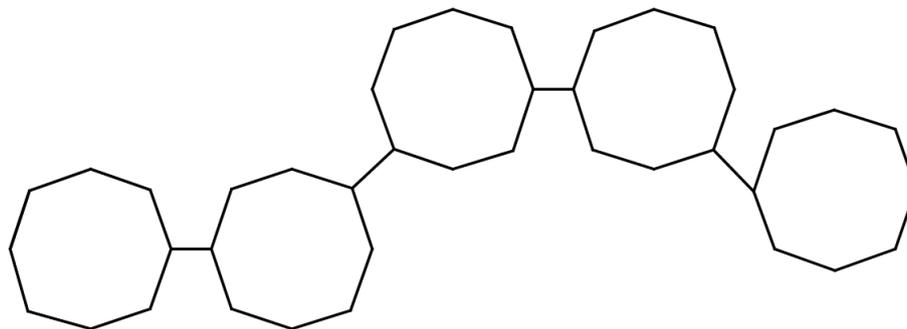


Figure 2 – Cyclooctane chain COC_5^3

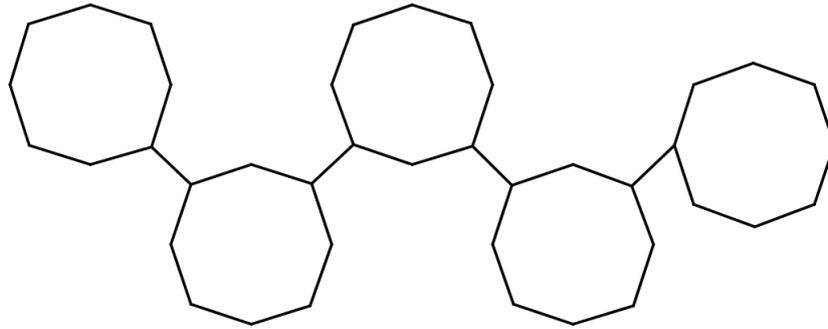


Figure 3 – Cyclooctane chain COC_8^2

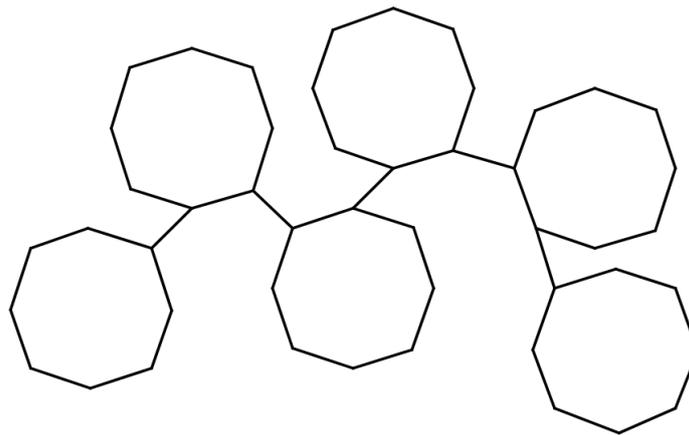


Figure 4 – Cyclooctane chain COC_6^1

Research results

Preliminaries

At the beginning of this section, we will consider k -dominance on one octagon O_8 , $k \in \{1, 2, 3\}$. We denote the set of nodes (vertices) in each graph G by $V(G)$. A set $D \subset V(G)$ is said to be a k -dominant set in the graph G if for every node y outside the set D there is at least one node $x \in D$ such that $d(x, y) \leq k$ where with $d(x, y)$ labeled distance between the nodes x and y . The number of elements of the smallest k -dominant set is called the k -dominance number and is denoted by γ_k .

Lemma 1: The 1-domination number for the octagon is $\gamma_1(O_8) = 3$.
 Proof: Let us denote the nodes of the octagon with x_1, x_2, \dots, x_8 (Figure 5).

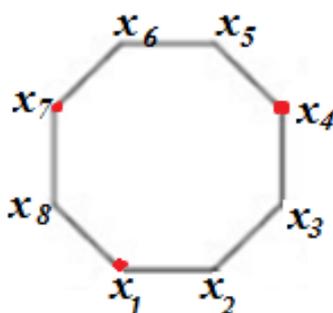


Figure 5 – 1-dominant set on an octagon

One node of the octagon dominates two neighboring nodes. Let us take the node x_1 . It dominates the nodes x_2 and x_8 . There are 5 nodes left in the octagon. Based on the proof of Lemma 2.1 presented in the paper (Carević, 2022), the 1-dominance number for 5 nodes is 2. Let these be the nodes x_4 and x_7 in the given octagon. Thus, the set $D = \{x_1, x_4, x_7\}$ is a 1-dominant set for the given octagon, but it is not the only one. They are also sets containing any 3 nodes of an octagon with the mutual distance $d = 2$ and $d = 3$. Based on the proof of Lemma 2.1 in the mentioned paper, there is no 1-dominating set D' of lesser cardinality. Therefore, the minimal 1-dominant set on the octagon is a three-membered set, so the 1-dominant number for the octagon is $\gamma_1(O_8) = 3$.

Lemma 2: The 2-domination number for the octagon is $\gamma_2(O_8) = 2$.
 Proof: Let us denote the nodes of the octagon with x_1, x_2, \dots, x_8 (Figure 6).

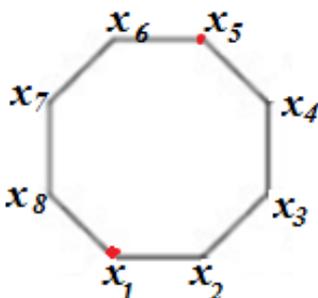


Figure 6 – 2-dominant set on an octagon

The node x_1 has 2-dominance over the nodes x_2 and x_3 , on the one hand, and over the nodes x_8 and x_7 , on the other hand. For the remaining nodes x_4, x_5, x_6 , it is necessary to determine one 2-dominant node. Let it be a node x_5 . So the set $D = \{x_1, x_5\}$ is a 2-dominant set for the given octagon, but it is not the only 2-dominant set whose cardinality is equal to 2, analogous to the previous consideration, where the distance between the dominant nodes must be 3 or 4. Let us prove that there is no set D' of lesser cardinality which is a 2-dominating set on the octagon. Assuming it exists, its cardinality would be 1. But one node cannot 2-dominate the 7 remaining nodes in the octagon. Therefore, the minimal 2-dominant set on the octagon is a two-membered set, so the 2-dominant number for the octagon is $\gamma_2(O_8) = 2$.

Lemma 3: The 3-domination number for the octagon is $\gamma_3(O_8) = 2$.

Proof: Let us look at Figure 6. The node x_1 has 3-dominance over the nodes x_2, x_3 and x_4 , on the one hand, and over the nodes x_8, x_7 and x_6 , on the other hand. The node x_5 is not dominated. So the set $D = \{x_1, x_5\}$ is a 3-dominant set for the given octagon, but it is not the only 3-dominant set whose cardinality is equal to 3, analogous to the previous consideration. Analogous to the proof of Lemma 2, there is no set D' of lesser cardinality which is a 3-dominating set on the octagon. Therefore, the minimal 3-dominant set on the octagon is a two-membered set, so the 3-dominant number for the octagon is $\gamma_3(O_8) = 2$.

Let us now define the coverage index of the nodes of the graph by the dominating node:

Definition 1: The node coverage index by the dominating node is the total number of nodes covered by the dominance including the dominant node. For k -dominance, we denote the coverage index by $index_k$.

Based on what was stated in Lemma 1, Lemma 2 and Lemma 3, in the octagon there is: $index_1 = 3$, $index_2 = 5$, $index_3 = 7$.

In the next part of the presentation, we consider k -dominance, for $k \in \{1, 2, 3\}$, on cyclooctane chains $COC_n^1, COC_n^2, COC_n^3$ and COC_n^4 , $n \in N$, $n \geq 2$.

It is known that two isomorphic graphs have equal dominance numbers (Vukičević & Klobučar, 2007). Based on this, we will present cyclooctane chains $COC_n^1, COC_n^2, COC_n^3$ and COC_n^4 in a convenient, isomorphic way and determine the k -dominance, for $k \in \{1, 2, 3\}$.

Cyclooctane chain COC_n^1

Theorem 1. The 1-dominance number on the cyclooctane chain COC_n^1 is

$$\gamma_1(COC_n^1) = \begin{cases} 8 \cdot \frac{n}{3} & , \text{ for } n = 3k, k \in \mathbb{N} \\ 8 \cdot \left\lceil \frac{n}{3} \right\rceil + 6 & , \text{ for } n = 3k - 1, k \in \mathbb{N} \\ 8 \cdot \left\lceil \frac{n}{3} \right\rceil + 3 & , \text{ for } n = 3k - 2, k \in \mathbb{N} \end{cases}$$

Proof: We observe the isomorphic graph of the cyclooctane chain COC_n^1 in Figure 7:

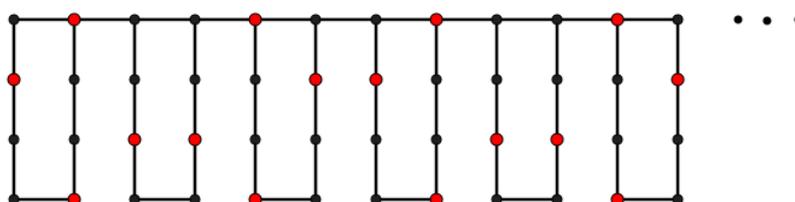


Figure 7 – 1-dominance on COC_n^1

Based on Lemma 1, the 1-dominance number in the first octagon is 3. Let us assume that the third dominant node is a cut node. Since in COC_n^1 the distance between cut nodes is $p = 1$, the third dominant node of the first octagon will dominate over the first cut node in the second octagon. In the same way, the first cut node in the third octagon will dominate the second cut node in the second octagon. Therefore, in the second octagon, two nodes will be enough to dominate the remaining 6 nodes because the coverage index of one node is $index_1 = 3$. In the third octagon, 3 nodes are necessary for dominance, and based on Lemma 1, they cannot be adjacent. Therefore, in the fourth octagon we must have 3 dominant nodes, one of them will be a cut node as in the first octagon. In this way, we have a periodic repetition of the position of the dominant nodes with a period of $\omega = 3$ octagons. If $n = 3k - 1$, $k \in \mathbb{N}$, the last octagon cannot have only 2 dominant nodes because $index_1 = 3$, so it will have 3 dominant nodes. Based on Lemma 1 and everything presented, we get that:

$$\gamma_1(COC_n^1) = \begin{cases} 8 \cdot \frac{n}{3} & , \text{ for } n = 3k, k \in \mathbb{N} \\ 8 \cdot \left\lceil \frac{n}{3} \right\rceil + 6 & , \text{ for } n = 3k - 1, k \in \mathbb{N} \\ 8 \cdot \left\lceil \frac{n}{3} \right\rceil + 3 & , \text{ for } n = 3k - 2, k \in \mathbb{N} \end{cases}$$

Theorem 2. The 2-dominance number on the cyclooctane chain COC_n^1 is

$$\gamma_2(COC_n^1) = \begin{cases} 3 \cdot \frac{n}{2}, & \text{for } n = 2k, k \in N \\ 3 \cdot \left\lceil \frac{n}{2} \right\rceil + 2, & \text{for } n = 2k - 1, k \in N \end{cases}$$

Proof: We observe the isomorphic graph of the cyclooctane chain COC_n^2 in Figure 8. As the coverage index for 2-dominance is $index_2 = 5$, in the first octagon one node will dominate over five nodes while 3 nodes remain without dominance. Let us choose a suitable dominating node so that the nodes not covered by dominance are the intersected node and its neighboring nodes.

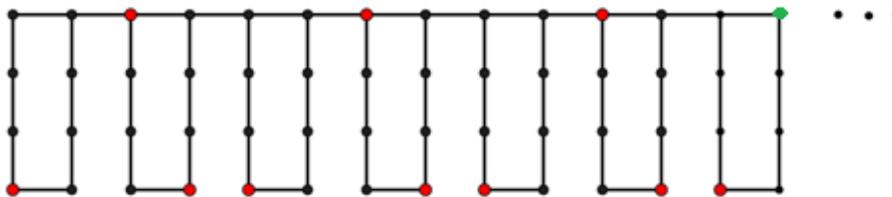


Figure 8 – 2-dominance on COC_n^1

In the second octagon, we take the dominant node so that it dominates the uncovered nodes of the previous octagon. In this octagon, we must have one more dominant node that will dominate the remaining nodes of that octagon. In the first two octagons, we have a total of 16 nodes dominated by 3 nodes (marked in red). The dominance repeats with a period of $\omega = 2$ octagons. If n is an odd number, the last octagon will have one more dominant node (marked in green in Figure 8) because $index_2 = 5$. Based on Lemma 2 and everything presented, we get that:

$$\gamma_2(COC_n^1) = \begin{cases} 3 \cdot \frac{n}{2}, & \text{for } n = 2k, k \in N \\ 3 \cdot \left\lceil \frac{n}{2} \right\rceil + 2, & \text{for } n = 2k - 1, k \in N \end{cases}$$

Theorem 3. The 3-dominance number on the cyclooctane chain COC_n^1 is

$$\gamma_3(COC_n^1) = \begin{cases} 5 \cdot \frac{n}{4}, & \text{for } n = 4k, k \in N \\ 5 \cdot \left\lceil \frac{n}{4} \right\rceil + 4, & \text{for } n = 4k - 1, k \in N \\ 5 \cdot \left\lceil \frac{n}{4} \right\rceil + 3, & \text{for } n = 4k - 2, k \in N \\ 5 \cdot \left\lceil \frac{n}{4} \right\rceil + 2, & \text{for } n = 4k - 3, k \in N \end{cases}$$

Proof: As the coverage index for 3-dominance is $index_3 = 7$, in the first octagon one node will dominate all nodes except one. Let us choose a suitable dominating node so that the node that is not covered by the dominance is the intersected node (Figure 9).

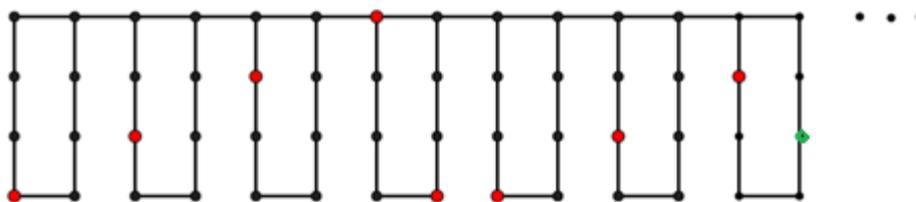


Figure 9 – 3-dominance on COC_n^1

In the second octagon, we take the dominant node so that it dominates the uncovered node of the previous octagon. Analogously, this applies in the third and fourth octagons. In four octagons, there are a total of 32 nodes where $index_3 = 7$, so it follows that there must be 5 dominant nodes. These 5 dominant nodes completely cover the first 4 octagons with dominance, so from the fifth octagon there is a repetition of dominance. The dominance repeats with a period of $\omega = 4$ octagons. If n is not divisible by 4 in the last octagon, we must have another dominant node (marked in green in Figure 9) because $index_3 = 7$. Based on Lemma 3 and everything presented, we get that:

$$\gamma_3(COC_n^1) = \begin{cases} 5 \cdot \frac{n}{4}, & \text{for } n = 4k, k \in N \\ 5 \cdot \left\lceil \frac{n}{4} \right\rceil + 4, & \text{for } n = 4k - 1, k \in N \\ 5 \cdot \left\lceil \frac{n}{4} \right\rceil + 3, & \text{for } n = 4k - 2, k \in N \\ 5 \cdot \left\lceil \frac{n}{4} \right\rceil + 2, & \text{for } n = 4k - 3, k \in N \end{cases}$$

Cyclooctane chain COC_n^2

Theorem 4. The 1-dominance number on the cyclooctane chain COC_n^2 is $\gamma_1(COC_n^2) = 3n$.

Proof: We observe the isomorphic graph of the cyclooctane chain COC_n^2 in Figure 10:

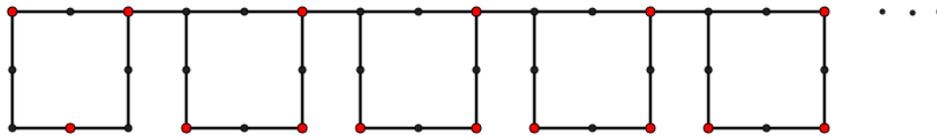


Figure 10 – 1-dominance on COC_n^2

By Lemma 1, the 1-dominance number in the first octagon is 3. Let us assume that the third dominant node is a cut node. As the distance between the cut nodes in COC_n^2 is $p = 2$, the third dominant node of the first octagon will dominate over the first cut node in the second octagon, but not over its neighboring nodes. In the second octagon, there are 7 nodes left, for which 2 dominant nodes are not enough, which would dominate over 6 nodes because $index_1 = 3$. Therefore, in the second octagon, we must have 3 dominant nodes, where one of them will be a cut node as in the first octagon. In this way, we have a periodic repetition of the position of the dominant nodes in each subsequent octagon. Based on Lemma 1 and everything presented, we get that $\gamma_1(COC_n^2) = 3n$.

Theorem 5. The 2-dominance number on the cyclooctane chain COC_n^2 is

$$\gamma_2(COC_n^2) = \begin{cases} 3 \cdot \frac{n}{2}, & \text{for } n = 2k, k \in N \\ 3 \cdot \left\lceil \frac{n}{2} \right\rceil + 2, & \text{for } n = 2k - 1, k \in N \end{cases}$$

Proof: We observe the isomorphic graph of the cyclooctane chain COC_n^2 in Figure 11. As the coverage index for 2-dominance is $index_2 = 5$, in the first octagon one node will dominate over five nodes while 3 nodes remain without dominance. Let us choose a suitable dominating node so that the nodes that are not covered by dominance are the cut node and its neighboring nodes.

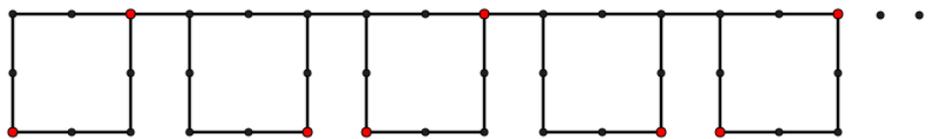


Figure 11 – 2-dominance on COC_n^2

This cut node will dominate the first cut node in the second octagon and its adjacent nodes. In the second octagon, we must have another dominant node that will dominate the remaining 5 nodes. As $index_2 = 5$, this node will complete the dominance in the second octagon. In the first two octagons we have a total of 16 nodes dominated by 3 nodes (marked in red). The dominance repeats with a period of $\omega = 2$ octagons. Based on Lemma 2 and everything presented, we get that:

$$\gamma_2(COC_n^2) = \begin{cases} 3 \cdot \frac{n}{2}, & \text{for } n = 2k, k \in N \\ 3 \cdot \left\lceil \frac{n}{2} \right\rceil + 2, & \text{for } n = 2k - 1, k \in N \end{cases}$$

Theorem 6. The 3-dominance number on the cyclooctane chain COC_n^2 is $\gamma_3(COC_n^2) = n + 1$.

Proof: As the coverage index for 3-dominance is $index_3 = 7$, in the first octagon one node will dominate all nodes except one. Let us choose a suitable dominating node so that the node that is not covered by dominance is a cut node (Figure 12).

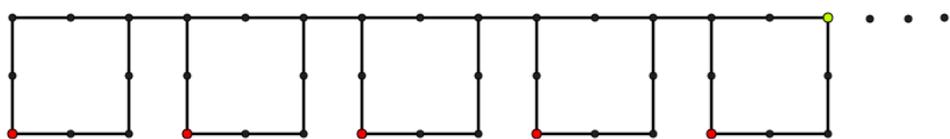


Figure 12 – 3-dominance on COC_n^2

In the second octagon, we select the dominating node so that it dominates the intersected node in the first octagon (Figure 12). This node, similar to the previous one, will dominate all the nodes of the second octagon except the second cut node in it. In this way, the previously described dominance is repeated, so it follows that in each octagon we have one dominant node, except in the last octagon in the chain, where we must have two nodes

(the node marked in green in Figure 12). Based on Lemma 3 and everything presented, we get that $\gamma_3(COC_n^2) = n + 1$.

Cyclooctane chain COC_n^3

Theorem 7. The 1-dominance number on the cyclooctane chain COC_n^3 is $\gamma_1(COC_n^3) = 3n$.

Proof: We observe the isomorphic graph of the cyclooctane chain COC_n^3 in Figure 13.

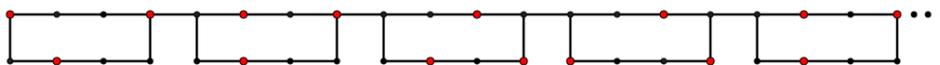


Figure 13 – 1-dominance on COC_n^3

By Lemma 1, the 1-dominance number in the first octagon is 3. Assume that the third dominant node is a cut node. Since in COC_n^3 the distance between intersected nodes is $p = 3$, the third dominant node of the first octagon will dominate over the first cut node in the second octagon, but not over its neighboring nodes. In the second octagon, there are 7 nodes left, for which 2 dominant nodes are not enough, it would dominate over 6 nodes because $index_1 = 3$. Therefore, in the second octagon, we must have 3 dominant nodes with the mutual distance of $d = 2$ and $d = 3$ as proved in Lemma 1. In the same way, we must have 3 dominant nodes in each subsequent octagon. Based on everything presented, we get that $\gamma_1(COC_n^3) = 3n$.

Theorem 8. The 2-dominance number on the cyclooctane chain COC_n^3 is:

$$\gamma_2(COC_n^3) = \begin{cases} 3 \cdot \frac{n}{2}, & \text{for } n = 2k, k \in N \\ 3 \cdot \left\lceil \frac{n}{2} \right\rceil + 1, & \text{for } n = 2k + 1, k \in N \end{cases}$$

Proof: We observe the isomorphic graph of the cyclooctane chain COC_n^3 in Figure 14:



Figure 14 – 2-dominance on COC_n^3

As the coverage index for 2-dominance is $index_2 = 5$, in the first octagon one node will dominate over five nodes while 3 nodes remain without dominance. Let us choose the first intersected node of the second octagon

as the dominant node. It will dominate the remaining 3 nodes of the first octagon and a total of 5 nodes of the second octagon because $index_2 = 5$. In the second octagon, we must have another dominant node that will dominate the second intersected node and the remaining 2 nodes. Assume that the dominant node is the second cut node. It will also dominate 3 nodes in the third octagon, so one dominant node will be enough in the third octagon. The dominance repeats with a period of $\omega = 2$ octagons. Based on Lemma 2 and everything presented, we get that:

$$\gamma_2(COC_n^3) = \begin{cases} 3 \cdot \frac{n}{2}, & \text{for } n = 2k, k \in N \\ 3 \cdot \left\lceil \frac{n}{2} \right\rceil + 1, & \text{for } n = 2k + 1, k \in N \end{cases}$$

Theorem 9. The 3-dominance number on the cyclooctane chain COC_n^3 is $\gamma_3(COC_n^3) = n + 1$.

Proof: We observe the isomorphic graph of the cyclooctane chain COC_n^3 in Figure 15:



Figure 15 – 3-dominance on COC_n^3

As the coverage index for 3-dominance is $index_3 = 7$, in the first octagon one node will dominate all nodes except one. Let us choose a suitable dominating node so that the node not covered by the dominance is the intersected node. In the second octagon, we select the dominating node so that it dominates the intersected node in the first octagon (Figure 15). This node, similar to the previous one, will dominate all the nodes of the second octagon except the second intersected node in it. In this way, the previously described dominance is repeated, so it follows that in each octagon we have one dominant node, except in the last octagon in the chain, where we must have two nodes (the node marked in green in Figure 15). Based on Lemma 3 and everything presented, we get that $\gamma_3(COC_n^3) = n + 1$.

Cyclooctane chain COC_n^4

Theorem 10. The 1-dominance number on the cyclooctane chain COC_n^4 is:

$$\gamma_1(COC_n^4) = \begin{cases} 8 \cdot \frac{n}{3} & , \text{ for } n = 3k, k \in N \\ 8 \cdot \left\lceil \frac{n}{3} \right\rceil + 6 & , \text{ for } n = 3k - 1, k \in N \\ 8 \cdot \left\lceil \frac{n}{3} \right\rceil + 3 & , \text{ for } n = 3k - 2, k \in N \end{cases}$$

Proof: We observe the isomorphic graph of the cyclooctane chain COC_n^4 in Figure 16:

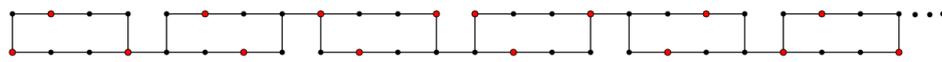


Figure 16 – 1-dominance on COC_n^4

By Lemma 1, the 1-dominance number in the first octagon is 3. Assume that the third dominant node is a cut node. The third dominant node of the first octagon will dominate the first cut node in the second octagon. In the same way, the first cut node in the third octagon will dominate the second cut node in the second octagon. Therefore, in the second octagon, two nodes will be sufficient to dominate the remaining 6 nodes because the coverage index of one node is $index_1 = 3$. In the third octagon, 3 nodes are necessary for dominance, and based on Lemma 1, they cannot be adjacent. Therefore, in the fourth octagon we must have 3 dominant nodes, one of which will be a cut node as in the first octagon. It will dominate the first cut node of the fifth octagon. Also, the first cut node in the sixth octagon will dominate the second cut node in the fifth octagon. Therefore, in the fifth octagon, 2 nodes will be enough to dominate the remaining 6 nodes. In the sixth octagon, 3 dominant nodes are necessary. In this way, we have a periodic repetition of the position of the dominant nodes with a period of $\omega = 3$ octagons. If $n = 3k - 1, k \in N$, the last octagon cannot have only 2 dominant nodes because $index_1 = 3$, will already have 3 dominant nodes. Based on Lemma 1 and everything presented, we get that:

$$\gamma_1(COC_n^4) = \begin{cases} 8 \cdot \frac{n}{3} & , \text{ for } n = 3k, k \in N \\ 8 \cdot \left\lceil \frac{n}{3} \right\rceil + 6 & , \text{ for } n = 3k - 1, k \in N \\ 8 \cdot \left\lceil \frac{n}{3} \right\rceil + 3 & , \text{ for } n = 3k - 2, k \in N \end{cases}$$

Theorem 11. The 2-dominance number on the cyclooctane chain COC_n^4 is $\gamma_2(COC_n^4) = n + 1$.

Proof: We observe the isomorphic graph of the cyclooctane chain COC_n^4 in Figure 17.

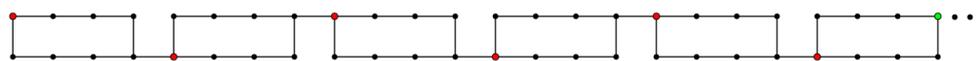


Figure 17 – 2-dominance on COC_n^4

As the coverage index for 2-dominance is $index_2 = 5$, in the first octagon one node will dominate over five nodes while 3 nodes remain without dominance. Let us choose a suitable dominating node so that nodes that are not covered by dominance are a cut node and its neighboring nodes. In the second octagon, we take the dominant node so that it dominates the uncovered nodes of the previous octagon. This node will dominate over 5 nodes of the second octagon, leaving 3 nodes without dominance (as in the first octagon). Therefore, in the third octagon, we take the first cut node as the dominant node. It will dominate the remaining 3 nodes of the second octagon and the 5 nodes of the third octagon. In this way, the previously described dominance is repeated, so it follows that in each octagon we have one dominant node, except in the last octagon in the chain, where we must have two nodes (the node marked in green in Figure 17). Based on Lemma 2 and everything presented, we get that $\gamma_2(COC_n^4) = n + 1$.

Theorem 12. 3-dominance number on the cyclooctane chain COC_n^4 is $\gamma_3(COC_n^4) = n + 1$.

Proof: We observe the isomorphic graph of the cyclooctane chain COC_n^4 in Figure 18.



Figure 18 – 3-dominance on COC_n^4

As the coverage index for 3-dominance is $index_3 = 7$, in the first octagon one node will dominate all nodes except one. Let us choose a suitable dominating node so that the node not covered by the dominance is the cut node. In the second octagon, we select the dominating node so that it dominates the cut node in the first octagon (Figure 18). This node, similar to the previous one, will dominate all but one of the nodes of the second octagon. In the third octagon, we take the first cut node as the dominant node. It will dominate the aforementioned node of the second octagon and the 7 nodes of the third octagon. In this way, the previously described dominance is repeated, so it follows that in each octagon we have one dominant node, except in the last octagon in the chain, where we must

have two nodes (the node marked in green in Figure 18). Based on Lemma 3 and everything presented, we get that $\gamma_3(COC_n^4) = n + 1$.

Conclusion

Numerous physical and chemical properties of molecules are highly correlated with graph theoretical invariants. One of the theoretical invariants is the dominance number. In this paper, we determined k -dominance numbers, $k \in \{1, 2, 3\}$, for cyclooctane chains COC_n^1 , COC_n^2 , COC_n^3 and COC_n^4 , $n \geq 2$. The obtained results have a potential practical application in molecular graphs of cyclooctane rings containing saturated hydrocarbons. In computational chemistry, cyclooctane chains are an important class of cycloalkanes. There are numerous applications of cyclooctane in the chemical and biological industry.

Also, the obtained results can be applied in the manufacturing industry, transport and other branches of industry where series of connected elements are present.

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Número de dominancia en las cadenas de ciclooctano

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CAMPO: materiales, tecnologías químicas, matemáticas

TIPO DE ARTÍCULO: artículo científico original

Resumen:

Introducción/objetivo: Las estructuras químicas se representan convenientemente mediante gráficos donde los átomos son nodos (vértices) y los enlaces químicos son ramas (líneas) en el gráfico. Una representación gráfica de una molécula proporciona mucha información útil sobre las propiedades químicas de la molécula. Se sabe que numerosas propiedades físicas y químicas de las moléculas están altamente correlacionadas con invariantes teóricas de las gráficas, que llamamos índices topológicos. Uno de esos invariantes teóricos es el número de dominancia. El objetivo de esta investigación es determinar el número de k -dominancia para las cadenas de ciclooctano COC_n^1 , COC_n^2 , COC_n^3 y COC_n^4 , for $k \in \{1,2,3\}$, $n \in \mathbb{N}$.

Métodos: La cadena de ciclooctano es una cadena de octágonos conectados por una sola línea. Los vértices del octágono se tratan como nodos del gráfico, y los lados y la línea que los conecta, como ramas del gráfico. Utilizando métodos matemáticos, se determinó la k -dominancia en un octágono, $k \in \{1,2,3\}$. Luego, al representar las cadenas de ciclooctano COC_n^1 , COC_n^2 , COC_n^3 y COC_n^4 , de una manera conveniente e isomorfa, determinamos su número de k -dominancia, $k \in \{1,2,3\}$.

Resultados: Determinando la k -dominancia, $k \in \{1,2,3\}$, para 4 cadenas de ciclooctano COC_n^1 , COC_n^2 , COC_n^3 y COC_n^4 , Obtuvieron 12 fórmulas diferentes para calcular su número de k -dominancia. Todas las fórmulas se componen de varias expresiones algebraicas alternativas, cuya selección está condicionada por la divisibilidad del número n por el número 2, 3 o 4, según el tipo de cadena de ciclooctano y k -dominancia a determinar. Los resultados de la investigación se presentan íntegramente en el artículo a través de teoremas matemáticamente probados y representaciones gráficas.

Conclusión: Los resultados muestran que los números de k -dominancia, $k \in \{1,2,3\}$, en las cadenas de ciclooctano COC_n^1 , COC_n^2 , COC_n^3 y COC_n^4 , están determinados y expresados explícitamente mediante expresiones matemáticas. También indican la posibilidad de su aplicación en gráficos moleculares de anillos de ciclooctano, en química computacional, industria química y biológica.

Palabras claves: ciclooctano, cadena de ciclooctano, número de dominancia.

Число доминирования в циклооктановых цепочках

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РУБРИКА ГРНТИ: 27.45.17 Теория графов,
61.13.21 Химические процессы

ВИД СТАТЬИ: оригинальная научная статья

Резюме:

Введение/цель: Химические структуры удобно представлять в виде графов, причем атомы являются узлами (вершинами), а химические связи – ветвями (линиями) графа. Графическое представление молекулы предоставляет полезную информацию о химических свойствах молекулы. Как известно, многочисленные физические и химические свойства молекул сильно коррелируют с теоретическими инвариантами графов, которые мы называем топологическими индексами. Одним из таких теоретических инвариантов является число доминирования. Цель данного исследования – определить k -числа доминирования циклооктановых цепочек COC_n^1 , COC_n^2 , COC_n^3 и COC_n^4 , причем $k \in \{1, 2, 3\}$, $n \in \mathbb{N}$.

Методы: Циклооктановая цепочка представляет собой цепочку восьмиугольников, соединенных одной линией. Вершины восьмиугольника рассматриваются как узлы графа, а стороны и соединяющая их линия – как ветви графа. Используя математические методы, было определено k -доминирование в одном восьмиугольнике, $k \in \{1, 2, 3\}$. Затем, представляя циклооктановые цепи COC_n^1 , COC_n^2 , COC_n^3 и COC_n^4 , соответствующим изоморфным образом было определено их k -число доминирования, $k \in \{1, 2, 3\}$.

Результаты: Определив k -доминирование, $k \in \{1, 2, 3\}$ по 4 циклооктановым цепочкам COC_n^1 , COC_n^2 , COC_n^3 и COC_n^4 , получено 12 разных формул для вычисления их k -числа доминирования. Все формулы состоят из нескольких альтернативных алгебраических выражений, выбор которых обусловлен делимостью числа n на числа 2, 3 или 4, в зависимости от типа циклооктановой цепи и определяемого k -доминирования. Результаты исследования полностью представлены в статье с помощью математически доказанных теорем и графических изображений.

Выводы: Результаты показывают, что k -числа доминирования $k \in \{1, 2, 3\}$, в циклооктановой цепочке COC_n^1 , COC_n^2 , COC_n^3 и COC_n^4 получены и эксплицитно выражены математическими выражениями. Они также указывают на возможность их

применения в молекулярных графах циклооктановых колец, в вычислительной химии, а также в химической и биологической промышленности.

Ключевые слова: циклооктан, циклооктановая цепочка, число доминирования.

Доминацијски број за циклооктанске ланце

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Сажетак:

Увод/циљ: Хемијске структуре се најпогодније приказују графовима при чему су атоми чворови (врхови), а хемијске везе гране (линије) у графу. Графичко представљање молекула пружа многобројне корисне информације о њиховим хемијским својствима. Познато је да су многобројна физичка и хемијска својства молекула у високој корелацији са теоријским инваријантама графова које називамо тополошки индекси. Једна од таквих теоријских инваријанти је доминацијски број. Циљ овог истраживања јесте одређивање k -доминацијског броја за циклооктанске ланце COC_n^1 , COC_n^2 , COC_n^3 и COC_n^4 , где је $k \in \{1, 2, 3\}$, $n \in \mathbb{N}$.

Методе: Циклооктански ланац је ланац осмоуглова повезаних по једном линијом. Темена осмоугла су третирана као чворови графа, а странице и линија која их спаја као гране у графу. Применом математичких метода одређена је k -доминација на једном осмоуглу $k \in \{1, 2, 3\}$. Затим је, представљањем циклооктанских ланаца COC_n^1 , COC_n^2 , COC_n^3 и COC_n^4 на погодан, изоморфан начин, одређен њихов k -доминацијски број $k \in \{1, 2, 3\}$.

Резултати: Одређујући k -доминацију $k \in \{1, 2, 3\}$ за 4 циклооктанска ланца COC_n^1 , COC_n^2 , COC_n^3 и COC_n^4 добили смо 12 различитих формула за израчунавање њиховог k -доминацијског броја. Све формуле су састављене од више алтернативних алгебарских израза чији одабир је условљен дељивошћу броја n бројем 2, 3 или 4, зависно од врсте циклооктанског ланца и k -доминације која се одређује. Резултати истраживања су комплетно изложени у раду путем теорема, које су математички доказане, и графичких приказа.

Закључак: Резултати показују да су k -доминацијски бројеви $k \in \{1, 2, 3\}$ на циклооктанским ланцима COC_n^1 , COC_n^2 , COC_n^3 и COC_n^4 одређени и експлицитно исказани математичким изразима. Такође, упућују на могућност њихове примене у молекуларним графовима

циклооктанских прстенова, у рачунарској хемији, хемијској и биолошкој индустрији.

Кључне речи: циклооктан, циклооктански ланац, доминацијски број.

Paper received on: 16.12.2023.

Manuscript corrections submitted on: 04.03.2024.

Paper accepted for publishing on: 05.03.2024.

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