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Equitable Domination in Chemical Structural Graph

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Abstract: Let G be a finite, connected graph. Atoms 0f Linear Benzenoid Graph is indicated by vertices and its bonds are indicated by edges. This Paper initiates about Equitable Domination in Linear Benzenoid Graph L (n) with n Hexagons.

Keywords: Dominating set, Equitable Dominating Set, Near Equitable Dominating Set.

1. INTRODUCTION

Molecular graphs are a special form of chemical graph that represent the constitution of molecules. Topological illustration of a molecule is often described through molecular graph. A chemical graph may be a model of a chemical system, wont to characterize the intersections among its components: atoms, bonds. A structural formula of a substance will be set out by a Chemical graph [4,3,10,11].

Definition [1,9]

A set D which is a subset of V (*G*) is known as Dominating Set if each vertex not in D is joined to a minimum of one member in D. The smallest cardinality of a dominating set of graph *G* is called Domination number and is symbolized by γ (*G*).

Definition [2, 8, 12, 13]

A set D which is a subset of V (*G*) is called an Equitable Dominating Set of a graph *G* if for each vertex v not in D, there is a vertex u in D such that u is joined with v and $|deg(u)-deg(v)| \leq 1$.The smallest cardinality of an Equitable Dominating Set of *G* is called an Equitable Domination Number of G and is symbolized by γ^{e} (*G*).

Definition [3]

A set D which is a subset of V (*G*) and u is a vertex in D. The out degree of u is symbolized by $out\ deg_{D}(u)$, is described as $out\ deg_{D}(u) = |N(u)-(V-D)|$. The out degree of v not in D is symbolized by $out\ deg_{(V-D)}(v)$, is defined as $out\ deg_{(V-D)}(v) = |N(v) - D|$.

Definition [3,12,13]

A set D which is a subset of V (*G*) is called a Near Equitable Dominating Set of *G* if for each v not in D, There is a vertex u in D such that u is joined with v and $|out\ deg_{D}(u)-$ *out*

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deg $_{(V-D)}$ *(v)* $| \leq 1$.The smallest cardinality of a Near Equitable Dominating Set of *G* is called a Near Equitable Domination Number of *G* and is symbolized by $\gamma_{ne}(G)$.

2. EQUITABLE DOMINATION IN MOLECULAR GRAPH OF LINEAR BENZENOID GRAPH

Let L (n) be a Linear Benzenoid Graph with n hexagons. Naming vertices of the followingas L (n):

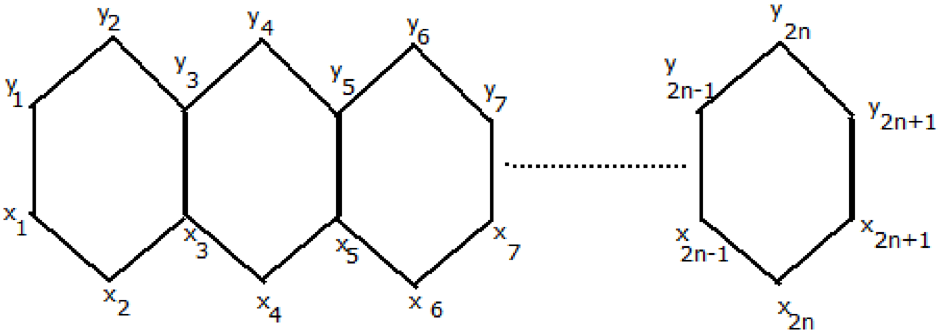

Figure 1 Linear Benzenoid Graph L (n)

Let $X = \{x_1, x_2, x_3 \ldots\ldots\ldots x_{2n+1}\}$ (2.1)

and $Y = \{y_1, y_2, y_3, \ldots\ldots\ldots y_{2n+1}\}$ (2.2)

We have G = X U Y which has (2n+1) vertices in X and (2n+1) vertices in Y.

From Equation (1), Dominating set $D_1 = \{x_1, x_5, x_9, \ldots\ldots\ldots x_{2n-1}\}$.

From Equation (2), Dominating set $D_2 = \{y_3, y_7, y_{11}, \ldots\ldots\ldots y_{2n+1}\}$.

Take $D=D_1UD_2$. Knowing a result from[6], *We can write* $D=\{x_1,y_3,x_5,y_7,\ldots\ldots,x_{2n-1}, y_{2n+1},x_{2n+1},y_{2n+3}\}$ *is a dominating set.*

In particular, consider Anthracene' Molecular Structure Graph [6,7]

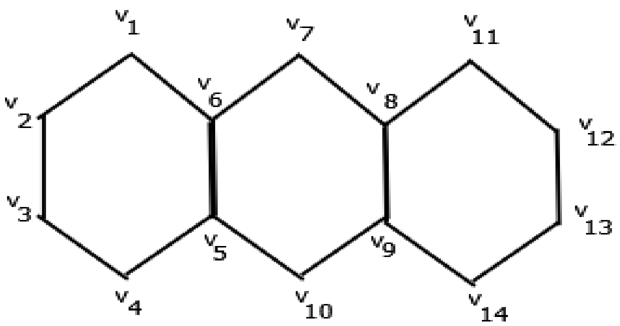

Figure 2 Anthracene' Molecular Structure Graph

Here $deg(v_3)= deg(v_9) = 3$ and $deg(v_6) = deg(v_{12}) = 2$.

This gives Molecular graph of Anthracene satisfying equitable condition.

Theorem 2.1. *The Linear Benzenoid Graph L (n) with n Hexagons satisfy equitable domination condition.*

Proof

For L(n), $D=\{x_1,y_3,x_5,y_7,\ldots\ldots,x_{2n-1},y_{2n+1}\}$ is a dominating set where $D = D_1UD_2$,

$D_1=\{x_1,x_5,x_9,\ldots\ldots x_{2n-1}\}$ from X and $D_2=\{y_3,y_7,y_{11}, \ldots\ldots y_{2n+1}\}$ from Y. [5,6]

Case(i) *.Let* $u \in D_1$ *such that* $uv \in E$.

Here $D_1=\{x_1,x_5,x_9,\ldots\ldots x_{2n-1}\}$.
First we take $u = x_1$ where $x_1 \epsilon D_1$.
x_1 is joined with y_1 and x_2 ,where y_1, $x_2 \epsilon$ (V-D).

$$deg\ x_1 = 2\ ,deg\ x_2 = deg\ y_1 = 2.$$

Therefore, $|deg(u)-deg(v)| = |2-2| = 0 < 1.$
Next, we take $u \epsilon \{x_5,x_9,\ldots\ldots x_{2n-1}\}$ and $v \epsilon \{x_4, x_6, x_8\ldots x_{2n}\}$ which contains $uv \epsilon E$.
Therefore, $|deg(u)-deg(v)| = |3-2| = 1.$
Then Take $u \epsilon \{x_5,x_9,\ldots\ldots x_{2n-1}\}$ and $v \epsilon \{y_5,y_9,\ldots\ldots y_{2n-1}\}$ which contains $uv \epsilon E$.
Therefore, $|deg(u)-deg(v)| = |3-3| = 0 < 1.$
Case (ii).*Let* $u \epsilon D_2$ which contains $uv \epsilon E$.
Here $D_2= \{y_3,y_7,y_{11},\ldots\ldots y_{2n+1}\}$.
First we take $u = y_{2n+1}$ where $y_{2n+1} \epsilon D_2$.
We get $deg\ y_{2n+1} = 2$ and $deg\ y_{2n} = deg\ x_{2n+1} = 2$.
Therefore, $|deg(u)-deg(v)| = |2-2| = 0 < 1.$
Then, take $u \epsilon \{y_3,y_7,y_{11},\ldots\ldots y_{2n-3}\}$ and $v \epsilon \{y_4, y_6, y_8\ldots y_{2n}\}$ such that $uv \epsilon E$.
Therefore, $|deg(u)-deg(v)| = |3-2| = 1.$
Now, consider $u \epsilon \{y_3,y_7,y_{11},\ldots\ldots y_{2n-3}\}$ and $v \epsilon \{x_3,x_7,x_{11},\ldots\ldots x_{2n-3}\}$ such that $uv \epsilon E$. *Therefore,* $|deg(u)-deg(v)| = |3-3| = 0 < 1.$

From this, *we can say that the Linear Benzenoid Graph L(n) with n hexagons satisfy equitable domination condition.*

Example 2.2. From the Figure 2, in the molecular graph of Anthracene,
Here Dominating set $D= \{v_3,v_6,v_9,v_{12}\}$.
$outdeg_D(v_3) = 2$, $outdeg_D(v_6) = 3$, $outdeg_D(v_9) = 3$, $outdeg_D(v_{12}) = 2$.
$outdeg_{(V-D)}(v_1) = 1$, $outdeg_{(V-D)}(v_2) = 1$, $outdeg_{(V-D)}(v_4) = 1$, $outdeg_{(V-D)}(v_5) = 1$,
$outdeg_{(V-D)}(v_7) = 1$, $outdeg_{(V-D)}(v_8) = 1$, $outdeg_{(V-D)}(v_{10}) = 1$, $outdeg_{(V-D)}(v_{11}) = 1$,
$outdeg_{(V-D)}(v_{13}) = 1$, $outdeg_{(V-D)}(v_{14}) = 1$.
$|outdeg_D(v_3) - outdeg_{(V-D)}(v_2)| = |2-1| = 1.$
$|outdeg_D(v_3) - outdeg_{(V-D)}(v_4)| = |2-1| = 1.$
$|outdeg_D(v_6) - outdeg_{(V-D)}(v_1)| = |3-1| = 2 > 1.$

It shows that the molecular graph of Anthracene does not satisfy Near Equitable Domination condition.

Theorem 2.3.*The Linear Benzenoid Graph L (n) with n hexagons does not satisfy Near Equitable Domination Condition.*

Proof. *By definition (1.3), it is proved from the following steps.*

Step 1

For L(n),$D=\{x_1,y_3,x_5,y_7,\ldots\ldots,x_{2n-1},y_{2n+1}\}$ is a dominating set where $D = D_1UD_2$ [6].

Step 2

Take $u = x_1$ where $x_1 \epsilon$ D.so $outdeg_D(u) = |N(u)-(V-D)| = 2$.
Then we take $u \epsilon \{y_3,x_5,y_7,\ldots\ldots,x_{2n-1}\}$.here $outdeg_D(u) = 3$.
Consider $u = y_{2n+1}$ where $y_{2n+1} \epsilon$ D. so $outdeg_D(u) = 2$.
Now, for all $v\epsilon$ (V-D), $outdeg_{(V-D)}(v) = |N(v)- D| = 1$.

Step 3. *It is to prove the Linear Benzenoid Graph L(n) with n Hexagons does not satisfy Near Equitable Domination Condition.*

For $u = x_1$,$v \epsilon$ (V-D), $|outdeg_D(u) - outdeg_{(V-D)}(v)| = |2-1| = 1.$
For $u = y_{2n+1}$, $v \epsilon$ (V-D), $|outdeg_D(u) - outdeg_{(V-D)}(v)| = |2-1| = 1.$
For $u \epsilon \{y_3,x_5,y_7,\ldots\ldots,x_{2n-1}\}$, $v \epsilon$ (V-D), $|outdeg_D(u) - outdeg_{(V-D)}(v)| = |3-1| = 2 > 1$.

Hence the Linear Benzenoid Graph L (n) with n Hexagons does not satisfy Near Equitable Domination Condition.

3. CONCLUSION

In this paper, It shows that the Linear Benzenoid Graph L (n) with n Hexagons satisfy Equitable Domination Condition. It does not satisfy Near Equitable Domination Condition.

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