

Analysing Ice Crystalline Structure Using Domination And Fractals

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Abstract: Water plays an important role within the evolution and survival of life. Ice is a solid substance which is obtained by water in its frozen state. Fractals are capable of describing many irregularly shaped objects. The aim of this Paper is about the Crystalline Structure of Ice which is a connected simple graph and identifies that its Structure is a dominating set and it exhibits the fractal structure of the graph.

Keywords: Ice Crystalline Structure, Dominating set, Self Similarity.

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I.INTRODUCTION

Water is one among the essential substance present within the earth. Water is out there in nature in three forms-solid, Liquid, Vapour. Water molecules within the solid state like in ice and snow, form hydrogen bonds to at least one another. Ordering water ice forms under ambient conditions and has two poly types, hexagonal ice and cubic ice. These ordered arrangements end in the symmetrical hexagonal shape of the snowflake. The molecular structure of the ice crystal is considered as a collection of overall water molecule arranged in a lattice structure. The structure of ice hexagonal form if water crystallizes at normal pressure and structure of ice is cubic in nature if water crystallizes at very coldness [1, 2 ,3]. A graph 'G' is a set of vertex which are connected by edges. Graphs play a vital role in real life applications [4,5,6,7]. A molecular graph will be related to a set if it will be shown that a topological structure is outlined upon its vertex set [8,9]. Fractals are elegant structures made by nature. Instead shapes that show inherent and continuation similarities are the most essential for being classified as a fractal. Self-Similarity is the property that describes a substructure which is itself similar to an overall structure [10,11,12].

II. MAIN RESEULTS

As a crystalline inorganic solid with an ordered structure, ice is taken into account to be a mineral. It possesses a daily crystalline structure supported the molecular structure of water. The scientific name for water is H₂O. It's called H₂O because it's two atoms of hydrogen (H) and one atom of oxygen (O).

The following figure 1(a) and 1(b) shows that Structure of water molecule and crystalline structure of ice respectively.

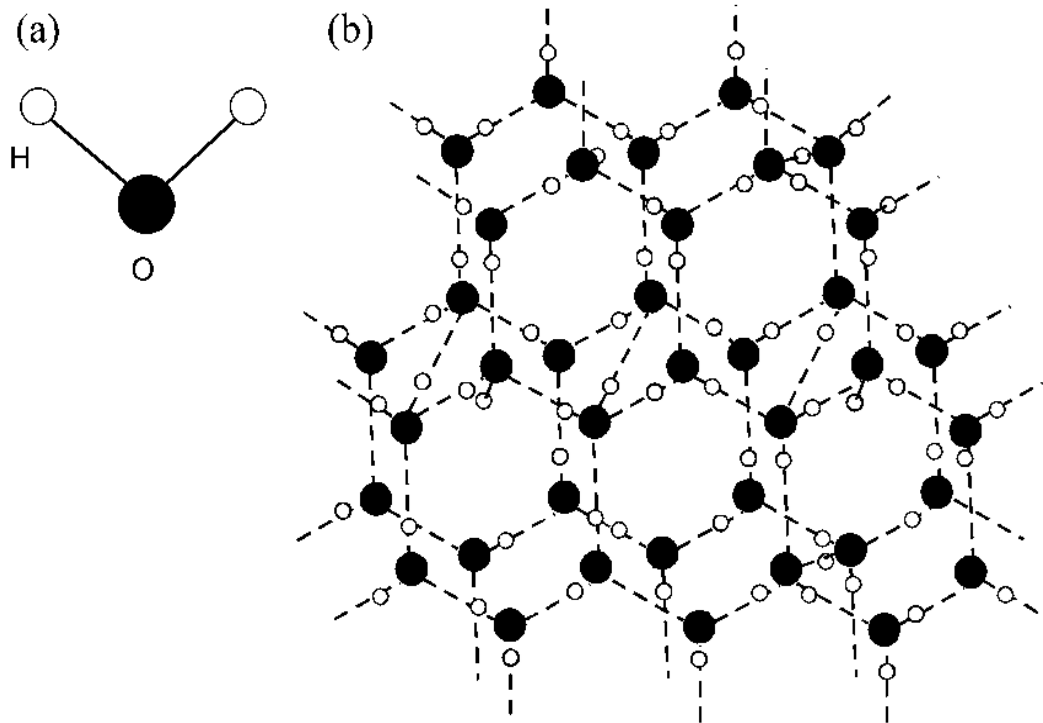


Figure 1. (a) Water molecule structure (b) Ice molecule structure.

Here oxygen atoms are represented by dark circles and hydrogen bonds by lines which link the corresponding faded circles. Our assumption of this paper is that each Oxygen atom as vertices and hydrogen bonds as edges. The connectivity of molecular structure of ice is fundamental to the functioning of connected simple graph. Here vertex set and edge set are considered as infinite sets because of open Ice crystalline structure.

Proposition 2.1 Let G_I be a simple connected graph with Ice crystalline structure at normal pressure, then (i) G_I contains no cut vertex.

(ii) Every vertex in the graph G_I is a dominating vertex.

Proof.

Given G_I is a simple connected graph with Ice crystalline structure at normal pressure.

Let us assume that each oxygen atom as a vertex and hydrogen bond as an edge.

Let O be a vertex set with o_i vertices and E be an edge set with e_i edges in the graph G_I .

(i) To prove : G_I contains no cut vertex.

Suppose one vertex is a cut vertex.

By definition of cut vertex, when removed it from a graph makes more components in the graph.

Then the graph $G_I - o_i$ is disconnected for some i .

From this, we get two components of the graph.

This is not possible in Ice hexagonal crystalline structure.

Therefore, there is no cut vertex in G_I for all i .

(ii) To prove : every vertex in the graph G_I is a dominating vertex.

We have claim that $V(G_I)$ is a dominating set.

Since the graph G_I has no isolated vertices, Each and every vertex in the graph G_I has an adjacency by hydrogen bond.

Therefore every vertex in the graph G_I is a dominating vertex.

Proposition 2.2 Let G_I be a simple connected graph with Ice crystalline structure, then every vertex cover is a dominating set.

Proof.

Let G_I be a simple connected graph with infinite vertex set and infinite edge set.

Let us assume that $V(G_I)$ be a vertex set and $E(G_I)$ be an edge set.

Let $S(G_I)$ be a vertex cover.

It is enough to show that $S(G_I)$ is a dominating set.

Let u and v be a vertex in G_I .

Suppose v does not belong to $S(G_I)$ and u belongs to $S(G_I)$.

We know that G_I has no isolated vertices.

Then v has some neighbor u .

Since $S(G_I)$ is a vertex cover, it must contain one of v, u .

Since v does not belong to $S(G_I)$, there is u which belongs to $S(G_I)$.

So v has a neighbor u which is in $S(G_I)$.

Therefore $S(G_I)$ is a dominating set.

Proposition 2.3 *Let G_I be a simple connected graph with Ice crystalline structure at normal pressure, then the graph G_I exhibits the fractal structure.*

Proof.

Clearly Ice crystalline structure at normal pressure forms Hexagonal Structure from Figure 1.

This Ice crystalline Hexagonal Structure is exactly similar to a part of itself.

So this graph G_I satisfies Self Similarity property.

Then the graph G_I forms recurring pattern of Hexagonal structure.

Since the graph G_I is infinite vertex set of open Ice crystalline structure.

From this, we can conclude that this Ice crystalline Hexagonal Structure has never ending recursion pattern.

Hence there exists similar pattern of Hexagonal Structure of the graph G_I .

Therefore, the graph G_I exhibits the fractal structure.

III. CONCLUSION

Chemical graph theory is one of the parts of mathematical chemistry which put in graph theory to mathematical modeling for molecular graph of chemical compounds. This paper obtains the Crystalline Structure of Ice is a dominating set and it preserves self-similarity. Hence it concludes that Ice Crystalline Structure exhibits the fractal structure.

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