Journal of Physics: Conference Series

PAPER • OPEN ACCESS

EMD of Linear Benzenoid Chain Using Chemical Graph

To cite this article: M Raji and G Jayalalitha 2019 *J. Phys.: Conf. Ser.* **1377** 012004

EMD of Linear Benzenoid Chain Using Chemical Graph

M Raji[1] and G Jayalalitha[2]

[1] Research Scholar, Department of Mathematics, VELS Institute of Science, Technology & Advanced Studies, Chennai, Tamil Nadu, India.
[2] Professor, Department of Mathematics, VELS Institute of Science, Technology & Advanced Studies, Chennai, Tamil Nadu, India.

E-mail: [1] rajialagumurugan@gmail.com, [2] ragaji94@yahoo.com

Abstract. Let G_m be a undirected graph. Having a Molecule, atoms indicate by vertices and bonds indicate by edges. The main aim of this paper explains Extended Medium Domination on Linear Benzenoid Chain like Benzene, Naphthalene, Anthracene and their generalisation will be proved.
Key Words: Distance in Graph, $u - v$ path, Extended Medium Domination Number.
AMS Subject Classification: 05C12

1. Introduction

Chemical graph theory depends on the combination of graphs and chemistry. A Molecular Graph or Chemical Graph may be an illustration of the molecular formula of a matter in terms of graph theory. A chemical graph may be a connected graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds [7]. Let $\mathcal{L}_{\mathfrak{h}}$ be the Linear Benzenoid Chain with $\mathfrak{h}$ hexagons [6, 8]. In this paper, Considering G_m as a finite connected simple graph.

1.1. Connected Graph [2]

A graph G_m is connected if there is at least one path between every pair of vertices.

1.2. Distance (u, v) [1, 2]

The Length of a shortest $u-v$ path in a connected graph G_m is called the distance from a vertex u to a vertex v.

1.3. $EDOM(u, v)$ [3, 8]

$edom(u, v)$ is the summation of number of $u - v$ paths of length one, two and three.

1.4. Extened Total Dominating Vertices $(ETDV(G_m))$ [3, 8]

Total number of vertices that dominate every pair of two vertices is defined as

$$(ETDV(G_m)) = \sum_{\forall u,v \in V(G_m)} edom(u, v)$$

1.5. $EMD(G_m))$ [3, 8]
Extended Medium Domination Number is defined as $EMD(G_m)) = \frac{2ETDV(G_m)}{n(n-1)}$

2. Extended Medium Domination Number

This section describes the Extended Medium Domination number for Linear Benzenoid Chain. Also It explains the Extended Medium Domination Number of Linear Benzenoid Chain $\mathcal{L}_{\mathfrak{h}}$ is

$$EMD(\mathcal{L}_{\mathfrak{h}}) = 2\sum_{k=1}^{\mathfrak{h}} \frac{25k-7}{(4k+2)(4k+1)}$$

by Induction method.

2.1. Benzene [8]

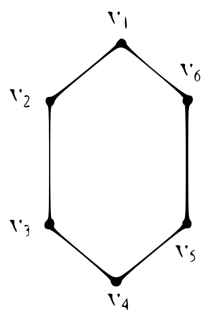

Figure 1. $\mathcal{L}_1$

$edom(v_1, v_2) = 1;$ $edom(v_1, v_3) = 1;$ $edom(v_1, v_4) = 2;$ $edom(v_1, v_5) = 1;$
$edom(v_1, v_6) = 1;$ $edom(v_2, v_3) = 1;$ $edom(v_2, v_4) = 1;$ $edom(v_2, v_5) = 2;$
$edom(v_2, v_6) = 1;$ $edom(v_3, v_4) = 1;$ $edom(v_3, v_5) = 1;$ $edom(v_3, v_6) = 2;$
$edom(v_4, v_5) = 1;$ $edom(v_4, v_6) = 1;$ $edom(v_5, v_6) = 1$

$$ETDV(\mathcal{L}_1) = 18$$

So,

$$EMD(\mathcal{L}_1) = \frac{6}{5}$$

2.2. Napathalene [5, 8]

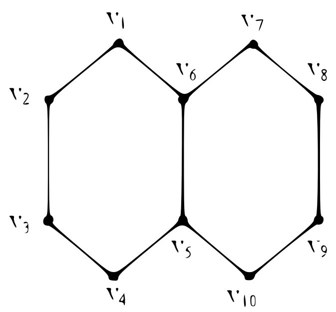

Figure 2. $\mathcal{L}_2$

$edom(v_1, v_2) = 1;$ $edom(v_1, v_3) = 1;$ $edom(v_1, v_4) = 2;$ $edom(v_1, v_5) = 1;$
$edom(v_1, v_6) = 1;$ $edom(v_1, v_7) = 1;$ $edom(v_1, v_8) = 1;$ $edom(v_1, v_9) = 0;$
$edom(v_1, v_{10}) = 1;$ $edom(v_2, v_3) = 1;$ $edom(v_2, v_4) = 1;$ $edom(v_2, v_5) = 2;$
$edom(v_2, v_6) = 1;$ $edom(v_2, v_7) = 1;$ $edom(v_2, v_8) = 0;$ $edom(v_2, v_9) = 0;$
$edom(v_2, v_{10}) = 0;$ $edom(v_3, v_4) = 1;$ $edom(v_3, v_5) = 1;$ $edom(v_3, v_6) = 2;$
$edom(v_3, v_7) = 0;$ $edom(v_3, v_8) = 0;$ $edom(v_3, v_9) = 0;$ $edom(v_3, v_{10}) = 1;$
$edom(v_4, v_5) = 1;$ $edom(v_4, v_6) = 1;$ $edom(v_4, v_7) = 0;$ $edom(v_4, v_8) = 0;$
$edom(v_4, v_9) = 1;$ $edom(v_4, v_{10}) = 1;$ $edom(v_5, v_6) = 1;$ $edom(v_5, v_7) = 1;$
$edom(v_5, v_8) = 2;$ $edom(v_5, v_9) = 1;$ $edom(v_5, v_{10}) = 1;$ $edom(v_6, v_7) = 1;$
$edom(v_6, v_8) = 1;$ $edom(v_6, v_9) = 2;$ $edom(v_6, v_{10}) = 1;$ $edom(v_7, v_8) = 1;$
$edom(v_7, v_9) = 1;$ $edom(v_7, v_{10}) = 2;$ $edom(v_8, v_9) = 1;$ $edom(v_8, v_{10}) = 1;$
$edom(v_9, v_{10}) = 1$

$$ETDV(\mathcal{L}_2) = 43$$

Therefore,

$$EMD(\mathcal{L}_2) = \frac{43}{45}$$

2.3. Anthracene [4, 8]

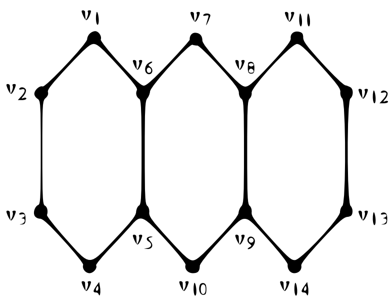

Figure 3. $\mathcal{L}_3$

$edom(v_1, v_2) = 1;$ $edom(v_1, v_3) = 1;$ $edom(v_1, v_4) = 2;$ $edom(v_1, v_5) = 1;$
$edom(v_1, v_6) = 1;$ $edom(v_1, v_7) = 1;$ $edom(v_1, v_8) = 1;$ $edom(v_1, v_9) = 0;$
$edom(v_1, v_{10}) = 1;$ $edom(v_1, v_{11}) = 0;$ $edom(v_1, v_{12}) = 0;$ $edom(v_1, v_{13}) = 0;$
$edom(v_1, v_{14}) = 0;$ $edom(v_2, v_3) = 1;$ $edom(v_2, v_4) = 1;$ $edom(v_2, v_5) = 2;$
$edom(v_2, v_6) = 1;$ $edom(v_2, v_7) = 1;$ $edom(v_2, v_8) = 0;$ $edom(v_2, v_9) = 0;$
$edom(v_2, v_{10}) = 0;$ $edom(v_2, v_{11}) = 0;$ $edom(v_2, v_{12}) = 0;$ $edom(v_2, v_{13}) = 0;$
$edom(v_2, v_{14}) = 0;$ $edom(v_3, v_4) = 1;$ $edom(v_3, v_5) = 1;$ $edom(v_3, v_6) = 2;$
$edom(v_3, v_7) = 0;$ $edom(v_3, v_8) = 0;$ $edom(v_3, v_9) = 0;$ $edom(v_3, v_{10}) = 1;$
$edom(v_3, v_{11}) = 0;$ $edom(v_3, v_{12}) = 0;$ $edom(v_3, v_{13}) = 0;$ $edom(v_3, v_{14}) = 0;$
$edom(v_4, v_5) = 1;$ $edom(v_4, v_6) = 1;$ $edom(v_4, v_7) = 1;$ $edom(v_4, v_8) = 0;$
$edom(v_4, v_9) = 1;$ $edom(v_4, v_{10}) = 1;$ $edom(v_4, v_{11}) = 0;$ $edom(v_4, v_{12}) = 0;$
$edom(v_4, v_{13}) = 0;$ $edom(v_4, v_{14}) = 0;$ $edom(v_5, v_6) = 1;$ $edom(v_5, v_7) = 1;$
$edom(v_5, v_8) = 2;$ $edom(v_5, v_9) = 1;$ $edom(v_5, v_{10}) = 1;$ $edom(v_5, v_{11}) = 0;$
$edom(v_5, v_{12}) = 0;$ $edom(v_5, v_{13}) = 0;$ $edom(v_5, v_{14}) = 1;$ $edom(v_6, v_7) = 1;$
$edom(v_6, v_8) = 1;$ $edom(v_6, v_9) = 2;$ $edom(v_6, v_{10}) = 1;$ $edom(v_6, v_{11}) = 1;$
$edom(v_6, v_{12}) = 0;$ $edom(v_6, v_{13}) = 0;$ $edom(v_6, v_{14}) = 0;$ $edom(v_7, v_8) = 1;$
$edom(v_7, v_9) = 1;$ $edom(v_7, v_{10}) = 2;$ $edom(v_7, v_{11}) = 1;$ $edom(v_7, v_{12}) = 1;$
$edom(v_7, v_{13}) = 0;$ $edom(v_7, v_{14}) = 1;$ $edom(v_8, v_9) = 1;$ $edom(v_8, v_{10}) = 1;$
$edom(v_8, v_{11}) = 1;$ $edom(v_8, v_{12}) = 1;$ $edom(v_8, v_{13}) = 2;$ $edom(v_8, v_{14}) = 1;$
$edom(v_9, v_{10}) = 1;$ $edom(v_9, v_{11}) = 1;$ $edom(v_9, v_{12}) = 2;$ $edom(v_9, v_{13}) = 1;$

$edom(v_9, v_{14}) = 1$; $edom(v_{10}, v_{11}) = 1$; $edom(v_{10}, v_{12}) = 0$; $edom(v_{10}, v_{13}) = 1$;
$edom(v_{10}, v_{14}) = 1$; $edom(v_{11}, v_{12}) = 1$; $edom(v_{11}, v_{13}) = 1$; $edom(v_{11}, v_{14}) = 2$;
$edom(v_{12}, v_{13}) = 1$; $edom(v_{12}, v_{14}) = 1$; $edom(v_{13}, v_{14}) = 1$

$$ETDV(\mathcal{L}_3) = 68$$

Hence,

$$EMD(\mathcal{L}_3) = \frac{68}{91}$$

Theorem 2.1. *The Extended Medium Domination Number of Linear Benzenoid Chain* $\mathcal{L}_\mathfrak{h}$ *is* $EMD(\mathcal{L}_\mathfrak{h}) = 2\sum_{k=1}^{\mathfrak{h}} \frac{25k-7}{(4k+2)(4k+1)}$

Proof. Let $\mathcal{L}_\mathfrak{h}$ be Linear Benzenoid Chain with $\mathfrak{h}$ Hexagones.
To Prove: $EMD(\mathcal{L}_\mathfrak{h}) = 2\sum_{k=1}^{\mathfrak{h}} \frac{25k-7}{(4k+2)(4k+1)}$ by Induction

Step 1:
Put $\mathfrak{h} = 1$ in the equation of $\mathcal{L}_\mathfrak{h}$, we get
By Calculation, we get $ETDV(\mathcal{L}_1) = 18$.
So, Extended Medium Domination Number of Linear Benzenoid Chain $\mathcal{L}_1$ is $EMD(\mathcal{L}_1) = \frac{6}{5}$.

Step 2:
Take $\mathfrak{h} = 2$ in the equation of $\mathcal{L}_\mathfrak{h}$, we get
By Calculation, $ETDV(\mathcal{L}_2) = 43$.
Hence Extended Medium Domination Number of Linear benzenoid Chain ($\mathcal{L}_2$) is $EMD(\mathcal{L}_2) = \frac{43}{45}$.
Assume that $\mathcal{L}_{\mathfrak{h}-1}$ is Linear Benzenoid Chain with $\mathfrak{h} - 1$ Hexagons where $\mathfrak{h} \geq 2 \in N$ [8]
Then the Extended Medium Domination Number of Linear Benzenoid Chain $\mathcal{L}_{\mathfrak{h}-1}$ is $EMD(\mathcal{L}_{\mathfrak{h}-1}) = 2\sum_{i=2}^{\mathfrak{h}} \frac{25i-7}{(4i+2)(4i+1)}$.

We have to show $EMD(\mathcal{L}_\mathfrak{h}) = 2\sum_{i=1}^{\mathfrak{h}} \frac{25i-7}{(4i+2)(4i+1)}$ for $\mathcal{L}_\mathfrak{h}$, Linear Benzenoid Chain with $\mathfrak{h}$ Hexagons, where $\mathfrak{h} \geq 1 \in N$.
The Total number of vertices that dominate every pair of two vertices is $25\mathfrak{h} - 7$ for $\mathfrak{h}$ hexagons.

$$\begin{aligned}
\text{Hence, } EMD(\mathcal{L}_\mathfrak{h}) &= \frac{2(18)}{6(5)} + 2\sum_{i=2}^{\mathfrak{h}} \frac{25i-7}{(4i+2)(4i+1)} \\
&= 2\left\{\frac{25(1)-7}{(4(1)+2)(4(1)+1)} + \sum_{i=2}^{\mathfrak{h}} \frac{25i-7}{(4i+2)(4i+1)}\right\} \\
&= 2\sum_{i=1}^{\mathfrak{h}} \frac{25i-7}{(4i+2)(4i+1)}
\end{aligned}$$

By the Principle of Mathematical induction,

$$EMD(\mathcal{L}_\mathfrak{h}) = 2\sum_{k=1}^{\mathfrak{h}} \frac{25k-7}{(4k+2)(4k+1)}$$

for $\mathfrak{h}$ Hexagons where $\mathfrak{h} \geq 1 \in N$.

3. Conclusion

In this Paper, the Extended Medium Domination Number for Benzene, Naphthalene and Anthracene's Molecular Graphs are obtained. Also It explained Extended Medium Domination Number of Linear Benzenoid Chain $\mathcal{L}_{\mathfrak{h}}$ is

$$EMD(\mathcal{L}_{\mathfrak{h}}) = 2\sum_{k=1}^{\mathfrak{h}} \frac{25k-7}{(4k+2)(4k+1)}$$

by Induction Method.

References

[1] Duygu Vargorn and Pinar Dundar 2011 The Medium Domination Number Of a Graph *International Journal of Pure and Applied Mathematics* **70** No. 3 pp 297-306
[2] Arumugam S 2014 Invitation to Graph Theory Scitech Publications(India) Pvt Limited ISBN 139788187328469
[3] Mahadevan G, Vijaylakshmi V and Sivagnanam C 2017 Further Results of Extended Medium Domination Number of some special Types of Graphs *International Journal of Engineering Science, Advanced Computing and Bio-Technology* **8** No. 2 pp 55-74
[4] Vijayalakshmi S, Raji M and Jayalalitha G 2018 Degree based in Molecular Graph of Organic compounds on Domination, *Journal of Advanced Research in Dynamical and Control Systems* **10** 6 pp 962-66
[5] Jayalalitha G, Raji M and Senthil S 2019 Hosoya Polynomial and Wiener Index of Molecular Graph of Naphthalene Based On Domination *International Journal of Scientific Research and Review* **8** 1 pp 1238-41
[6] Nisreen Bukhary 2010 Domination in Benzenoids, Virginia Commonwealth University, VCU Scholars Compass
[7] Nenad Trinajstic 1983 Chemical Graph Theory, Second Edition, CRC Press
[8] Venkatesan S, Raji M and Jayalalitha G 2019 Medium Domination Number in Linear Polyacene *International Journal of Innovative Technology and Exploring Engineering* **8** 9S2 pp 459-61