Degree Based In Molecular Graph of Organic Compounds on Domination

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Abstract -Let G(V,E) be a 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, We obtain Hosoya polynomial, Wiener Index, Wiener Number of Anthracene based on Distance Matrix.
KEYWORDS: Distance in Graphs, Connectivity, Dominating set, Minimum dominating Distance matrix, Hosoya polynomial, Wiener Index

1. Introduction

A graph G = (V, E) consists of a nonempty set V of vertices and a set E of edges. 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. Any dominating set with minimum cardinality is called a minimum dominating set. Let D be a minimum dominating set of a graph G. The adjacency matrix of a molecular graph having N vertices is a square N x N symmetric matrix which is defined as

$$[A]_{ij} = \begin{cases} 1 \; if \; i \neq j \text{ and } e_{ij} \in E(G) \\ 0 \; if \; i = j \text{ and } e_{ij} \in E(G) \end{cases}$$

Where e_{ij} is the edge between I and j and E(G) is the set of edges of the graph G.

The Distance Matrix (D) of a Molecular graph having N vertices is a real symmetric $N \times N$ Matrix, whose elements $[D]_{ij}$ represent the minimum distance or minimum length of the path between the vertices I and j in terms of the number of edges between them.

$$[D]_{ij} = \begin{cases} \min\left(l(p)_{ij}\right) \text{if } i \neq j \\ 0 \; if \;\; i = j \end{cases}$$

Where p_{ij} is the number of edges separating the vertices i and j.[6]

The minimum dominating distance matrix of G is N x N matrix defined by

$A_{Dd}(G) = (d_{ij})$ where $d_{ij} = \begin{cases} 1 \;\; if \;\; i = j \text{ and } v_i \in D \\ d(v_i, v_j) \text{otherwise} \end{cases}$. [8]

2. Molecular Graph Of Organic Compounds

Graph theory can be used to model many relations in real time systems. A chemical graph is a mathematical structure which provides a pictorial representation of a molecule, taking into account the internal connectivity of atoms in the molecule through bonds. Benzenoid graphs are graphs pertaining to the network constructed by arranging congruent regular hexagons in a plane, so that two hexagons are either disjoint or have one edge in common[1]. Benzenoid graph is formed by the vertices in edges lying on C and in the interior of C.A linear benzenoid chain is a set of hexagons arranged on a horizontal line where each pair of adjacent hexagons share a vertical edge. Let L (h) be the linear benzenoid chain with h hexagons. Knowing that If L (h) is a linear benzenoid chain with h hexagons, then n(L(h))=4h+2.If L(h) is a linear benzenoid chain with h hexagons ,then Y(L(h))=h+1.where No. of vertices is n(L(h)) and Domination No. of Linear Benzenoid chain is Y(L(h))[5].

Molecular graph of Anthracene

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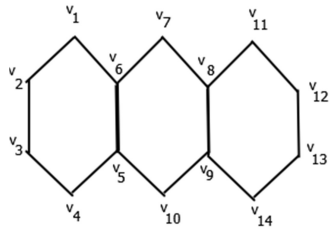

Figure 1

Here V = { v_1,v_2,v_3,v_4,v_5,v_6,v_7,v_8,v_9,v_{10},v_{11},v_{12},v_{13},v_{14}}

Dominating set D= { v_3 ,v_6,v_9,v_{12}}

V-D ={ v_1,v_2, v_4,v_5, v_7,v_8, ,v_{10},v_{11},v_{13},v_{14}}

Connecting the vertices of Dominating set D, we get a connected acyclic graph which is a tree with 4 vertices and 3 edges.

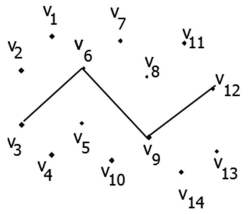

Figure 2

In this Paper, For the following theorem, Let us consider as L(n) is a Linear Benzenoid chain with n hexagons[7].

THEOREM 2.1: If L(n) is linear benzenoid chain with n hexagons where n ϵ N, then connecting the vertices of dominating set of L(n) is a connected acyclic graph which is a tree with (n+1)vertices and n edges.

Proof: Let L (n) be a linear benzenoid chain with n hexagons.Consider this linear benzenoid chain with n times.

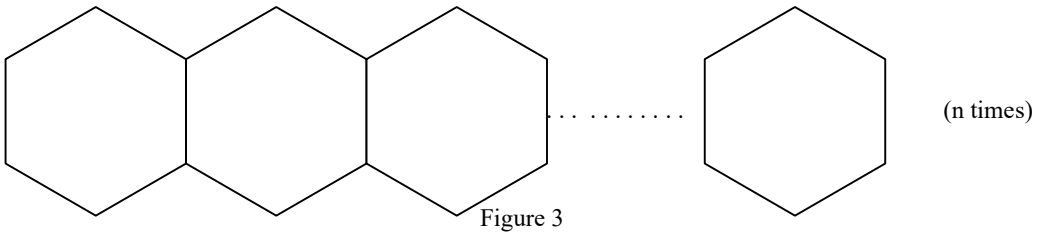

Figure 3

Assigning vertices of the above linear benzenoid chain L(n)

Let X= {x_1, x_2, x_3…x_{2n+1}} and Y= {y_1, y_2, y_3 ,……y_{2n+1}}

Take G =X U Y, D_1={x_1,x_5,x_9,……x_{2n-1}} from X and D_2={y_3,y_7,y_{11}, …….y_{2n+1}} from Y.

Number of vertices in $D_1 = \frac{n-1}{2} + 1$ and No. of vertices in $D_2 = \frac{n-1}{2} + 1$.

Take D = D_1 U D_2. Now D = D_1 U D_2 is a dominating set of G =X U Y.

Number of vertices in D =n +1.

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We have to show that when we connect the vertices of dominating set D= D_1 U D_2, it is a connected acyclic graph which is a tree with (n+1) vertices and n edges.

Connecting the vertices of Dominating set D = D_1 U D_2.

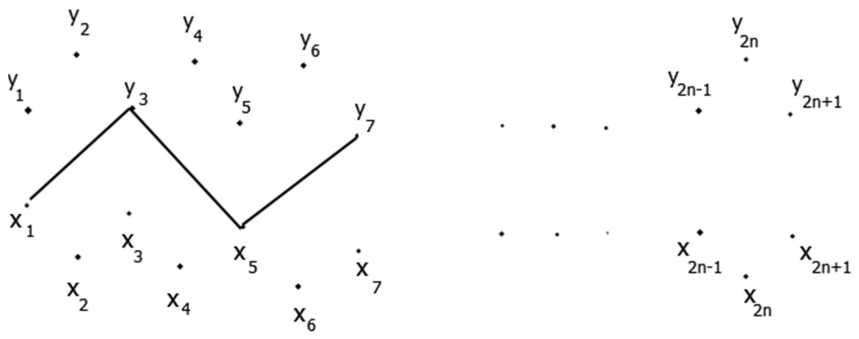

Figure 4

Here we get a connected acyclic graph from connecting the vertices of Dominating set

D = D_1 U D_2.

Knowing the result, A connected acyclic graph which is a tree. [4]

Using Induction Hypothesis, the above statement is true for all n hexagons where n ϵ N.

Using Induction, It is true for L(1) with n=1 hexagons.

That is, D= D_1 U D_2 = { x_1, y_3} is a dominating set which is connected acyclic graph for n=1.

Assume that it is true for n = k hexagons. we have to prove this for n = k+1.

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

Then Dominating set of L(k) with n = k hexagons is $\{x_1,y_3,x_5,y_7,\ldots..,x_{2n-1},y_{2n+1}\}$.

Now Dominating set of L(k+1) with n = k+1 hexagons is

$\{x_1 ,y_3,x_5,y_7,\ldots..,x_{2n-1},y_{2n+1}\}$ U $\{x_{2n+1}, y_{2n+3}\}$.

We can write D=$\{x_1 ,y_3,x_5,y_7,\ldots..,x_{2n-1},y_{2n+1},x_{2n+1},y_{2n+3}\}$ is a dominating set which is connected acyclic graph for n=k+1.

Therefore, Connecting the vertices of Dominating set D ,there is a connected acyclic graph which is a tree with (n+1) vertices and n edges is true for all n hexagons where n ϵ N.

3. Wiener Number And Index For Minimum Dominating Distance Matrix Of Anthracene

Topological indices are real numbers related to a structural graph of a molecule. Such indices based on the distances in graph are widely used for establishing relationships between the structure of a molecular graph and their physicochemical properties. Topological indices are used in biology and chemistry between physicochemical properties of organic compounds and the index of their molecular graphs.

The Wiener number W and Wiener index W.I are computed by the definitions

$$W= 1/2\sum_{i=1}^{N} \quad \sum_{j=1}^{N} d_{ij} \qquad (3.1)$$

and W.I = 2W/N(N-1) (3.2)

Where N is the number of vertices and d_{ij} is the distance between the vertices in terms of number of edges.[3] .H.Hosoya[2] ,[9]introduced The Hosoya polynomial in 1988 and define as follows:

$$H(G,X) = \frac{1}{2}\sum_{v\epsilon V(G)}\sum_{u\epsilon V(G)} X^{d(u,v)} \quad (3.3)$$

$$\text{and } W(G) = \frac{\partial H(G,X)}{\partial X} / X=1 \quad (3.4)$$

The following table gives the degree of each vertex for the molecular graph of Anthracene.

Table 1

Vertex	V_1	V_2	V_3	V_4	V_5	V_6	V_7	V_8	V_9	V_{10}	V_{11}	V_{12}	V_{13}	V_{14}
Degree	2	2	3	2	3	3	2	3	3	2	2	2	2	2

Minimum Dominating Distance Matrix of Anthracene

	V_1	V_2	V_3	V_4	V_5	V_6	V_7	V_8	V_9	V_{10}	V_{11}	V_{12}	V_{13}	V_{14}
V_1	0	1	2	3	2	1	2	3	4	3	4	5	6	5
V_2	1	0	1	2	3	2	3	4	5	4	5	6	7	6
V_3	2	1	1	1	2	3	4	5	4	3	6	7	6	5
V_4	3	2	1	0	1	2	3	4	3	2	5	6	5	4
V_5	2	3	2	1	0	1	2	3	2	1	4	5	4	3
V_6	1	2	3	2	1	1	1	2	3	2	3	4	5	4
V_7	2	3	4	3	2	1	0	1	2	3	2	3	4	3
V_8	3	4	5	4	3	2	1	0	1	2	1	2	3	2
V_9	4	5	4	3	2	3	2	1	1	1	2	3	2	1
V_{10}	3	4	3	2	1	2	3	2	1	0	3	4	3	2
V_{11}	4	5	6	5	4	3	2	1	2	3	0	1	2	3
V_{12}	5	6	7	6	5	4	3	2	3	4	1	1	1	2
V_{13}	6	7	6	5	4	5	4	3	2	3	2	1	0	1
V_{14}	5	6	5	4	3	4	3	2	1	2	3	2	1	0

From Equation (3.1) and(3.2),we get the Wiener Number for minimum dominating distance matrix of Anthracene=281 and Wiener Index for minimum dominating distance matrix of Anthracene=3.088.

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From equations(3.3) and(3.4),Hosoya polynomial for minimum dominating distance matrix of Anthracene = $18X + 22X^2 + 21X^3 + 14X^4 + 10X^5 + 6X^6 + 2X^7$ and Wiener Index(Anthracene) for minimum dominating distance matrix=281

References

[1] S. Klavzar, I. Gutman (1996). A Comparison of the Schultz Topological Index with the Wiener Index, J. Chem. Inf. Comput. Sci., 36, 1001-1003.

[2] H.Hosoya, (1988) Discreteappli.Math.19239-257.

[3] R.Sundareswaran, Mathavimanisekar, S.Lalitha, (2017) Removal Of Degeneracy In The Topological Indices Of Cospectral Graphs Using Edge Weighted Molecular Graphs.Journal Of Advances In Chemistry.Volume23.Number17. 6322-6326.

[4] J.Gross and Yellen , (2006), J. *Graph Theory and Its Applications*,CRC Press.

[5] NisreenBukhary,(2010)Domination in Benzenoids. Virginia Commonwealth University, VCU Scholars Compass.

[6] Qian-Nan Hu, Yi-Zeng Liang and Kai-Tai Fang, (2003) The Matrix Expression. Topological Index and Atomic Attribute of Molecular Topological Structure, Journal of Data Science1.361-369.

[7] Damir Vukicevic, Nenad Trinajstic. (2004)Wiener Indices of Benzenoid Graphs. Bulletin of the Chemists and Technologists of Macedonia, Vol.23, No.2,pp.113-129.

[8] M.R.Rajesh Kanna, B.N.Dharmendra, G.Sridhara. (2014)Minimum Dominating Distance Energy Of a Graph.J.Indones.Math.Soc.Vol.20, No.1, pp.19-29.

[9] Wei Gao, Mohammed Reza Furahani,[..],M.R.Rajesh Kanna, (2016) Springerplus,5(1):1563.