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Roman Domination of Some Chemical Graphs

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Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

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ABSTRACT

The concept of Domination in graphs has application to the study of DNA structures. For *investigating the chemical and physical properties, several topological indices used are Wiener index, Randic index, Zagreb index, Kier & Hall index that depends on vertex degree and distance sum, and have been used extensively for QSAR and QSPR studies.*
A Roman Dominating Function of G is function f: V→ {0, 1, 2} such that every vertex v for which f (v) = 0 has a neighbor u with f(u) = 2. The weight of a Roman dominating function f is w (f) = $\sum_{v\in V} f(v)$*. The Roman domination number of a graph G is denoted by* γ_R*(G) and is the minimum weight of all possible Roman dominating functions. In this paper, we find Roman domination number of some chemicals graphs such as saturated hydrocarbons and unsaturated hydrocarbons, hexagonal chain, pyrene, Hexabenzocoronene, H-Phenylenic nanotube and N-Napthelenic nanotube.*

Keywords: Domination number; Roman domination number; molecular graphs; Hexabenzocoronene; H-Phenylenic nanotube and N-Napthelenic nanotube.

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1. INTRODUCTION

Graph theory has wide application in the study of the properties of molecules. Graphs are used to represent chemical structures. A molecule consisting of atoms and atomic bound is correlated to the graph with vertices and edges where atom corresponds to vertex and atomic bound corresponds to edge and valance of atom corresponds to degree of vertex.

This graphical representation reveals many chemical properties of molecules. Pharmaceutical company's manufactures and examines for new compounds in the investigation for new antibacterial and numerous other medicinal drugs, characterizing in detail those compounds that show some prominent properties. Testing for biological activity is costly, therefore many theoretical approaches have been devised for associating structures with biological activities or physical-chemical properties. Graph theory is used for the investigation of the properties through QSAR and QSPR models through graph invariants such as topological indices. The tool for encryption methods like, basic method and insertion method encrypting any chemical formula uses graph domination. Nanotechnology uses Chemical graph theory to create new devices and materials that have applications in computers, electronics, and medicines.

Let G = (V, E) be a graph with a non-empty vertex set and unordered pairs of distinctive vertices set of G called edges. V (G) indicates vertex set and E (G) indicates the edge set. N_G(v) = N_G(v) ∩ {v} is open neighborhood of a vertex v ∈ V (G) and N_G[v] = N_G(v) ∪ {v} is the closed neighborhood of a vertex v ∈ V (G) [1]. In a subset D ⊆ V for each vertex v ϵ V is adjacent to an element of D. i.e. $N[D] = V(G)$ is a dominating set. The dominating set with the least cardinality gives domination number and is symbolized as γ (G) [2]. The graph G with the function f : V→{ 0,1,2} supporting for each vertex **v** assigned f(v) = 0 has a neighbor u assigned f(u) = 2 and w(f) = $\sum_{v\in V} f(v)$ is called the weight of a Roman dominating function. Let us denote Roman dominating function as RDF.

The Roman domination number of a graph G is the minimum weight of all possible Roman dominating functions and is denoted by γ_R(G) [3]. During Roman Empire, to optimize the military strategies this concept was applied by Emperor. The article by Ivan [4] which contained this concept, was the motivation to further study it relating to graph theory aspects. Area is compared to vertex v is considered unstable if no armies are positioned there i.e f(v) = 0 and stable (f(v)∈{1,2}). Area joining routes are compared to edges. An unstable area vertex v will be safe by sending an army to v from a neighboring area (u). Yet, Ruler announced that an army can't be sent from a tied-down area to an unstable area if doing as such leaves that area unstable. In this manner, two armies should be positioned at an area (f(v)=2) before one of the armies can be shipped off an adjoining area. Along these lines, the Ruler can guard the Roman Empire. Since it is costly to keep an army in an area, the Emperor might want to station a couple of armies as could be expected, while as yet guarding the Roman Empire. An RDF compares to a particularly ideal task of optimization of armies to areas.

The Hexagonal chains are natural graph representations of Benzenoid hydrocarbons. Pyrene is a polycyclic aromatic hydrocarbon and is used in the preparation of dyes, plastics, and pesticides. Carbon nanotubes are briskly out spreading our capability to make Nanoscale devices by providing molecular probes, tubes, wires, bearings and spirals. They have many budding applications in various technologies, as they are the tautest and most solid, durable materials. Chloroquine and hydroxychloroquine are considered as antiviral drug and are used in the treatment of viral-related diseases as they control fever and disease progression. H-Phenylenic nanotubes HPH[m, n] are graphs that are made up of C6, C4 and C8 [1]. In the H-Phenylenic HPH[m, n] nanotube, m represents the number of hexagons (rows) in each column and n represents the number of hexagons(columns) in each row.

2. BRIEF SURVEY ON APPLICATION OF CHEMICAL GRAPH THEORY

From the study of Chemical graph theory about its applications and development, one can analyze relations between chemical configuration and molecular properties which provides approval for the planning of energetic elements on the idea of quantitative structure-activity relationships (QSARs). A number of the best tools for QSAR square measure topological indices are discussed in [5]. For researchers investigating bounds of invariants of chemical graphs by investigating upper bounds for the domination number of a Benzenoid is presented in Automated Conjecturing VI: Domination Number of Benzenoid [6]. The domination number of a catacondensed hexagonal system

given in is solved in [7]. Moreover, lower bounds for the domination number in catacondensed hexagonal systems using the number of hexagons and the number of branching hexagon sis obtained. The Domination number and the bondage number for pyrene torus, Balaban 10-cage is obtained in Domination in certain graphs [8]. The domination number, the total domination number and the connected domination number for some chemical graphs is obtained in [9].

2.1 Preliminary Results

Theorem 3.1. [6] A benzenoid with h hexagons has $\gamma(G) \leq 2h$.

Theorem 3.2. [6] For any catacondensed benzenoid, $\gamma(G) \leq \frac{n}{2}$

Theorem 3.3. [6] For any catacondensed benzenoid, $\gamma(G) \leq \frac{m}{2} - h$

Theorem 3.4. [6] Let H ∈ CHS(h) . Then, γ (H) ≤ $\frac{4h+2}{3}$

Theorem 3.5. [10] The total number of minimal and minimum dominating sets in the molecular graph of chloroquine is 648 and 6, respectively.

Theorem 3.6. [10] Suppose G is the molecular graph of chloroquine. Then

1. $DM_1^*(G)=12627$, $\gamma M_1^*(G)=98$,
2. $DM_2(G)=1728576$, $\gamma M_2(G)=25$,
3. $DF^*(G)=3633075$, $\gamma F^*(G)=504$,

Theorem 3.7. [9] Let Gn be a Hexagonal chain with dimension n, then

$$\gamma\,(\mathrm{Gn}) \;=\; n + \left\lfloor \frac{n}{6} \right\rfloor + 1$$

Lemma 3.8. [9] Let Gn be a Hexagonal chain with dimension n, then $\gamma_t(G_n) = 2n + 2$ and $\gamma_c(G_n) = 2n + 2$

Proposition 3.9. [4] For the classes of paths $\gamma_R(P_n) = \left\lceil \frac{2n}{3} \right\rceil$

3. RESULTS AND DISCUSSIONS

In pharmaceutical industries several drugs are tested for their physical and molecular structures to check their action on living being. Nature of chemical structures are very important to do analysis. They need the information regarding the properties such as boiling point, melting point, color, odor, density, hardness and toxicity, ph value, heat of combustion, radioactive decay rate, chemical stability, flammability to design the drug. Domination parameters are required for encryption of binary filament into a DNA sequence, domination can be applied to model of electrical networks made of positive and negative charges, positive and negative electronic spin, during network saturation, also used to find minimum number of routed call so that more number of call are not added. Study on packing of graphs are discussed in [12,13]. Various information on H-Phenylenic nanotube is given in [11,14]. Equivalence between chemical and mathematical terms in describing constitutional formulas and certain of the simplest tools for QSAR are topological indices are briefly discussed in [15]. A quantitative analysis of secondary RNA structure using domination based parameters on trees-7 is discussed in [16]. Thus many of domination parameters have real life application as well as chemical applications.

The molecular graphs are represented in two ways, hydrogen suppressed graphs and hydrogen filled graphs. In hydrogen suppressed graphs, the hydrogen are removed and only carbon atoms are presented as vertices where as in hydrogen filled graphs, carbons and hydrogen's both are presented as vertices. The molecular formula of alkane, alkene and alkyne are C_nH_{2n+2} , C_nH_{2n} and C_nH_{2n-2} respectively.

Example 1. C_8H_{18}

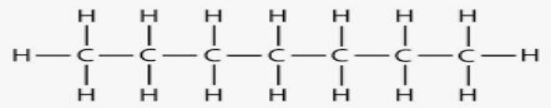

Fig. 1. Octane C_8H_{18}

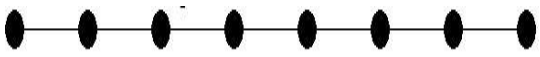

Fig. 2. Carbon tree of Octane in hydrogen suppressed form

Example 2. C_2H_6

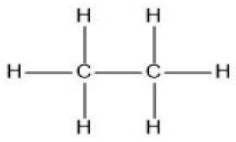

Fig. 3. Ethane C_2H_6

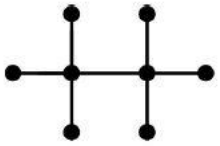

Fig. 4. Hydrogen filled form C_2H_6

3.1 Roman Domination of Alkane, Alkene and Alkyne in Hydrogen Suppressed form and Hydrogen Filled Form

Alkanes are saturated hydrocarbons with single bonding between carbon atoms and alkene, alkynes are unsaturated hydrocarbons with double or triple bonding between carbon atoms. Alkanes have higher number of carbon atoms. They are used in surfacing of roads, generation of compressed natural gas, LPG cylinders, electricity generation, heating and cooking. Alkenes are used in preparation of plastic, plastic products like polythene. Naturally occurring female hormones like estradiol and progesterone are alkynes. Birth control pills are made up of synthetic alkynes like Ethinylestradiol, mifepristone, norethindrone and levonorgestrel which inhibits ovulation and hence prevents pregnancy. Therefore some of the properties of hydrocarbons can be investigated with help of domination parameters for the drug preparation in the required state.

Proposition 4.1 For the graph $G = C_nH_{2n+2}$ or $G = C_nH_{2n}$ or $G = C_nH_{2n-2}$ in hydrogen suppressed form,

$$\gamma_R(G) = \left\lceil \frac{2n}{3} \right\rceil$$

Proof. In hydrogen suppressed from the alkane, alkene and alkyne all are converted into path graph of n vertices. We refer Proposition 3.9. [4] For the classes of paths $\gamma_R(P_n) = \left\lceil \frac{2n}{3} \right\rceil$
Therefore,

$$\gamma_R(C_nH_{2n+2} = C_nH_{2n} = C_nH_{2n-2}) = \left\lceil \frac{2n}{3} \right\rceil$$

3.2 Graphs in Hydrogen Filled form

Theorem 4.2 For the graph $G = C_nH_{2n+2}$ then, $\gamma_R(G) = 2n$

Proof. Let G be a graph with n carbon atoms and $2n + 2$ hydrogen atoms.

Let f: V→ {0, 1, 2} be the roman dominating function.

Algorithm

Input:

1) Let C_1, C_2, C_3,…, C_n be the carbon atoms, Let H_1, H_2, H_3,…, H_n be the hydrogen atoms.
2) Assign $f(C_i) = 2$ for $i = 1, 2, 3 \ldots n$
3) Assign $f(H_i) = 0$ for $i = 1, 2, 3, \ldots, n$

Output: $\gamma_R(G) = 2n$

Example 3. C_3H_8

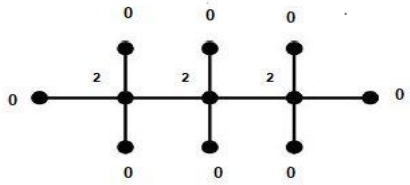

Fig. 5. $\gamma_R(C_3H_8) = 6$

Theorem 4.3 If $G = C_nH_{2n}$ then, $\gamma_R(G) = 2n$

Proof. Let G be a graph with n carbon atoms and $2n$ hydrogen atoms. Let f: V→ {0, 1, 2} be the roman dominating function.

Algorithm

Input:

1) Let C_1, C_2, C_3,…, C_n be the carbon atoms, Let H_1, H_2, H_3,…, H_n be the hydrogen atoms.
2) Assign $f(C_i) = 2$ for $i = 1, 2, 3, \ldots, n$
3) Assign $f(H_i) = 0$ for $i = 1, 2, 3, \ldots, n$

Output: $\gamma_R(G) = 2n$

Theorem 4.4 If $G = C_nH_{2n-2}$ then $\gamma_R(G) = 2n\text{-}2$

Proof. Let G be a graph with n carbon atoms and $2n - 2$ hydrogen atoms. Let f: V→ {0, 1, 2} be the roman dominating function.

Algorithm

Input:

1) Let C_1, C_2, C_3,…, C_n be the carbon atoms, Let H_1, H_2, H_3,…, H_n be the hydrogen atoms.
2) Assign $f(C_{2,\ldots,n-1}) = 2$
3) Assign $f(H_i) = 0$ for $i = 1, 2, 3, \ldots, n$
4) For the hydrogen atoms attached to C_1 and C_n assign the weight 1

Output: $\gamma_R(G) = 2n - 2$

Corollary 4.5. If $G = C_nH_{2n+2}$ then $\gamma_R(G) = 2\gamma(G)$.

Corollary 4.6. If $G = C_nH_{2n}$ then $\gamma_R(G) = 2\gamma(G)$.

Corollary 4.7. If G is the iso-alkane graph, $G= C_nH_{2n}$ then $\gamma_R(G) = 2n$.

3.2.1 Roman domination of hexagonal chain, Pyrene, Hexabenzocoronene, H-Phenylenic nanotube and N-Napthelenic nanotube

4.2.1.1 Saturation of vertex

In the molecular structure if there is a regular pattern consisting of K_2 or K_3 we consider the certain vertex of K_2 or K_3 as reference vertex to assign it the weight 2 and then assign all diagonally opposite vertices also 2. Thus named this step as saturation of vertex.

Theorem 4. 2.1. If G_n is a hexagonal chain with n hexagons then, $\gamma_R(G) = 2(n + 1)$

Proof. Let $h_1, h_2, \ldots h_n$ be the hexagons in G_n.

Algorithm

Input:

1) Consider a vertex of h_1 of degree 3
2) Assign it the weight 2
3) Then saturate all the diagonally opposite vertices with weight 2, till the last hexagon h_n
4) Remaining vertices assign weight 0.

Output: $\gamma_R(G) = 2(n + 1)$

Example 4: G_6

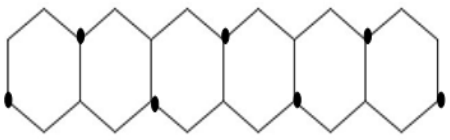

Fig. 6. $\gamma_R(G_6) = 14$

Theorem 4.2.2. If G = PY(n) is a pyrene of dimension n,

$$\gamma_R(G) = 2\begin{cases}\left(\frac{2n^2 + 4n}{4}\right) + 1 & n \text{ is even}\\ \left\lceil\frac{2n^2 + 4n}{4}\right\rceil & n \text{ is odd}\end{cases}$$

Proof: Consider a graph G a pyrene that is symmetric, with vertex ‘a’ at the top hexagon and vertex ’ b’ at the bottom hexagon.

Algorithm

Input:

1) Begin with saturating the vertex v and all diagonally opposite vertices until the vertex u is reached.
2) Assign the saturated vertices the weight 2
3) Other vertices are assigned weight 0
Satisfies the Roman domination function in both even and odd cases

Output:

$$\gamma_R(G) = 2\begin{cases}\left(\frac{2n^2 + 4n}{4}\right) + 1 & n \text{ is even}\\ \left\lceil\frac{2n^2 + 4n}{4}\right\rceil & n \text{ is odd}\end{cases}$$

Example 5. PY(5)

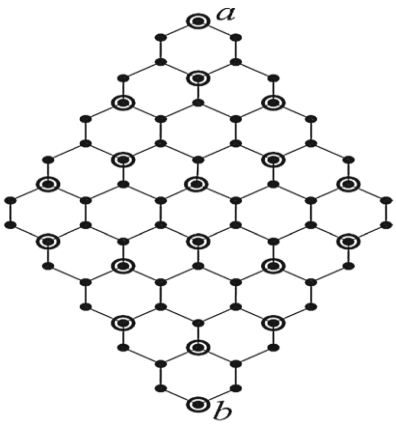

Fig. 7. Pyrene network PY (5)

Theorem 2.2.3. If G is a hexabenzocoronene of dimension n then

$$\gamma_R(G) = 2\gamma(G) = 2\left\{6\left\lfloor\frac{n^2 + 2n + 4}{4}\right\rfloor + 1\right\}$$

Proof: To the honeycomb, network add a layer of six hexagons to get Hexabenzocoronene HBC(n). In six hexagons the vertices of degree 2 are top vertices.

Algorithm

Input:

1) Request the packing HBC(n)($K_{1,3}K_{1,2}$) method
2) In $K_{1,3}$ vertex of degree 3 and in $K_{1,2}$ the vertex of degree 2, assign weight 2
3) Other vertices are assigned 0

Output: $\gamma_R(G) = 2\left\{6\left\lfloor\frac{n^2+2n+4}{4}\right\rfloor + 1\right\}$

Example 6. HBC(3)

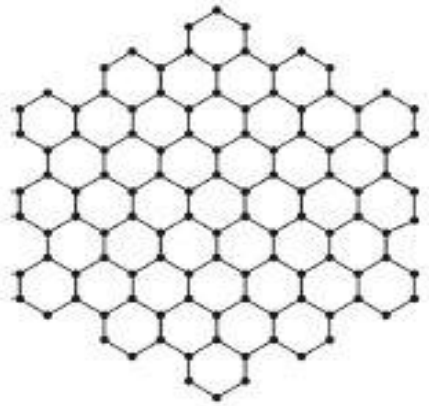

Fig. 8. Hexabenzocoronene HBC (3)

Theorem 2.2.4. If the graph G is a H-Phenylenic nanotube $C_6C_4C_8(m,n)$ then

$$\gamma_R(G) = \begin{cases} m(3n+1), n \text{ is odd} \\ m(3n), n \text{ is even} \end{cases}$$

Proof: Let every level is composed of two rows.

Algorithm

Input:

1) For every row i where i is odd, begin with a vertex u and saturate it.
2) Navigating through the row i (Ri) vertices select the next vertex v at distance 4 from u and saturate it.
3) For each level i where i is even, start at a vertex u and saturate it.
4) Navigating through the level i (Ri) vertices select the next vertex v at distance 4 from u and saturate it.
5) Carry on the practice till all the levels are navigated.
6) Assign weight 2 to all the saturated vertices other vertices assign the weight 0.

This satisfies the roman dominating function and gives the minimum weight.

Output:

$$\gamma_R(G) = \begin{cases} m(3n+1), n \text{ is odd} \\ m(3n), n \text{ is even} \end{cases}$$

Example 7. $C_6C_4C_8(m,n)$

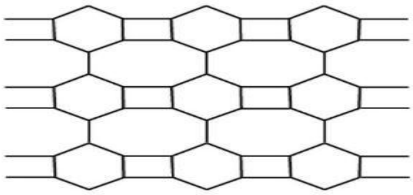

Fig. 9. H-Phenylenic nanotube $\mathbf{C_6C_4C_8(m,n)}$

Theorem2.2.5 If the graph G is a N-Napthelenic nanotube $C_6C_6C_4(m,n)$ then

$$\gamma_R(G) = \begin{cases} p(3q+1)q \text{ is odd} \\ p(3q)q \text{ is even} \end{cases}$$

Proof: The H-Phenylenic nanotube $C_6C_4C_8(m,n)$ and N-Napthelenic nanotube $C_6C_6C_4(m,n)$ are distinct in appearance but have the same number of vertices and procedure to assign the weight is as in above theorem and hence,

$$\gamma_R(G) = \begin{cases} p(3q+1)q \text{ is odd} \\ p(3q)q \text{ is even} \end{cases}$$

4. CONCLUSION

Domination parameters are widely used in the study of effect of drugs in protein - protein interaction (PPI) network in human as network are compared to graph, proteins are considered as vertices and connection between proteins are edges. Dominating sets are used to study the functioning of medicine to analyze the statistical significance, the enrichment of biological central genes and specificity protein genes, the enrichment in drug target for the proper cellular functioning. Domination number of pyrene, Balaban Cage-10, Hexabenzocoronene, H-Phenylenic nanotube and N-Napthelenic nanotube is been studied to find their chemical properties. Mat lab is used to find the graph properties such as domination number, vertices, edges, internal vertices, external vertices, vertices of degree two, three of benzoids such as anthracene, naphthalene, phenanthrene are studied to find the properties of their chemical structures. Benzoids which are made up of hexagons are studied for removal and non-removable hexagons. Domination number of benzoid are studied in terms of hexazons, domination of catacondensed benzoid are studied in terms of number of its vertices.

In this paper we have done a brief survey on application of chemical graph theory and obtained Roman domination number of alkane, alkene and alkyes in terms of number of carbon

atoms they contain along with their uses. We obtained Roman domination number of hexagonal chain pyrene, Hexabenzocor onene, H-Phenylenic nanotube and N-Napthelenic nanotube based on number of hexagon.

CONSENT

It is not applicable.

ETHICAL APPROVAL

It is not applicable.

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COMPETING INTERESTS

Authors have declared that no competing interests exist.

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