Medium Domination Number in Linear Polyacene

S.Venkatesan, M.Raji, G.Jayalalitha

Abstract— *Let G(V,E) be a finite, connected graph. The set of vertices and edges of G are denoted by V=V(G) and E=E(G) respectively. In such a Molecular graph, vertices represent atoms and edges represent bonds. In this paper, it obtains Medium Domination Number in the Molecular Graph of Organic Compounds and proves by induction method.*

Keywords: Dominating set, Medium Domination Number, Internally Disjoint Path, Molecular Graph.
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1. INTRODUCTION

For a Molecular Graph, vertices denote atoms and edges denote bonds[8]. The structure of Molecular graph may be connected, undirected, loop less graph. In a graph, each vertex is able to protect every vertex in its neighborhood and in domination every vertex needs to be prevented. In such case, it is required to inspect the number of vertices those are dominating each pair of vertices. The summation of vertices that dominate every set of vertices and mean value of this is defined as the medium domination number of a graph[2].

Chemical graph theory is based on Mathematics which mixes graph concepts and chemistry. Graph theory is applied to mathematically model molecules so as to achieve insight into the physical properties of those chemical compounds. Chemical graph is a suitable model for any real or abstracted chemical system. Let L (h) be the Linear Polyacene with h hexagons. Knowing that If L (h) is a Linear Polyacene with h hexagons, then $n(L(h))=4h+2$.If L(h) is a Linear Polyacene with h hexagons ,then $Y(L(h))=h+1$.where No. of vertices is $n(L(h))$ and Domination No. of Linear Polyacene in is $Y(L(h))$[6].In this paper, all graphs are considered as a finite, undirected graph without loops and multiple edges. here it obtains the Medium Domination number in the molecular graph of organic compounds using Induction method.

2. PRELIMINARIES

2.1 GRAPH [1]:

A graph $G = (V, E)$ consists of a nonempty set V of vertices and a set E of edges.

2.2 DOMINATING SET [2]:

A set D in a graph 'G' is a dominating set if each vertex is either in D or adjacent to a vertex in D.

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2.3 K - CONNECTED[2]

Two vertices u and v in a graph G are said to be **k - connected** if there are k or more pairwise internally disjoint paths between them.

2.4 DOMINATES EACH OTHER [2,3]

If u and v are adjacent in a graph G, they **dominates each other**, then at least

dom(u,v)=1 where dom(u,v) denotes the number of vertices that dominate both of u & v.

2.5 TOTAL DOMINATING VERTICES (TDV(G)) [2,3]

The summation of vertices that dominate every set of two vertices is defined as

$$TDV(G)=\sum_{\forall u,v \,\in V(G)} dom(u,v)\,.$$

2.6 MEDIUM DOMINATION NUMBER(MD(G))[2,3]

If the order of G is n, then Medium Domination Number is defined as

$$MD(G)=\frac{2\,TDV(G)}{n(n-1)}.$$

3. MOLECULAR GRAPH OF ORGANIC COMPOUNDS & RESULTS

In this section, it obtains Medium Domination Number for the Molecular Graph of Benzene, Naphthalene and Anthracene and also obtains Medium Domination Number Of Linear Polyacene L_h is MD(L_h) $=2 \sum_{k=1}^{h} \frac{13k-1}{(4k+2)(4k+1)}$ .Using *Theorem dom(u,v)= k_1(u,v) + k_2(u,v) where k_1 and k_2 denote the number of u-v internally disjoint paths of length 1 and 2 respectively, for calculating dominates each other of joining vertices u and v[2].*
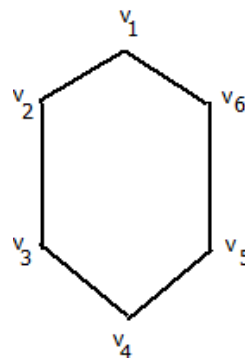
3.1 MOLECULAR GRAPH OF BENZENE

Figure 1.Molecular Graph of L_1 (Benzene)

In the Molecular Graph of Benzene ,from figure1,we get

dom $(v_1,v_2) = 1$; dom $(v_1,v_3)=1$; dom $(v_1,v_4) = 0$; dom $(v_1,v_5)= 1$; dom $(v_1,v_6)= 1$; dom $(v_2,v_3) = 1$;

dom $(v_2,v_4)= 1$; dom $(v_2,v_5) =0$; dom $(v_2,v_6) =1$; dom $(v_3,v_4)= 1$; dom $(v_3,v_5)=1$; dom $(v_3,v_6) = 0$;

dom $(v_4,v_5)= 1$; dom $(v_4,v_6)= 1$; dom $(v_5,v_6) = 1$.

TDV(G)= 12.

Medium Domination Number $= \frac{2(12)}{6(5)} = \frac{4}{5}$.
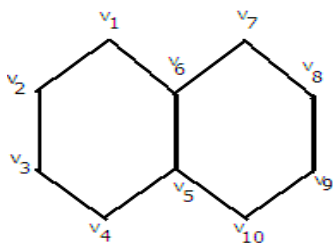
3.2 MOLECULAR GRAPH OF NAPATHALENE[5]

Figure 2.Molecular Graph of Naphthalene

In the Molecular Graph of Naphthalene, from figure 2, we get

dom $(v_1,v_2) = 1$; dom $(v_1,v_3)= 1$; dom $(v_1,v_4) = 0$; dom $(v_1,v_5)= 1$; dom $(v_1,v_6)= 1$; dom $(v_1,v_7)= 1$;

dom $(v_1,v_8)= 0$; dom $(v_1,v_9)= 0$; dom $(v_1,v_{10})= 0$; dom $(v_2,v_3) = 1$; dom $(v_2,v_4)= 1$; dom $(v_2,v_5) = 0$;

dom $(v_2,v_6) =1$; dom $(v_2,v_7)= 0$; dom $(v_2,v_8) = 0$;dom $(v_2,v_9)= 0$; dom $(v_2,v_{10}) = 0$; dom $(v_3,v_4) = 1$;

dom $(v_3,v_5) =1$; dom $(v_3,v_6) = 0$; dom $(v_3,v_7) = 0$; dom $(v_3,v_8) = 0$; dom $(v_3,v_9)= 0$; dom $(v_3,v_{10}) = 0$;

dom $(v_4,v_5) = 1$; dom $(v_4,v_6)= 1$; dom $(v_4,v_7) = 0$; dom $(v_4,v_8) = 0$; dom $(v_4,v_9) = 0$; dom $(v_4,v_{10}) = 1$;

dom $(v_5,v_6) = 1$; dom $(v_5,v_7)= 1$; dom $(v_5,v_8) = 0$; dom $(v_5,v_9) = 1$; dom $(v_5,v_{10}) = 1$;dom $(v_6,v_7) = 1$;

dom $(v_6,v_8) = 1$; dom $(v_6,v_9) =0$; dom $(v_6,v_{10}) = 1$;dom $(v_7,v_8) = 1$; dom $(v_7,v_9) = 1$; dom $(v_7,v_{10}) = 0$;

dom $(v_8,v_9)= 1$; dom $(v_8,v_{10})= 1$; dom $(v_9,v_{10}) = 1$.

TDV(G)= 25.

Medium Domination Number $= \frac{2(25)}{10(9)} = \frac{5}{9}$.
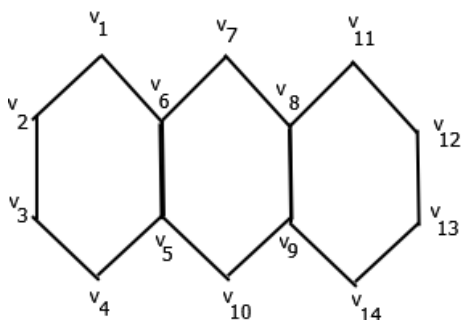
3.3 MOLECULAR GRAPH OF ANTHRACENE [4]:

Figure 3.Molecular Graph of Anthracene

In the Molecular Graph of Anthracene, from figure 3,we get

dom $(v_1,v_2) = 1$; dom $(v_1,v_3)= 1$; dom $(v_1,v_4) = 0$; dom $(v_1,v_5)= 1$; dom $(v_1,v_6)= 1$; dom $(v_1,v_7) = 1$;

dom $(v_1,v_8)= 0$; dom $(v_1,v_9)= 0$; dom $(v_1,v_{10})= 0$; dom $(v_1,v_{11}) = 0$; dom $(v_1,v_{12})= 0$; dom $(v_1,v_{13}) = 0$; dom $(v_1,v_{14})= 0$; dom $(v_2,v_3) = 1$; dom $(v_2,v_4)= 1$; dom $(v_2,v_5) = 0$; dom $(v_2,v_6) =1$; dom $(v_2,v_7)= 0$; dom $(v_2,v_8) = 0$;dom $(v_2,v_9)= 0$; dom $(v_2,v_{10}) = 0$; dom $(v_2,v_{11})= 0$; dom $(v_2,v_{12}) = 0$; dom $(v_2,v_{13})= 0$; dom $(v_2,v_{14})= 0$; dom $(v_3,v_4) = 1$; dom $(v_3,v_5) =1$; dom $(v_3,v_6) = 0$; dom $(v_3,v_7) = 0$; dom $(v_3,v_8) = 0$; dom $(v_3,v_9)= 0$; dom $(v_3,v_{10}) = 0$; dom $(v_3,v_{11})= 0$; dom $(v_3,v_{12}) = 0$; dom $(v_3,v_{13})= 0$;dom $(v_3,v_{14}) = 0$;

dom $(v_4,v_5) = 1$; dom $(v_4,v_6)= 1$; dom $(v_4,v_7) = 0$; dom $(v_4,v_8) = 0$; dom $(v_4,v_9) = 0$; dom $(v_4,v_{10}) = 1$;

dom $(v_4,v_{11}) =0$; dom $(v_4,v_{12})= 0$; dom $(v_4,v_{13}) = 0$;dom $(v_4,v_{14})= 0$; dom $(v_5,v_6) = 1$; dom $(v_5,v_7) = 1$; dom $(v_5,v_8) = 0$; dom $(v_5,v_9) =1$; dom $(v_5,v_{10}) = 1$; dom $(v_5,v_{11}) = 0$; dom $(v_5,v_{12}) = 0$; dom $(v_5,v_{13}) =0$; dom $(v_5,v_{14}) = 0$; dom $(v_6,v_7) = 1$; dom $(v_6,v_8) = 1$; dom $(v_6,v_9) =0$; dom $(v_6,v_{10}) = 1$; dom $(v_6,v_{11}) = 0$; dom $(v_6,v_{12}) = 0$; dom $(v_6,v_{13})= 0$; dom $(v_6,v_{14}) = 0$; dom $(v_7,v_8) = 1$; dom $(v_7,v_9) = 1$;dom $(v_7,v_{10}) = 0$;

dom $(v_7,v_{11}) = 1$; dom $(v_7,v_{12})= 0$; dom $(v_7,v_{13}) = 0$; dom $(v_7,v_{14}) = 0$; dom $(v_8,v_9)= 1$; dom $(v_8,v_{10})= 1$;

dom $(v_8,v_{11}) = 1$; dom $(v_8,v_{12}) = 1$; dom $(v_8,v_{13}) = 0$; dom $(v_8,v_{14}) = 1$; dom $(v_9,v_{10}) = 1$;dom $(v_9,v_{11}) = 1$; dom $(v_9,v_{12})= 0$; dom $(v_9,v_{13}) = 1$;dom $(v_9,v_{14}) = 1$;dom $(v_{10},v_{11}) = 0$; dom $(v_{10},v_{12}) = 0$;dom $(v_{10},v_{13}) = 0$; dom $(v_{10},v_{14})= 1$;dom $(v_{11},v_{12})= 1$;dom $(v_{11},v_{13}) = 1$;dom $(v_{11},v_{14}) = 0$;dom $(v_{12},v_{13}) = 1$;dom $(v_{12},v_{14}) = 1$; dom $(v_{13},v_{14}) = 1$.

TDV(G)= 38.

Medium Domination Number $= \frac{2(38)}{14(13)} = \frac{38}{91}$.

THEOREM 3.4: The Medium Domination Number of Linear Polyacene L_h is

$$MD(L_h) = 2 \sum_{k=1}^{h} \frac{13k-1}{(4k+2)(4k+1)}.$$

Proof

Let L_h be Linear Polyacene with h Hexagones.

It is enough to show that the Medium Domination Number of Linear Polyacene L_h is

$$MD(L_h) = 2 \sum_{k=1}^{h} \frac{13k-1}{(4k+2)(4k+1)} \qquad \text{(I)}$$

by Induction.

Step 1:

Put h=1 in equation(I),we get

L_1 -Linear Polyacene with one Hexagone(Benzene).

There are 6 vertices v_1,v_2,v_3,v_4,v_5,v_6(Figure 1).

By 3.1,The summation of vertices that dominate every set of two vertices is 12.

Therefore, By Definition 2.6, the Medium Domination Number of Linear Polyacene L_1 is

$$MD(L_1) = \frac{2(12)}{6(5)} = \frac{4}{5}.$$

Step 2:

Put h=2 in equation(I),we get

L_2 - Linear Polyacene with two Hexagons(Naphthalene).

By 3.2,The summation of vertices that dominate every set of two vertices is 25.

Therefore, By Definition 2.6 and 3.2, the Medium Domination Number of Linear

Polyacene L_2 is $MD(L_2) = \frac{2(25)}{10(9)} = \frac{5}{9}$.

Assume that L_{h-1} is Linear Polyacene with *h-1* Hexagons where $h \geq 2 \in N$.

Then the Medium Domination Number of Linear Polyacene L_{h-1} is

$$MD(L_{h-1}) = 2 \sum_{i=2}^{h} \frac{13i-1}{(4i+2)(4i+1)}.$$

We have to show $MD(L_h) = 2 \sum_{i=1}^{h} \frac{13i-1}{(4i+2)(4i+1)}$ for L_h , Linear Polyacene with *h* Hexagones

where $h \geq 1 \in$ N.

By hypothesis, summation of vertices that dominate every set of two vertices is 13*h*-1

for *h* hexagones.

By step 1, summation of vertices that dominate every set of two vertices is 12.

Now , the summation of vertices that dominate every set of two vertices for *h* hexagons is equal to the sum of total number of vertices that every set of two vertices for *one* hexagon and total number of vertices that dominate every set of two vertices for *h-1* hexagons

where $h \geq 2$.

Hence $MD(L_h) = \frac{2(12)}{6(5)} + 2 \sum_{i=2}^{h} \frac{13i-1}{(4i+2)(4i+1)}$

$= 2\left\{\frac{13(1)-1}{(4(1)+2)(4(1)+1)} + \sum_{i=2}^{h} \frac{13i-1}{(4i+2)(4i+1)}\right\}$

$= 2 \sum_{i=1}^{h} \frac{13i-1}{(4i+2)(4i+1)}$.

By Induction Principle, $MD(L_h) = 2 \sum_{k=1}^{h} \frac{13k-1}{(4k+2)(4k+1)}$ for

h Hexagons where $h \geq 1 \in N$.

4. CONCLUSION

In this Paper, the Molecular Graph such as Benzene, Naphthalene and Anthracene obtained Medium Domination Number for them. It also explained Medium Domination Number of Linear Polyacene L_h is $MD(L_h) = 2 \sum_{k=1}^{h} \frac{13k-1}{(4k+2)(4k+1)}$ by Induction method.

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