RESEARCH PAPER

Application of Connected Distance 2 Dominating Set in Chemical Structures

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Abstract

A subset D □ V(G) is called a dominating set if every vertex in V(G)\D is adjacent to at least one vertex in D. If the subgraph "D" produced by D is connected in G, then D is said to be a connected dominating set. The distance-2 dominating set D□V if G = (V, E) is a connected distance –k dominating set if the induced subgraph <D> is connected. It is denoted by □c≤k(G). This study identifies the dominating number γ(G), connected dominating number γc(G), distance 2 dominating number γ≤2(G) and connected distance 2 domination number (CD2D) γc≤2 (G) for some chemical structural graph.

AMS Classification: 05C69, 05C90, 92E10

Keywords: Dominating set, chemical graph, Connected dominating set, Connected distance – k domination number

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1. INTRODUCTION

Graph theory serves as a fundamental framework for modeling the intricate topological properties of molecular systems, allowing researchers to quantify structural complexity through various distance-based and connectivity-driven parameters [1]. By mapping atoms to vertices and chemical bonds to edges, this mathematical approach provides essential insights into molecular stability and reactivity [2]. While traditional topological indices such as the Zagreb indices have proven effective in QSPR modeling [3], there remains a critical research gap in exploring more sophisticated neighborhood constraints like the connected distance-2 dominating set. This parameter offers a nuanced perspective on molecular reachability by extending dominance beyond immediate neighbors to secondary atoms while ensuring internal structural coherence [4]. This investigation specifically addresses this gap by formalizing the utility of distance-2 dominating sets in predicting topological variations within carbon-based nanostructures [5]. This approach effectively bridges the gap between discrete mathematical optimization and the predictive modeling of molecular behavior, which remains a primary objective in contemporary chemical graph theory [6]. Furthermore, exploring the connected distance-2 dominating set allows for a more granular assessment of structural motifs compared to existing indices [7], thereby extending the utility of traditional domination-based parameters [8].

In the study of chemical structures, graph theory has proved a valuable tool, with atoms being modeled as nodes, and bonding being modeled as edges. A major concept in graph theory is domination whereby some structural properties of these chemical graphs are described [9].

Atoms are depicted with small circles and chemical bonds are expressed as lines connecting the related circles. In the graph theory, points or nodes are defined as the objects labeled with small circles. The connecting lines are referred to as edges or lines [10]. Chemical compounds can be represented using molecular graphs, and numerous conventions exists, depending upon the application.

Graphs will be different in families of some chemicals which makes a stark contrast to the graphs of alkanes, alkenes, and cycloalkanes, as their bonding and structure are different. In addition to plain domination a number of associated parameters have been found helpful in examining these structures:

Distance Domination Number: This generalizes the domination where the number of vertices is considered equivalent where each other vertex is considered at a certain distance of each vertex [11][9].

Connected Domination Number: This indicator not only makes the dominating set minimal but also a connected subgraph to indicate the continuity of the chemical links [11].

Connected Distance 2 Domination Number: In this, the first extension to range is to hold vertices within distance two (i.e. connected) in the graph and thus a further spread of atomic influence is expressed in the domination, but with outstanding connectivity, particularly in cyclic systems such as cycloalkanes

[12].

Within this article we have domination number, connected domination number, distance 2 domination number and connected distance two domination number of certain chemical graphs and also a generalization by using the Ceiling function represented by ⌈ ⌉ and Floor function represented by ⌊ ⌋ [13].

The following notation is used throughout the paper.

D = Domination number γ(G) ,
D2D = Distance-2 domination number γ≤2(G),
CD = Connected domination number γc(G),
CD2D = Connected distance-2 domination number γc≤2 (G).

2. APPLICATION OF CD2D IN ALKANES

Alkanes are a class of compounds consisting of hydrogen and carbon atoms joined by a single covalent link. "saturated hydrocarbons" is the word used to describe these. This class of molecules is made up of hydrogen and carbon atoms bound together by a single covalent link. Includes a similar sequence with the chemical formula C_nH_{2n+2}.

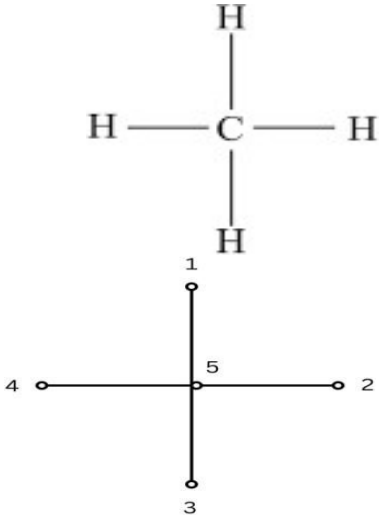
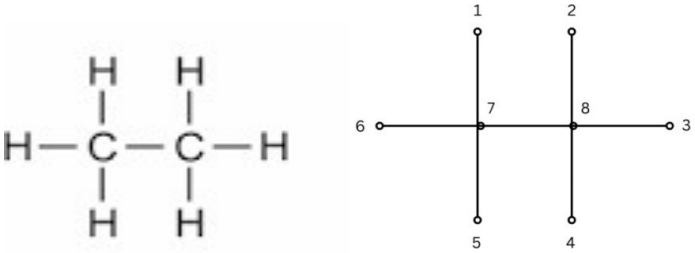


FIGURE 1. Methane (CH_4)

i. D = {5} γ(G) =1
ii. D2D = {5} γ≤2(G) =1
iii. CD ={5} γc(G) =1
iv. CDD ={5} γc≤2 (G) =1

FIGURE 2. Ethane(C_2H_6)



i. D = {7,8} γ(G) =2
ii. D2D = {8} γ≤2(G) =1
iii. CD ={7,8} γc(G)=2
iv. CDD ={7} γc≤2 (G) =1

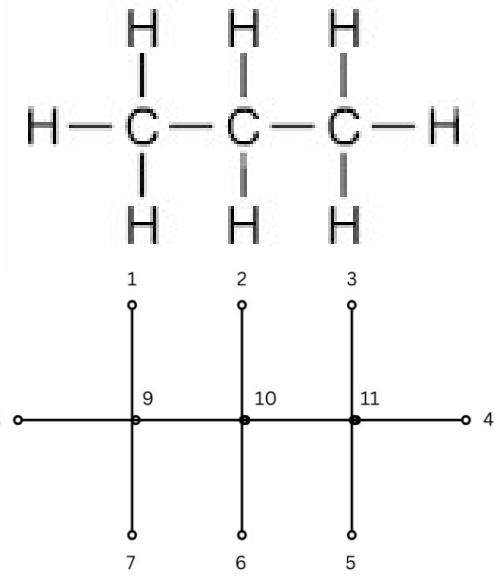
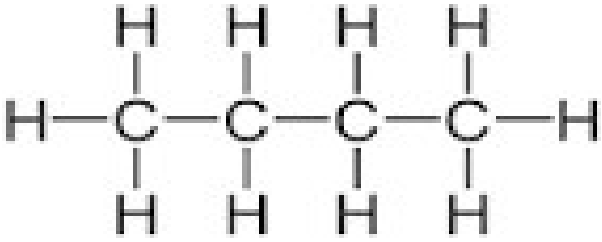


FIGURE 3. Propane(C_3H_8)

i. D = {9,10,11} γ(G) =3
ii. D2D = {10} γ≤2(G) =1
iii. CD ={9,10,11} γc(G) =3
iv. CDD ={10} γc≤2 (G) =1



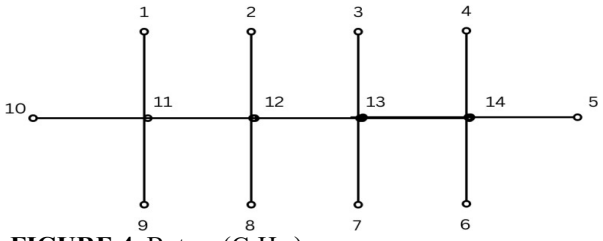


FIGURE 4. Butane(C_4H_{10})

i. D = {13,14,15,16,17} γ(G) =5
ii. D2D = {11,14} γ≤2(G) =2
iii. CD ={11,12,13,14} γc(G) =4
iv. CDD ={12,13} γc≤2 (G) =2

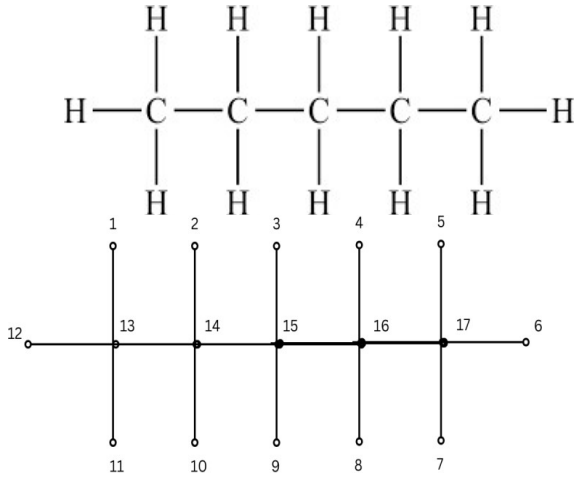


FIGURE 5. Pentane (C_5H_{12})

i. D = {13,14,15,16,17} γ(G) =5
ii. D2D = {13,16} γ≤2(G) =2
iii. CD ={13,14,15,16,17} γc(G)=5
iv. CDD ={14,15,16} γc≤2 (G)=3

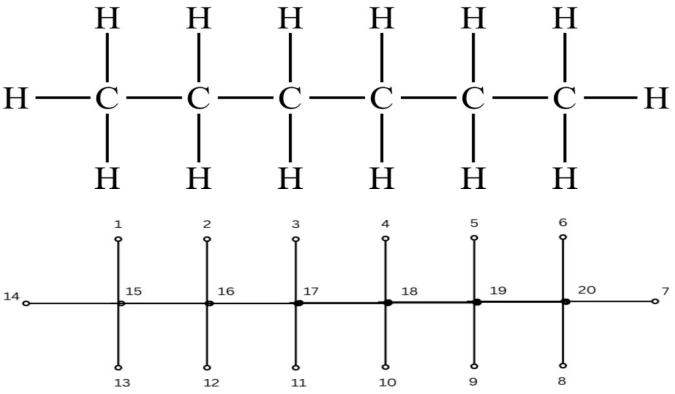


FIGURE 6. Hexane (C_6H_{14})

i. D = {15,16,17,18,19,20} γ(G) =6
ii. D2D = {16,19} γ≤2(G) =2
iii. CD ={15,16,17,18,19,20} γc(G)=6
iv. CDD ={16,17,18,19} γc≤2 (G) =4

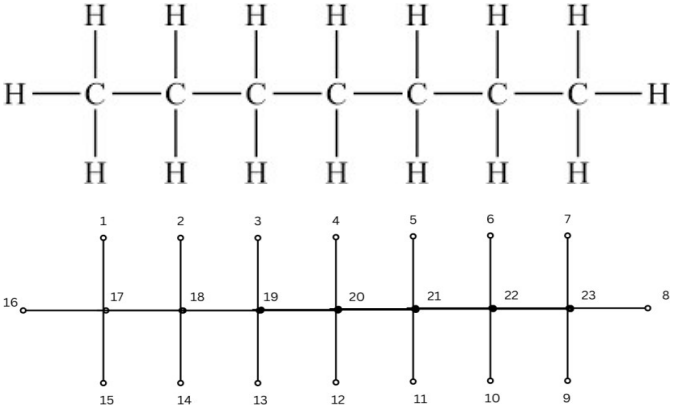


FIGURE 7. Heptane(C_7H_{16})

i. D = {17,18,19,20,21,22,23} γ(G) =7
ii. D2D = {18,20,22} γ≤2(G) =3
iii. CD ={17,18,19,20,21,22,23} γc(G) =7

iv. CDD ={18,19,20,21,22}
γc≤2 (G) =5

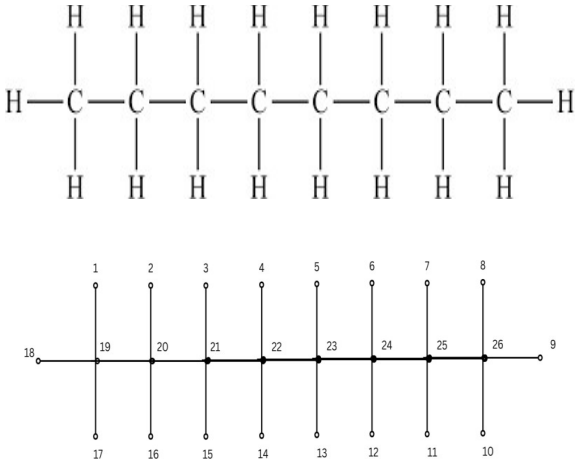


FIGURE 8. Octane(C8H18)

i. D = {19,20,21,22,23,24,25,26}
γ(G) =8
ii. D2D = {20,22,25}
γ≤2(G) =3
iii. CD ={19,20,21,22,23,24,25,26}
γc(G) =8
iv. CDD ={20,21,22,23,24,25}
γc≤2 (G) =6

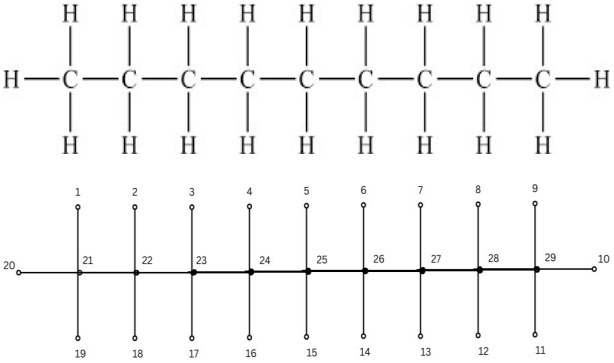


FIGURE 9. Nonane(C_9H_{20})

i. D = {21,22,23,24,25,26,27,28,29}
γ(G) =9
ii. D2D = {22,25,28}
γ≤2(G) =3
iii. CD ={21,22,23,24,25,26,27,28,29}
γc(G) =9
iv. CDD ={22,23,24,25,26,27,28}
γc≤2 (G) =7

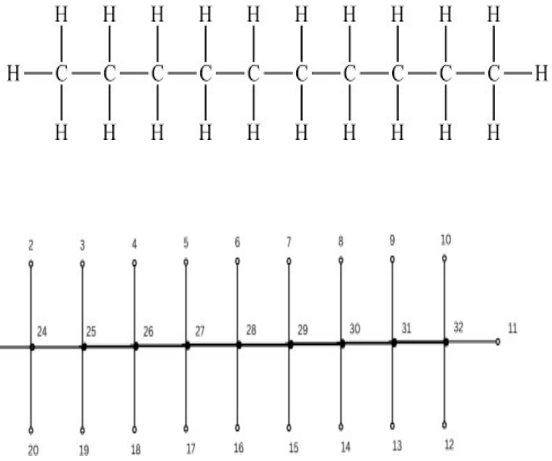


FIGURE 10. Decane ($C_{10}H_{22}$)

i.	D = {23,24,25,26,27,28,29,30,31,32}	γ(G) =10
ii.	D2D = {24,27,29,31}	γ≤2(G) =4
iii.	CD ={23,24,25,26,27,28,29,30,31,32}	γc(G)=10
iv.	CDD ={24,25,26,27,28,29,30,31}	γc≤2 (G) =8

The nth term for each graph-theoretic parameter was derived, providing a formulaic representation that applies to any alkane in the series. This allows not only computing these parameters of higher-order alkanes more easily but also provides an indication of the structural complexity of alkanes as it increases with longer chains. From Figures 1-10 the following table of recapitulation sets these findings clear in comparing the parameters of domination between the alkane series across methane to decane (Table 1).

TABLE 1. Analysis of Alkanes in Domination

Alkanes	γ(G)	γ≤2(G)	γc(G)	γc≤2(G)
Methane CH_4	1	1	1	1
Ethane C_2H_6	2	1	2	1
Propane C_3H_8	3	1	3	1
Butane C_4H_{10}	4	2	4	2
Pentane C_5H_{12}	5	2	5	3
Hexane C_6H_{14}	6	2	6	4
Heptane C_7H_{16}	7	3	7	5
Octane C_8H_{18}	8	3	8	6
Nonane C_9H_{20}	9	3	9	7
Decane $C_{10}H_{22}$	10	4	10	8
C_nH_{2n+2}	n	$\lceil n/3 \rceil$	n	$\lceil n/3 \rceil$, if n=1,2,3 i) n-2, if n≥4

3. APPLICATION OF CD2D IN ALKYNES

Alkenes are a class of hydrocarbons which are hydrogen and carbon molecules, and at least one molecule of carbon must be in a form of carbon-carbon double bond. This double bond causes an alkene to be unsaturated which implies that an alkene contains fewer hydrogen atoms than alkanes of equal carbon atoms. Since they are unsaturated, alkenes are more reactive than alkanes and are able to respond to more reactions. Their chemical formula is a homologous series and their overall chemical formula has the general formula C_nH_{2n} where n is the number of carbon atoms. Alkenes play a significant role in natural and artificial systems, where they are central intermediates in the polymerization, alcohols and other chemicals processes.

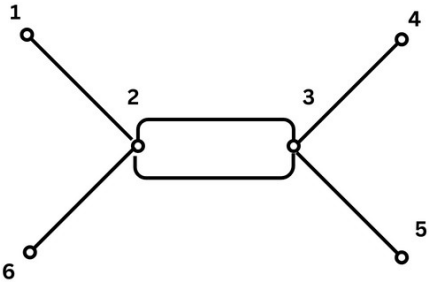
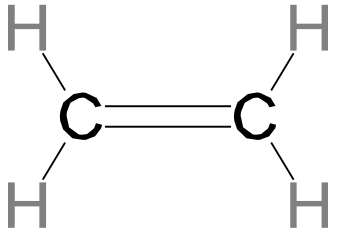
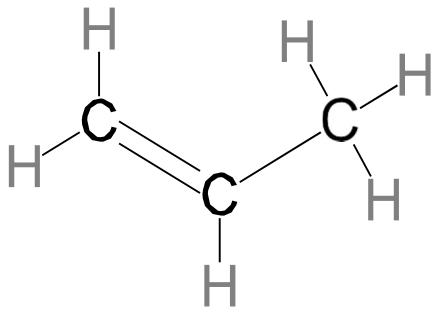


FIGURE 11. Ethylene(C_2H_4)

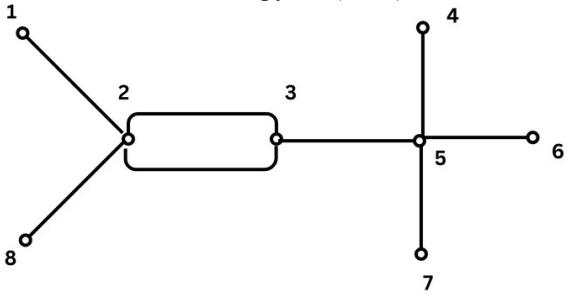


i. D = {2,3} γ(G) =2
ii. D2D = {2} γ≤2(G) =1
iii. CD ={2,3} γc(G) =2

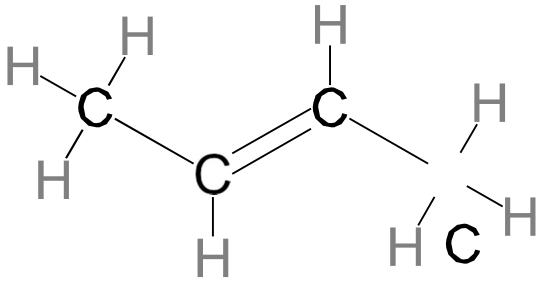


iv. CDD ={2} γc≤2 (G) =1

FIGURE 12. Propylene(C_3H_6)



i. D = {2,5} γ(G) =2
ii. D2D = {3} γ≤2(G) =1
iii. CD ={2,3,5} γc(G)=3



iv. CDD ={3} γc≤2 (G) =1

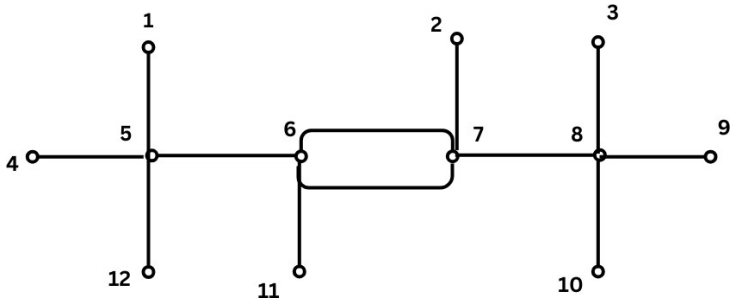


FIGURE 13. Butylene(C_4H_8)

i. D = {5,6,7,8} γ(G) =4
ii. D2D = {6,7} γ≤2(G) =2
iii. CD ={5,6,7,8} γc(G) =4
iv. CDD ={6,7} γc≤2 (G) =2

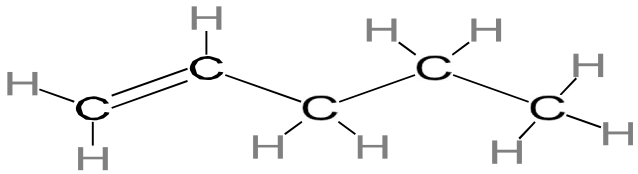
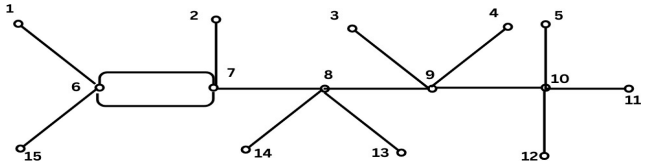
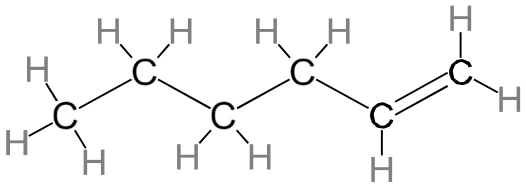


FIGURE 14. Pentylene(C_5H_{10})



i. D = {6,7,8,9,10} γ(G) =5
ii. D2D = {7,9} γ≤2(G) =2
iii. CD ={6,7,8,9,10} γc(G) =5
iv. CDD ={7,8,9} γc≤2 (G) =3



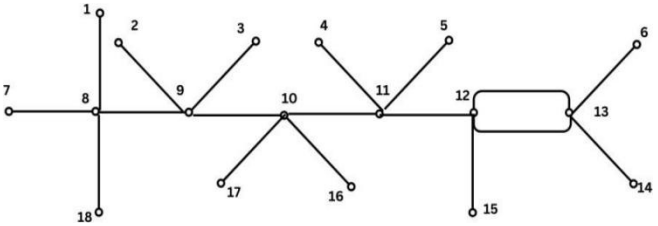


FIGURE 15. Hexylene(C_6H_{12})

i. D = {8,9,10,11,12,13} γ(G) =6
ii. D2D = {9,12} γ≤2(G) =2
iii. CD ={8,9,10,11,12,13} γc(G)=6
iv. CDD ={9,10,11,12} γc≤2 (G)=4

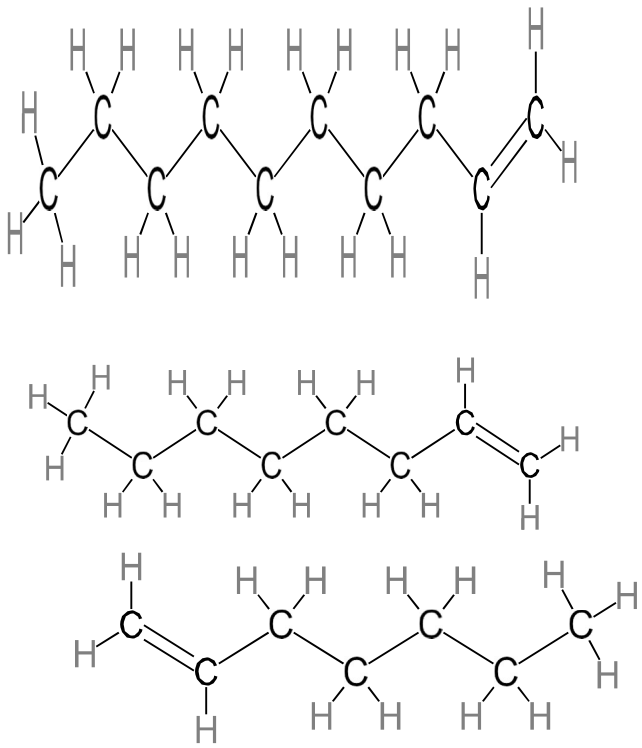


FIGURE 16. Heptylene(C_7H_{14})

i. D = {7,8,9,10,11,12,13} γ(G) =7

ii. D2D = {8,11,12} γ≤2(G) =3

iii. CD ={7,8,9,10,11,12,13} γc(G)=7

iv. CDD ={8,9,10,11,12} γc≤2 (G) =5

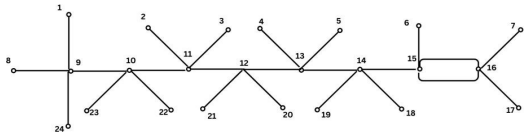


FIGURE 17. Octylene(C_8H_{16})

i. D = {9,10,11,12,13,14,15,16} γ(G) =8

ii. D2D = {10,13,15} γ≤2(G) =3

iii. CD ={9,10,11,12,13,14,15,16} γc(G) =8

iv. CD2D ={10,11,12,13,14,15} γc≤2 (G) =6

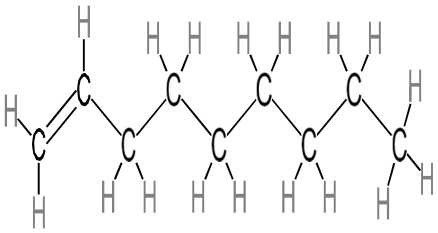
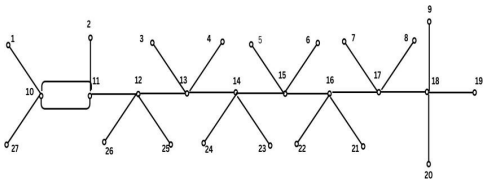


FIGURE 18. Nonylene(C_9H_{18})



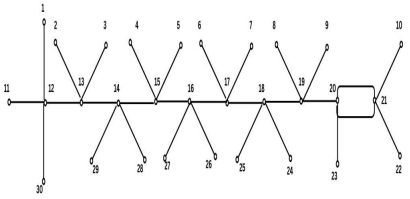
i. D = {10,11,12,13,14,15,16,17,18} γ(G) =9

ii. D2D = {11,14,17} γ≤2(G) =3

iii. CD ={10,11,12,13,14,15,16,17,18} γc(G) =9

iv. CDD ={11,12,13,14,15,16,17} γc≤2 (G) =7

FIGURE 19. Decylene($C_{10}H_{20}$)



i. D = {12,13,14,15,16,17,18,19,20,21}
γ(G) =10

ii. D2D = {13,16,19,20}
γ≤2(G) =4

iii. CD ={12,13,14,15,16,17,18,19,20,21}
γc(G) =10

iv. CDD ={13,14,15,16,17,18,19,20}
γc≤2 (G) =8
.

Each of the parameters that were computed was achieved using the nth term. this gives a short and expandable way to predict the domination-related properties of any alkyne of the range, not only ethene to decene. Investigating trends and structural complexities may be done with the nth term as the chain length grows (Figures 11-19). A comparison of these results in the table below provides an overview look of the domination parameters of the alkynes (Table 2).

TABLE 2. Analysis of Alkynes in Domination

Alkynes	**γ(G)**	**γ≤2(G)**	**γc(G)**	**γc≤2(G)**
Ethylene C2H4	2	1	2	1
Propylene C_3H_6	2	1	3	1
Butylene C_4H_8	4	2	4	2
Pentylene C_5H_{10}	5	2	5	3
Hexylene C_6H_{12}	6	2	6	4
Heptylene C_7H_{14}	7	3	7	5
Octylene C_8H_{16}	8	3	8	6
Nonylene C_9H_{18}	9	3	9	7
Decylene $C_{10}H_{20}$	10	4	10	8
C_nH_{2n}	n, if n≥4 2, if n=2,3	⌈n/3⌉	n	n-2, if n≥3 1, if n=2

4. APPLICATION OF CD2D IN CYCLOALKANES

The Cycloalkanes are some certain type of hydrocarbons which are made up of hydrogen and carbon atoms in the form of a ring like structure and have single covalent bonds. The chemical nature is saturated in these compounds because they are single bonded only unlike alkanes but with a twist of being cyclic. An overall equation of cycloalkanes is C_nH_{2n}, which means that the cycloalkanes have 2 less H compared to the straight-chain alkanes. Cycloalkanes have different chemical and physical properties because of their ring structure e.g. strain in small rings which influences their stability and reactivity. Cycloalkanes are widespread in natural products and widely employed in synthesis of several chemical compounds.

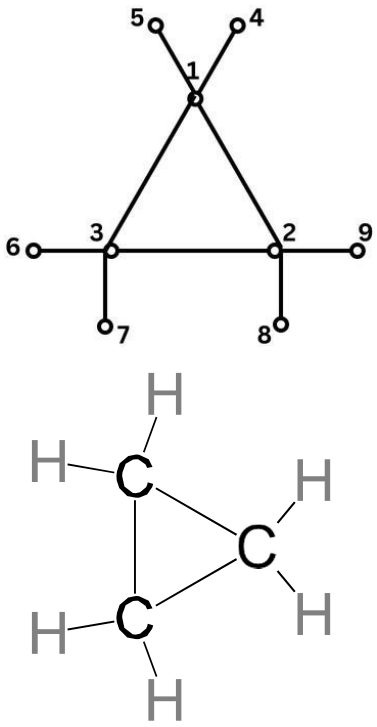


FIGURE 20. Cyclopropane(C_3H_6)

i.	D = {1,2,3}	γ(G) =3
ii.	D2D = {3}	γ≤2(G) =1
iii.	CD ={1,2,3}	γc(G) =3
iv.	CDD ={3}	γc≤2 (G) =1

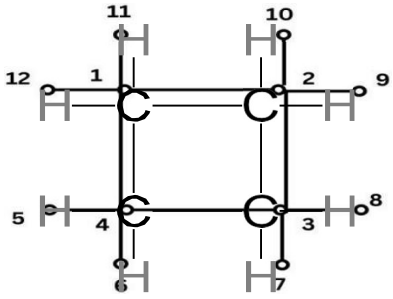


FIGURE 21. Cyclobutane (C_4H_8)

i.	D = {1,2,3,4}	γ(G) =4
ii.	D2D = {2,4}	γ≤2(G) =2
iii.	CD ={1,2,3,4}	γc(G)=4
iv.	CDD ={3,4}	γc≤2 (G) =2

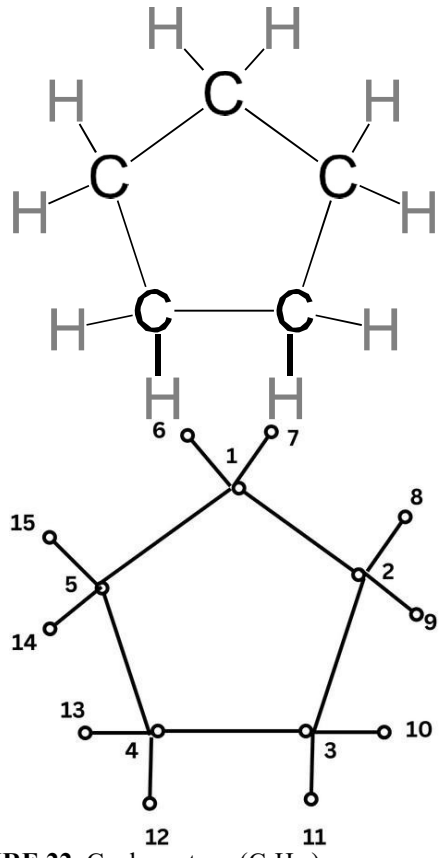


FIGURE 22. Cyclopentane (C_5H_{10})

i.	D = {1,2,3,4,5}	γ(G) =5
ii.	D2D = {1,3}	γ≤2(G) =2
iii.	CD ={1,2,3,4,5}	γc(G) =5
iv.	CDD ={1,2,3}	γc≤2 (G) =3

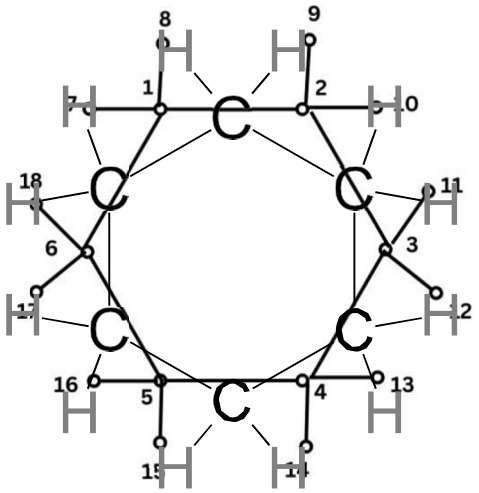


FIGURE 23. Cyclohexane(C_6H_{12})

i. D = {1,2,3,4,5,6} γ(G) =6
ii. D2D = {1,4} γ≤2(G) =2
iii. CD ={1,2,3,4,5,6} γc(G) =6
iv. CDD ={1,2,3,4} γc≤2 (G) =4

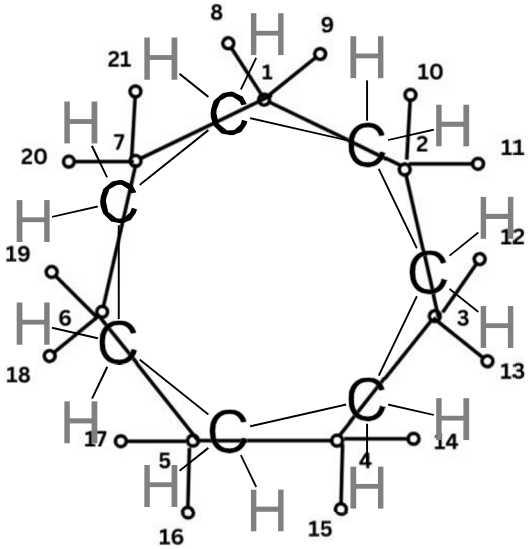


FIGURE 24. Cycloheptane(C_7H_{14})

i. D = {1,2,3,4,5,6,7} γ(G) =7
ii. D2D = {1,4,6} γ≤2(G) =3
iii. CD ={1,2,3,4,5,6,7} γc(G) =7
iv. CDD ={1,2,3,4,5} γc≤2 (G) =5

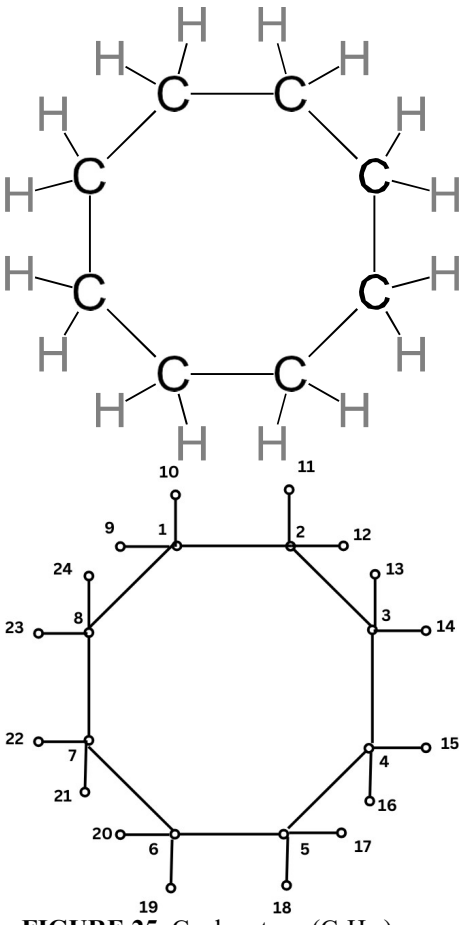


FIGURE 25. Cyclooctane (C_8H_{16})

i. D = {1,2,3,4,5,6,7,8} γ(G) =8
ii. D2D = {1,4,6} γ≤2(G) =3
iii. CD ={1,2,3,4,5,6,7,8} γc(G) =8
iv. CDD ={1,2,3,4,5,6} γc≤2 (G) =6

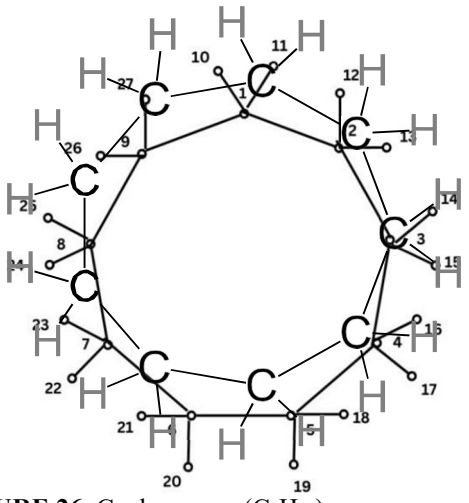


FIGURE 26. Cyclononane (C_9H_{18})

i. D = {1,2,3,4,5,6,7,8,9}
γ(G) =9
ii. D2D = {1,4,7}
γ≤2(G) =3
iii. CD ={1,2,3,4,5,6,7,8,9}
γc(G) =9
iv. CDD ={1,2,3,4,5,6,7}
γc≤2 (G) =7

The nth term for each graph-theoretic parameter was derived. This allows for the prediction of these domination-related values for any cycloalkane in the series, beyond just the ones explicitly calculated. by identifying these nth terms, it becomes easier to track the impact of increasing ring size on the structural complexity of cycloalkanes (Figure 21-26). The table below presents these findings, offering a clear comparison across the series from cyclopropane to cyclononane (Table 3).

TABLE 3. Analysis of Cycloalkanes in Domination

Cycloalkanes	γ(G)	γ≤2(G)	γc(G)	γc≤2 (G)
Cyclopropane C_3H_6	3	1	3	1
Cyclobutane C_4H_8	4	2	4	2
Cyclopentane C_5H_{10}	5	2	5	3
Cyclohexane C_6H_{12}	6	2	6	4
Cycloheptane C_7H_{14}	7	3	7	5
Cyclooctane C_8H_{16}	8	3	8	6
Cyclononane C_9H_{18}	9	3	9	7
CnH2n	n, if n≥3	⌈n/3⌉, if n≥3	n, if n≥3	n-2, if n≥3

CONCLUSION

This study investigates the domination number, distance domination number, connected domination number, and connected distance 2 domination number for the chemical structures of alkanes, alkenes, and cycloalkanes, employing graph-theoretic approaches. By modeling these chemical structures as graphs, where atoms represent vertices and bonds represent edges.

For each class of compounds, we derived general formulas for the n'th term of the respective domination-related parameters. These equations help to come to a better understanding of the influence the size and structure of molecular compounds have on the characteristics of domination. The results show that the differences in molecular connectivity particularly of alkanes, alkenes, and cycloalkanes and its cyclic or linear structure basically translated to significant control of parameter of domination.

This work has many implications in terms of the understanding the properties of the structure of chemical compounds viewed as a graph-theoretic one. They are also pointing to new research directions, including extension of these ideas to more complicated organic compound examples, or higher-order domination concepts, or whether they relate to chemical reactivity and stability.

Defining the parameters of domination in these families of compounds, the work serves the field of chemical graph theory as well as molecular property analysis, constituting a fundamental toolbox that could

be used in future endeavors related to chemistry and material science.

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