RESEARCH ARTICLE

Results on Domination and Chromatic Numbers of Rhombus Silicate Molecular Structure

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Abstract

In this article, we specially focused on rhombus silicate molecular structure. Graph is a data structure for describing complex systems, which contains a set of objects and relationships. A molecular graph, also known as a chemical graph, is a graph-theoretic representation of the structural formula of a chemical compound used in chemical graph theory and mathematical chemistry. A chemical graph is a labelled graph whose edges represent covalent bonds and vertices represent the atoms. A set of vertices (atoms) of a graph G is known as its dominating set with respect to the vertices, if every vertex other than that set is adjacent to some vertex in set. The vertex and edge dominating sets, total domination and chromatic number of rhombus silicate structure has been discussed in this article.

Keywords: domination set $\Upsilon(G)$, domination number with respect to vertices, total domination $\Upsilon_t(G)$, edge domination number $\Upsilon'(G)$, chromatic number, rhombus network.

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1 Introduction

A graph $G(V, E)$ with vertex set V and edge set E is connected if there exists a connection between any pair of vertices in G. A network is simply a connected graph having no multiple edges and loops. A chemical graph is a graph whose vertices denote atoms and edges denote bonds between that atoms of any underlying chemical structure. The degree of a vertex is the number of vertices that are connected to that fixed vertex by the edges. In a chemical graph, the degree of any vertex is at most 4.

Graph theory is used for mathematical gearing of the chemical compound in order to get deep unsightly observation of sensible properties of chemical compounds. Physical properties just like boiling point, are interconnected to the 3-dimensional structure of the chemical compounds. Chemical bonds are symbolized as edges and atoms symbolised as vertices in the graph. A graph can be recognised as a sequence of number, a matrix, a numeric number or a polynomial and these representations are uniquely defined for a graph [1].

To understand the whole network its essential to know about the basics of silicate structure SiO_4 tetrahedron. Silicates [12] are the largest most interesting and the most complex mineral type structure. SiO_4 is the fundamental unit of silicate [8]. When all the silicon

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nodes are deleted from a SiO_4 tetrahedron molecule, the obtained structure is an oxide structure.

Mathematical study of domination in graph theory began around 1960's. We discuss results related to domination of rhombus silicate molecular structure [16]. We also provide some fundamental definitions about graph in general, followed by a discussion of domination in graphs [3, 6, 11].

Chemical graph theory, often known as molecular [21] topology, is an interdisciplinary subject that uses graph theory to explore molecular structures. It makes an effort to pinpoint the structural elements involved in correlations between structure-property and activity relationships [20], utilising methods from graph theory, set theory, and statistics. The classification of molecules and modelling of unidentified structures with desired features are made possible by topological characterisation of chemical structures.

2 Domination Graphs

In this section, we discuss about the vertex and edge domination sets, total domination of graphs.

2.1 Vertex Domination

The concept of dominating sets with respect to the vertices [14, 15, 17, 18] is defined as a set D of vertices in a graph $G = (V, E)$ is a dominating set if every vertex $v \in V$ is a member of D or adjacent to the member other than D however, the member of subset D is not adjacent to each other. A dominating set D is a minimal dominating set if no proper subset $D' \subset D$ is a dominating set. The vertex domination number $\Upsilon(G)$ of a graph G is the minimum cardinality of a dominating set of G [10]. We call such a set as Υ-set of G.

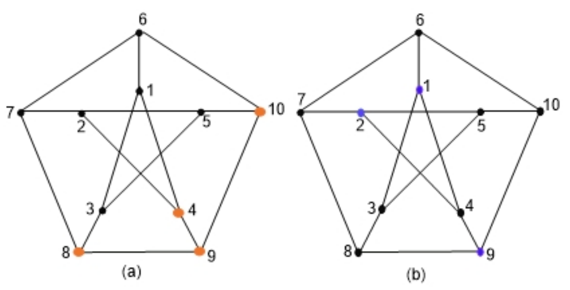

Figure 1. Domination number & total domination number of peterson graph.

2.2 Total Domination

The total domination number Υ_i of a graph is the magnitude of a smallest total dominating set [2, 7], where a total dominating set is a set of vertices of the graph such that all vertices (counting those in the set itself) have a neighbor in the set. Total dominating number [6] are defined for connected graphs.

For example, in the Peterson graph [5] illustrated above, $T(P) = 3$. Since the set $S = \{1, 2, 9\}$ is a least possible dominating set, as shown in Figure 1(a), while $T_t(p) = 4$ because $S^t = \{4, 8, 9, 10\}$ is the minimum total dominating set as shown in Figure 1(b).

For undirected simple graph G with no multiple edges, the total vertex domination number T^t and vertex domination number T satisfies [12]:

$$T \leq T_t \leq 2(T).$$

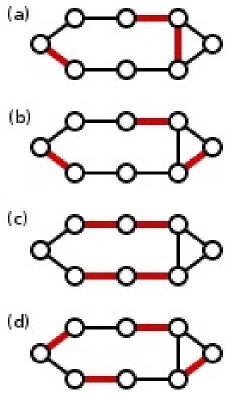

Figure 2. Edge domination.

2.3 Edge Dominating Set

Arumugam and Velammal [4] proposed the idea of edge domination number of graphs. If a subset of the edges of the graph S contain disjoint lines or disjoint edges of graph G, then S is known as edge dominating set. The edge domination number $T'(G)$ of the graph G is the minimum cardinality taken over all the edge dominating sets of graph.

The above Figures 2(a) and 2(c) shows the connected edge dominating number and Figure 2(b) shows the minimum edge dominating sets and Figure 2(d) are the dominating sets but not the dominating numbers because their cardinalities are equal to 4, which is not the least dominating set according definition. For literature about chromatic numbers, see [9].

In this section, we discuss the method of finding chromatic number of Rhombus type networks.

By far the most intriguing mineral class is silicate. Metal oxides or metal carbonates are fused with sand to produce these. As a basic unit, SiO_4 tetrahedra can be found in all silicates [22]. The corner vertices of the SiO_4 tetrahedron represent oxygen ions in chemistry, while the centre vertex represents silicon ions. In graph theory, the corner vertices are referred to as oxygen nodes, while the centre vertex is referred to as a silicon node. Different silicate structures can be obtained by arranging the tetrahedron silicate in different ways. Similarly, different silicate structures build different silicate networks [23]. Figure 3 depicts a three-dimensional rhombus silicate network of dimension 2. In general, the vertices and edges of a rhombus silicate of dimension n are $5n^2 + 2n$ and $12n^2$ respectively [13].

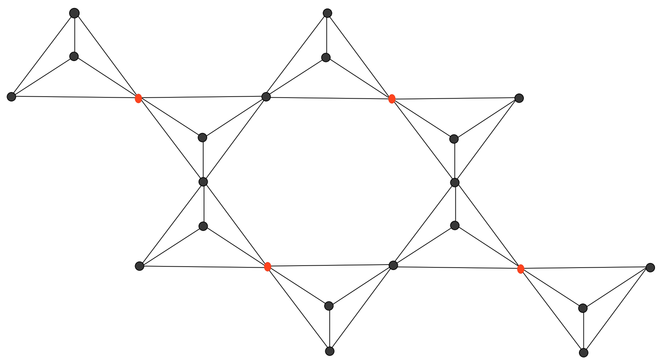

Figure 3. Rhombus silicate network $RhSl(2)$.

3 Algorithm for Graph Vertex Coloring

There is no well organized algorithm for coloring of the nodes in simple graph with least number of colors. The following algorithm is studied for locating the chromatic number of the graph G.

- Color first vertex with any color, say C_1. Then, color the remaining $(n-1)$ vertices one by one, by observing the following these instructions:
- Select a vertex and colored it with unadapted color of its adjacent vertices.
- If the has been adapted, then choose the next color for the vertex.
- If selected colors have been utilized, then allot a new or unused color to the presently chosen vertex.

3.1 Chromatic Number

The node colouring of a simple graph G with k (minimum number of colors) colours is the process of assigning colour to each of the node of G such that adjacent nodes does not have the identical colours. The chromatic number of a graph G is denoted by $\Upsilon(G)$.

4 Results for Rhombus Silicate Molecular Structure

In the following theorems, we computed the vertex and edge dominating sets, total domination and chromatic number of rhombus silicate structure.

Theorem 4.1. *For G be the Rhombus silicate network $RhSl(n)$, the domination number $\Upsilon(G) = n^2$, where $n \in \mathbb{N}$.*

Proof. By using mathematical induction:

For $n = 1$ it is $T(G) = 1 = n^2$, correct.

We have to add at the right hand side one, below one, and at the corner right below also one vertex: $1 + 1 + 1 + 1 = 4$.

Step induction assumption: For $n = k$ holds $T(G)) = k^2$. The "dimension" of Rhombus silicate network as the number of vertices existing in every side of the network as shown in Figures 3 and 4. Thus the $n = k$-network has k vertices at every side.

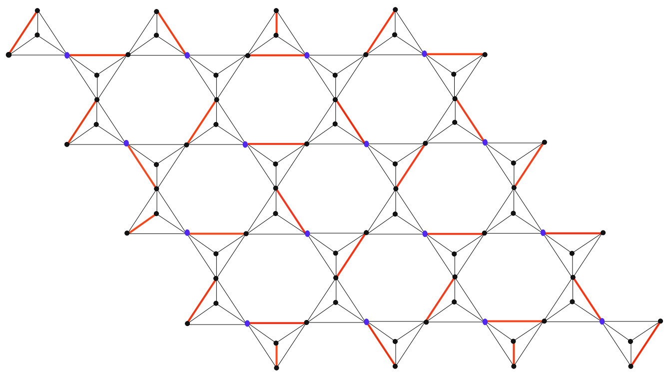

Figure 4. Rhombus oxide silicate network $RhSl(4)$.

Step induction proof: We claim that for $n = k+1$ holds $T(G) = (k+1)^2$.

We can look for the Rhombus type network in the cases k and $k+1$: the step to $k+1$ needs additional vertices: We have to add at the right hand side k, below k, and at the corner right below still one vertex: $k^2 + k + k + 1 = (k+1)^2$. □

Theorem 4.2. *Let G be a rhombus silicate network $RhSl(n)$, the $T'(G) = \frac{3}{2}n^2 + \frac{3}{2}n$, where $n \in \mathbb{N}$.*

Proof. To prove the statement first of all we have to determined the edge domination number [4] separately for each dimension by using the definition of edge domination. Dimension wise the sequence of edge domination is: $3, 9, 18, 30, 45, \cdots$ so on respectively. As red lines in Figure 4 represents the edge domination number of 4-Dimension of Rhombus oxide silicate network which can also be written as $RhSl(4)$. Now with the help of this sequence we proceeds toward the required result.

Step I Find the first difference between terms:

$$9-3=6, 18-9=9, 30-18=12, 45-30=15$$

Step II Find the second difference between terms:

$$9-6=3, 12-9=3, 15-12=3$$

Therefore, there is a common second difference of $+3$. We can therefore conclude that this is a quadratic sequence of the form:

$$T_n = un^2 + vn + w \quad (1)$$

Step III Determine general term to find u, v, w for equation (1). We look first three terms in the sequence.

$$n=1 : T_1 = u+v+w$$
$$n=2 : T_2 = 4u+2v+w$$
$$n=3 : T_3 = 9u+3v+w$$

We know that, $T_1 = 3, T_2 = 9, T_3 = 18$

$$n=1 : 3 = u+v+w \quad (2)$$
$$n=2 : 9 = 4u+2v+w \quad (3)$$
$$n=3 : 18 = 9u+3v+w \quad (4)$$

Subtract equation (2) from Equation (3), we have

$$\begin{aligned} T_2 - T_1 &= 4u+2v+w-(u+v+w) \\ & 9-3 = 4u-u+2v-v+w-w \\ & 6 = 3u+v \end{aligned} \quad (5)$$

Subtract equation (3) from equation (4), we have

$$\begin{aligned} T_3 - T_2 &= 9u+3v+w-(4u+2v+w) \\ & 18-9 = 9u-4u+3v-2v+w-w \\ & 9 = 5u+v \end{aligned} \quad (6)$$

Subtract equation (5) from equation (6), we have

$$9-6 = 5u+v-(3u+v)$$
$$3 = 5u-3u+v-v$$
$$3 = 2u$$
$$\frac{3}{2} = u$$

Put the value of u in equation (5), we have

$$6 = 3(\frac{3}{2}) + v$$
$$\frac{3}{2} = v$$

Put values of u and v in equation (2)

$$3 = \frac{3}{2} + \frac{3}{2} + w$$
$$w = 0$$

Now put values of u, v and w in equation (1)

$$T_n = \frac{3}{2}n^2 + \frac{3}{2}n + 0$$
$$\Rightarrow \Upsilon'(G) = \frac{3}{2}n^2 + \frac{3}{2}n$$

Hence, this is the required result for edge domination number of Rhombus Silicate network $RhSl(n)$. □

Theorem 4.3. *Let G be a rhombus silicate network $RhSl(n)$, the $\Upsilon_t(G) = 2n^2 - 1$, where $n \in \mathbb{N}$.*

Proof. Let $G \cong RhSl(n)$, for total dominating set, we are looking for the least cardinality subset of G, such that the elements of subset, adjacent to itself as well as to the elements other than that subset as shown in Figure 6. For first dimension, the vertex total domination number is 1.

By using mathematical induction.

For: $RhSl(1)$

$$\Upsilon_t(G) = 1$$

Which can also be written in the form: $\Upsilon_t(G) = 2-1$

$$\Upsilon_t(G) = 2(1)^2 - 1$$

Base Case (n=1): Consider $RhSl(1)$. As shown in Figure 5, the minimal total dominating set requires only one vertex. This vertex is adjacent to all other vertices in the network, satisfying the total domination condition. Thus: $\Upsilon_t(G) = 2n^2 - 1$

The result is true for $n = 1$.

By using the principal of induction. Suppose $\Upsilon_t(G)$ is correct for any $n = k \in W$. That is, $RhSl(k) = 2k^2 - 1$ represents an integer.

Now, we want to show that for $RhSl(k+1)$. For $n = k+1$, the statement becomes:

$$RhSl(k+1) = 2(k+1)^2 - 1 = 2k^2 + 4k + 2 - 1$$

As $2k^2 + 4k + 1$, $k \in W$. Hence, both the conditions are satisfied, we conclude that the given statement is true $\forall n \in \mathbb{N}$. □

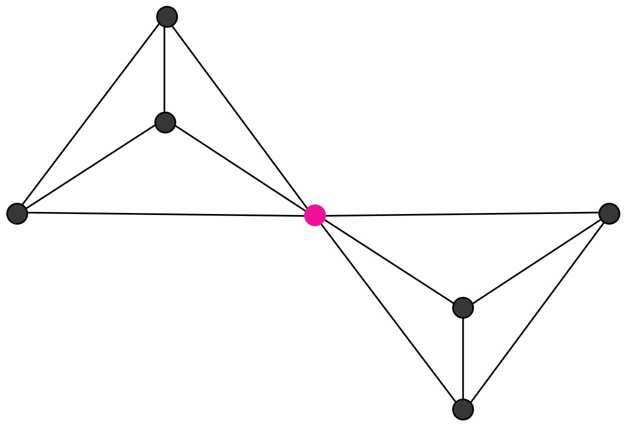

Figure 5. Vertex total domination of rhombus silicate network $RhSl(1)$.

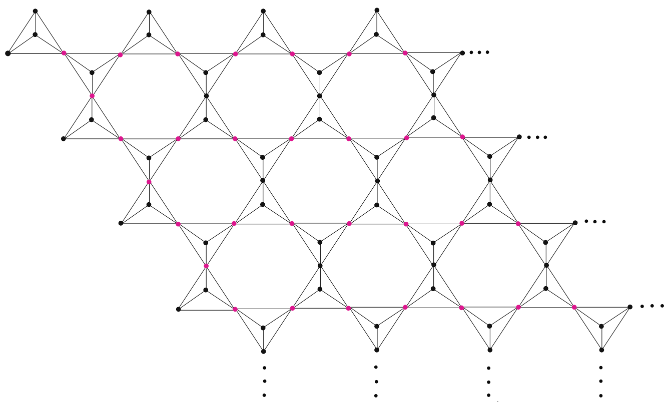

Figure 6. Vertex total domination of rhombus silicate network $RhSl(n)$ $(\Upsilon_t(G).)$

Theorem 4.4. *For Rhombus Silicate Network $RhSl(n)$, the chromatic number is 4.*

Proof. **Case I**

For $RhSl(1)$

Supposed that we have 1-dimension of Rhombus silicate network. To determine the chromatic number we need to colour all the vertices in such manner that adjacent vertices not having the selfsame colour. To fulfill such requirement their are minimum 4 colour to be needed for the colouring of the network. As shown in Figure 7.

Case II For $RhSl(2)$

Suppose that, we have 2-dimension of Rhombus silicate network. To determine the chromatic number

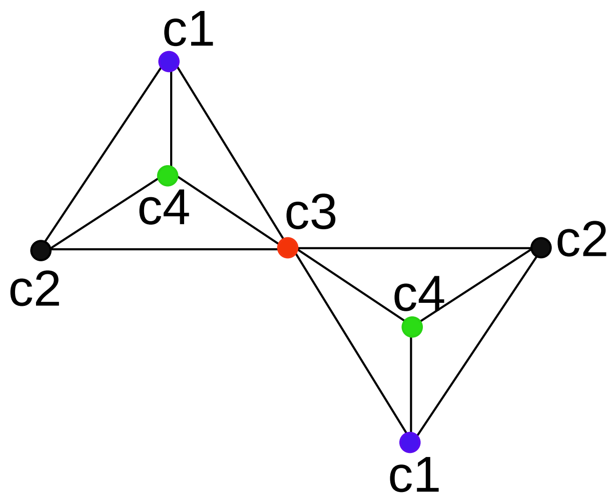

Figure 7. Colouring of $RhSl(1)$.

we need to colour all the vertices in such manner that adjacent vertices not having the same colour. To fulfill such requirement their are minimum 4 colour to be needed for the colouring of the network. As shown in Figure 8.

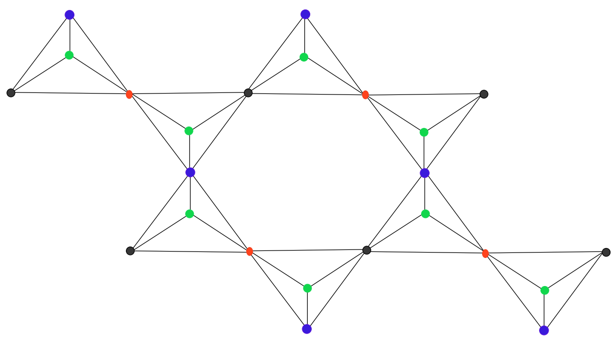

Figure 8. Colouring of $RhSl(2)$.

Case III

For $RhSl(3)$

Supposed that we have 3-dimension of Rhombus silicate network. To determine the chromatic number we need to colour all the vertices in such manner that adjacent vertices not having the identical colour. To fulfill such requirement their are minimum 4 colour to be needed for the colouring of the network. As shown in Figure 9.

- Blue→ C1.
- Black→ C2.

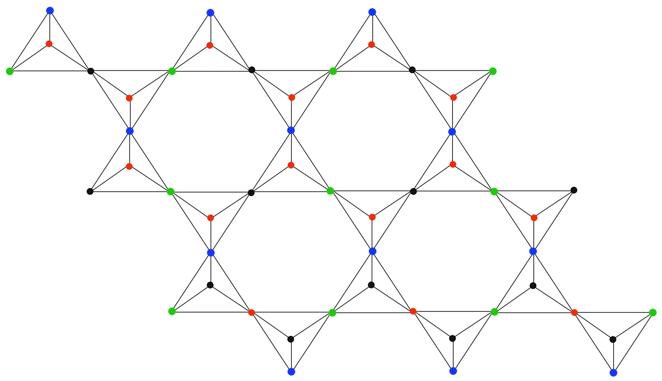

Figure 9. Colouring of $RhSl(3)$.

- Red $\rightarrow$ C3.
- Green$\rightarrow$ C4.

So, it is proved that to colour Rhombus silicate network Colouring of $RhSl(n)$. we need minimum 4 different colours in such manner that adjacent vertices not having identical colour and the statement is true for all $n \in \mathbb{N}$. □

5 Results for Rhombus Hex Derived network of type 3 Molecular Structure

In the following theorems, we computed the vertex and edge dominating sets, total domination and chromatic number of rhombus silicate structure.

Theorem 5.1. *For every n, if n is a natural number, then for $RhHDN_3(n)$ network $\Upsilon(G)$ is:*

$$\Upsilon(G) = \begin{cases} 3, & n = 1; \\ 2n^2, & n \geq 2; \end{cases}$$

Proof. **Case I**

Assume that $n = 1$ than, by definition of domination number we find only 3 vertices in 1st dimension of $RhHDN_3(n)$ which fulfill all the requirements of dominating vertices. Therefore, $\Upsilon(G) = 3$ for $n = 1$.

Case II

For $n = 2$ With out any lose of generality, by using the basic concept of domination we are locating for a subset of minimum vertices which satisfied the criteria of domination. In this case their are minimum 8 vertices as shown in Figure 9 the blue vertices. Mathematically, can be written as:

$$\Upsilon(G) = 8$$
$$\Upsilon(G) = 2(4) \Rightarrow 2(2)^2 \Rightarrow 2n^2$$

The structure of $RhHDN_3(2)$ is shown in Figure 10. Through systematic analysis, we identify that the minimum dominating set consists of 8 vertices, as indicated by the blue vertices. These vertices are strategically positioned such that every vertex not in the set is adjacent to at least one vertex in the set, satisfying the domination condition.

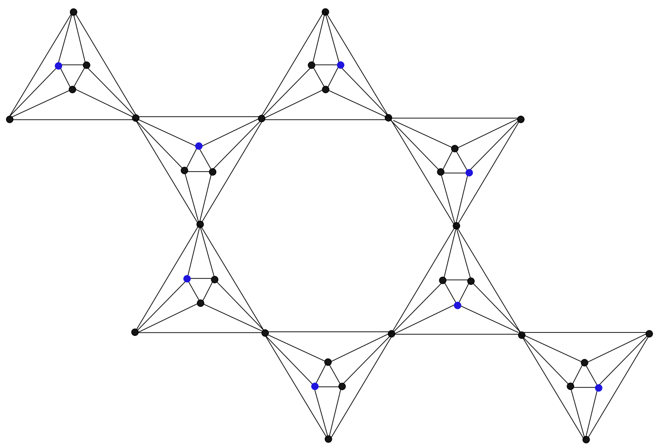

Figure 10. $RhHDN_3(2)$.

The cardinality calculation yields:

$$\Upsilon(G) = 8 = 2 \times 4 = 2(2)^2 = 2n^2$$

This result aligns with the proposed formula for $n \geq 2$.

Case III

For $n > 2$

Assume that $n = 3$ By using definition of domination number we get minimum 18 vertices which dominates the system. As shown in Figure 11 the blue vertices can be represented in mathematic form as:

$$\Upsilon(G) = 18$$
$$\Upsilon(G) = 2(9) \Rightarrow 2(3)^2 \Rightarrow 2n^2$$

For the third dimension, Figure 12 illustrates the structure of $RhHDN_3(3)$. By applying the domination criteria, we determine that the minimum dominating set requires 18 vertices, as marked in the figure. This result validates the general formula:

$$\Upsilon(G) = 18 = 2 \times 9 = 2(3)^2 = 2n^2$$

The pattern established in lower dimensions continues to hold for $n = 3$.

Concluding Remarks: By the observation of above three cases, the given statement is true for all $n \in \mathbb{N}$. In $RhHDN_3(n)$, which is the required result. □

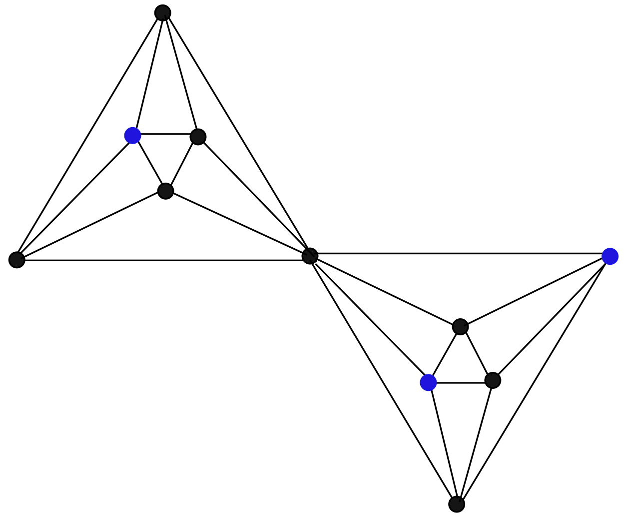

Figure 11. $RhHDN_3(1)$.

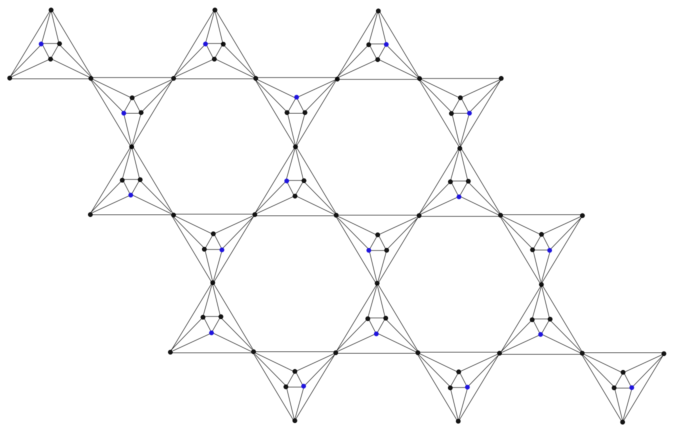

Figure 12. $RhHDN_3(3)$.

Theorem 5.2. *Let edge domination $\Upsilon'(G)$ of $RhHDN_3(n)$ is $3n^2+n$, iff the sequence of dimensions of $RhHDN_3(n)$ is $4, 14, 30, 52, \cdots$.*

Proof. Consider the sequence of $RhHDN_3(n)$ is $4, 14, 30, 52, \cdots$. Now we have to prove that the edge domination $\Upsilon'(G) = 3n^2+n$.

Step I Find the first difference between terms:

$$14-4=10, 30-14=16, 52-30=22$$

Step II Find the second difference between terms:

$$16-10=6, 22-16=6$$

So, there is a common second difference of $+6$. We can therefore conclude that this is a quadratic sequence of the form:

$$T_n = un^2+vn+w \tag{7}$$

Step III Determine general term to find u, v, w for equation (7). We look first three terms in the sequence.

$$n=1: T_1 = u+v+w$$
$$n=2: T_2 = 4u+2v+w$$
$$n=3: T_3 = 9u+3v+w$$

We know that, $T_1 = 4, T_2 = 14, T_3 = 30$

$$n=1: 4 = u+v+w \tag{8}$$
$$n=2: 14 = 4u+2v+w \tag{9}$$
$$n=3: 30 = 9u+3v+w \tag{10}$$

Subtract equation (8) from equation (9).

$$T_2 - T_1 = 4u+2v+w-(u+v+w)$$
$$14-4 = 4u-u+2v-v+w-w$$
$$10 = 3u+v \tag{11}$$

Subtract equation (9) from equation (10).

$$T_3 - T_2 = 9u+3v+w-(4u+2v+w)$$
$$30-14 = 9u-4u+3v-2v+w-w$$
$$16 = 5u+v \tag{12}$$

Subtract equation (11) from equation (12).

$$16-10 = 5u+v-(3u+v)$$
$$6 = 5u-3u+v-v$$
$$6 = 2u$$
$$3 = u$$

Put the value of u in equation (11).

$$10 = 3(3)+v$$
$$1 = v$$

Put values of u and v in equation (8).

$$4 = (3)+(1)+w$$
$$w = 0$$

So, put values of u, v and w in equation (7).

$$T_n = 3n^2+n$$
$$\Rightarrow \Upsilon'(G) = 3n^2+n$$

Hence, this is the required result.

Converse:

Now we have to that the converse of the statement also exist. So, we assume that the general for edge domination $\Upsilon'(G) = 3n^2 + n$ of $RhHDN_3(n)$, where $n = 1, 2, 3, 4, \cdots$.

For n=1

Applying the formula $\Upsilon'(G) = 3(1)^2 + 1 = 4$. This result is visually confirmed in Figure 13, which demonstrates the edge domination set for $RhHDN_3(1)$ consisting of exactly 4 edges that satisfy the edge domination criteria.

$$\Upsilon'(G) = 3(1)^2 + 1 \Rightarrow \Upsilon'(G) = 4$$

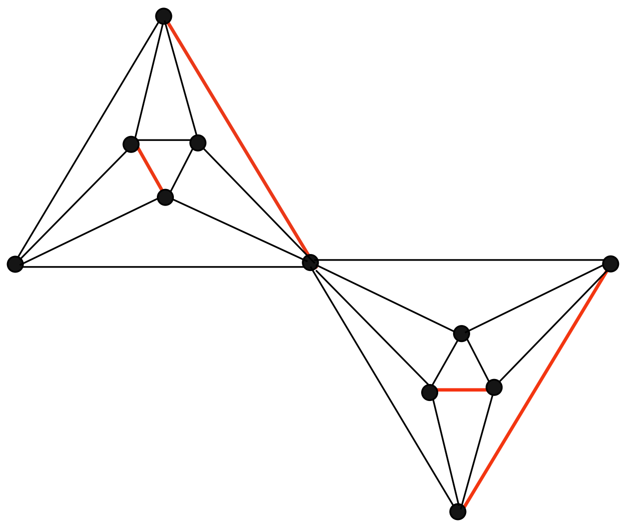

Figure 13. Dominating edges of $RhHDN_3(1)$.

For n=2

The edge domination pattern for $RhHDN_3(2)$ is illustrated in Figure 14. The diagram clearly shows 14 edges that form a minimal edge dominating set, confirming the computational result:

$$\Upsilon'(G) = 3(2)^2 + 2 = 12 + 2 = 14$$

This exact correspondence between the formula and the visual representation in Figure 14 strongly supports the validity of the general formula.

For n=3

The complexity of edge domination in higher dimensions is demonstrated in Figure 15, which shows the minimal edge dominating set for $RhHDN_3(3)$. The configuration consists of exactly 30 edges, validating the computational result:

$$\Upsilon'(G) = 3(3)^2 + 3 = 27 + 3 = 30$$

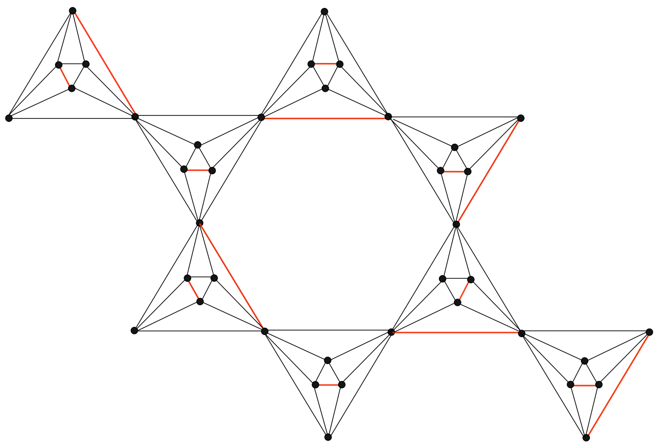

Figure 14. Dominating edges of $RhHDN_3(2)$.

The precise alignment between the formula and the visual evidence in Figure 15 confirms the pattern for $n = 3$.

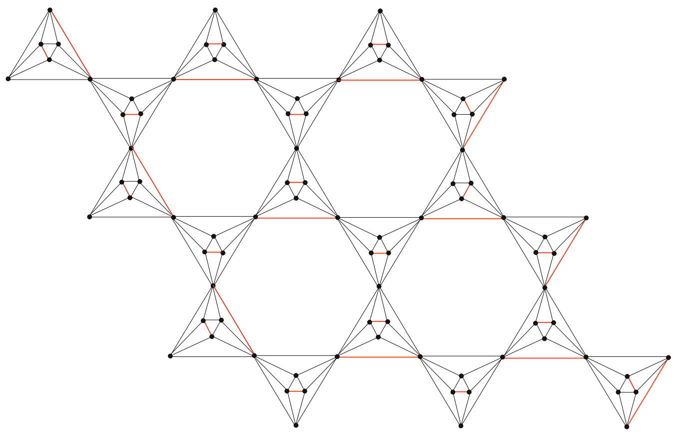

Figure 15. Dominating edges of $RhHDN_3(3)$.

For n=4

$$\Upsilon'(G) = 3(4)^2 + 4 \Rightarrow \Upsilon'(G) = 52$$

By the variation of n we get the sequence of terms : 4, 14, 30, 52,... which is our required sequence. Hence the conversed of the given statement is also true. □

Theorem 5.3. *For $RhHDN_3(n)$, the total domination is $\Upsilon_t(G) = 4n^2 - 1$, where $n \in \mathbb{N}$.*

Proof. Let $G \cong RhHDN_3(n)$ is the set of whole vertices, than for the total domination. we are locating for the least cardinality subset of $G(V)$ such that the elements of subset adjacent to them self as wall as to the elements other than that subset. By using mathematical induction.

For: $RhHDN_3(1)$

$$\Upsilon_t(G) = 3$$

According to the general formula: $\Upsilon_t(G) = 4n^2 - 1$

than, $\Upsilon_t(G) = 4(1)^2 - 1$

$$\Upsilon_t(G) = 4 - 1$$

$$\Upsilon_t(G) = 3$$

$$3 = 3 \text{ (True for } n = 1)$$

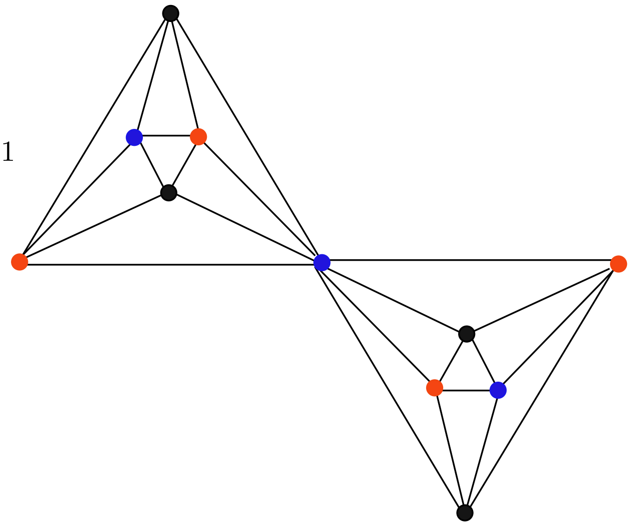

Figure 16. Colouring of $RhHDN_3(1)$.

(By using the principal of induction)let us imagine that $\Upsilon_t(G)$ is accurate for any $n = k\epsilon W$. That is, $RhSl(k) = 4k^2 - 1$ represents an integer.

Now we want to show that $RhHDN_3(k+1)$ is also an integer. For $n = k+1$,the statement becomes:

$$\begin{aligned} RhHDN_3(k+1) &= 4(k+1)^2 - 1 \\ &= 4(k^2 + 2k + 1) - 1 \\ &\Rightarrow 4k^2 + 8k + 4 - 1 \end{aligned}$$

As $4k^2 + 8k + 3$ is also an integer because we know that $k \in W$. Since both the conditions are satisfied, we conclude that the given statement is true $\forall n \in \mathbb{N}$. □

Theorem 5.4. *For Rhombus Network $RhHDN_3(n)$, the chromatic number is 3.*

Proof. **Case I**

For $RhHDN_3(1)$

Now we have to determine the chromatic number of 1-dimension. We need to colour all the vertices in such manner that no adjacent vertex having the identical colour. To fulfill such requirement their are minimum 3 colour to be needed for the colouring of the network, as shown in Figure 16.

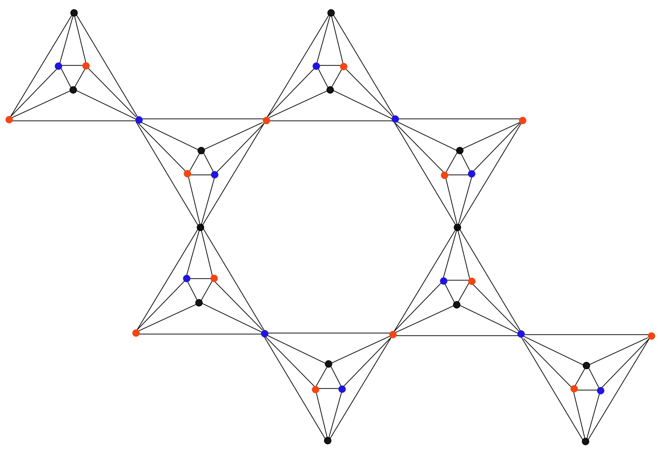

Figure 17. Colouring of $RhHDN_3(2)$.

Case II

For $RhHDN_3(2)$

Suppose that, we have 2-dimension of network. To determine the chromatic number we need to colour all the vertices in such manner that no adjacent vertex having the selfsame colour. To fulfill such requirement their are minimum 3 colour to be needed for the colouring of the network, as shown in Figure 17.

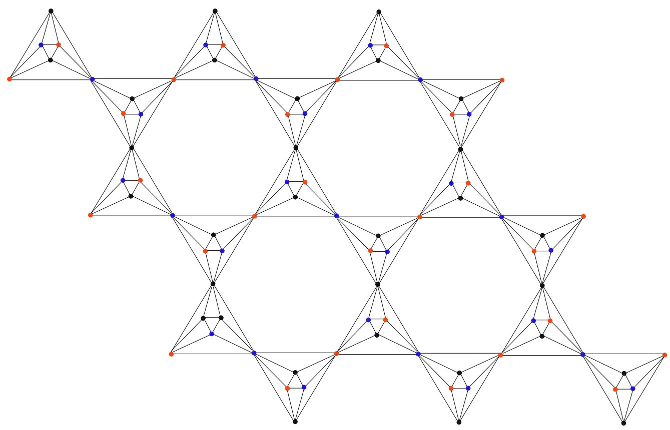

Figure 18. Colouring of $RhHDN_3(3)$.

Case III For $RhSl(3)$.

Suppose that, we have 3-dimension of network. To determine the chromatic number [19] we need to colour all the vertices in such manner that no adjacent vertex having the selfsame colour. To fulfill such requirement their are minimum 3 colour to be needed for the colouring of the network, as shown in Figure 18.

- Blue→ C1.

- Black→ C2.
- Red → C3.

So, it is proved that to colour the network Colouring of $RhHDN_3(n)$. we need minimum 3 different colours and the statement is true for all $n \in \mathbb{N}$. □

6 Conclusion

In this article, we focused on rhombus silicate molecular structure. Graph is a data structure for describing complex systems, which contains a set of objects and relationships. A molecular graph, also known as a chemical graph, is a graph-theoretic representation of the structural formula of a chemical compound used in chemical graph theory and mathematical chemistry. A chemical graph is a labelled graph whose edges represent covalent bonds and vertices represent the atoms. A set of vertices (atoms) of a graph G is known as its dominating set with respect to the vertices, if every vertex other than that set is adjacent to some vertex in set. The vertex and edge dominating sets, total domination and chromatic number of rhombus silicate structure has been discussed in this article.

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Data will be made available on request.

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Conflicts of Interest

The authors declare no conflicts of interest.

Ethical Approval and Consent to Participate

Not applicable.

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