Harary Index of Anthracene's Chemical Graph Using Domination

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Abstract

Consider a Anthracene's Chemical Graph as a connected finite simple graph. In such a chemical graph, vertices and edges signify atoms and bonds respectively. Harary Index is a distance based on the topological index. This paper obtains Harary Index of Chemical Graph of Anthracene using Reciprocal Minimum Dominating Distance Matrix.

Keywords

Chemical Graph, Dominating Set, Reciprocal Minimum Dominating Distance Matrix, Harary Index.

Introduction

Chemical Graph Theory is a graphical representation of molecular structure of Organic compounds. Topological indices can be calculated for the chemical graph of organic compounds based on their degree and distance [Klavžar. S & Gutman.I. ,1996]. Let G_A be a graph with nonempty set V of vertices and a set E of edge. Topological Indices have more applications in various fields of Chemistry, Physics, Mathematics and Informatics. The Harary index is defined as the sum reciprocals of distances between all pairs of vertices of a connected graph [(Plavšić et al., 1993) (Lučić et al., 2002)]. A set D_A in a graph 'G_A' is a Dominating Set if each vertex is either in $D_A$or adjacent to a vertex in D_A [Arumugam, S., 2014]. Any dominating Set with minimum cardinality is called a Minimum Dominating Set [Dharmendra. B, 2014]. Let D_A be a Minimum Dominating Set of a graphG_A. The Minimum Dominating Distance Matrix of G_A is a square matrix defined by,

$$\text{MDDM}(G_A) = (d_{ij}) \text{where } d_{ij} = \begin{cases} 1 \; if \; \text{i} = \text{j} \;\; \text{and } v_i \epsilon \, D_A. \\ \text{minimum distance d}(v_i, v_j) \text{ otherwise} \end{cases}$$

Throughout this paper, a finite simple connected Graph is taken. In this Paper, It obtains Reciprocal Minimum Dominating Distance Matrix of a Graph and Harary Index of Chemical Graph of Anthracene using Reciprocal Minimum Dominating Distance Matrix is calculated and describes a proposition.

Anthracene's Chemical Graph [(Vijayalakshmi et al., 2018) (Jayalalitha et al., 2019) (Raji et al, 2019)]

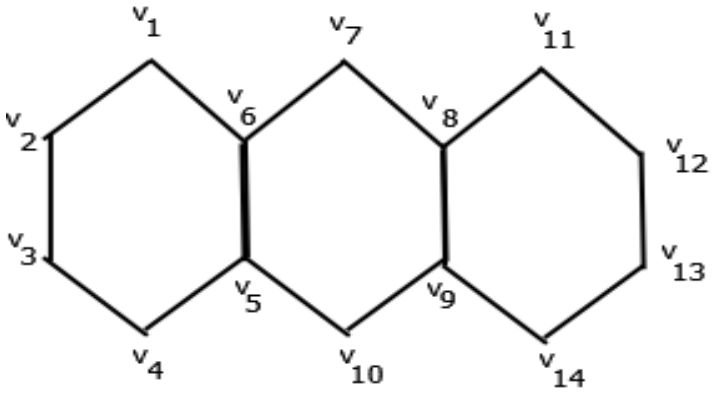

Figure 1 Anthracene

Harary Index of Chemical Graph of Anthracene

In this section, it defines (2.1) Reciprocal Minimum Dominating Distance Matrix (RMDDM) and describes Reciprocal Minimum Dominating Distance Matrix (Anthracene). Then it obtains Harary Index of Chemical Graph of Anthracene using RMDDM and a proposition.

Reciprocal Minimum Dominating Distance Matrix (RMDDM (G_A))

Let D_A be a minimum dominating set of a graph G_A. The Reciprocal Minimum Dominating Distance Matrix of $G_A$is a square matrix defined by,

$$\text{RMDDM(G)} = (md_{ij}) \text{where } md_{ij} = \begin{cases} 1 \; if \; \text{i} = \text{j} \;\; \text{and } v_i \, \epsilon \, D_A. \\ \frac{1}{\text{minimum distance d}(v_i, v_j)} \text{ otherwise} \end{cases}$$

Reciprocal Minimum Dominating Distance Matrix (ANTHRACENE)

Reciprocal Minimum Dominating Distance Matrix of Molecular Graph of Anthracene using (2.1)															
	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}	TOTAL
V_1	0	1	0.5	0.3	0.5	1	0.5	0.3	0.25	0.3	0.25	0.2	0.17	0.2	5.47
V_2	1	0	1	0.5	0.3	0.5	0.3	0.25	0.2	0.25	0.2	0.17	0.14	0.17	4.98
V_3	0.5	1	1	1	0.5	0.3	0.25	0.2	0.25	0.3	0.17	0.14	0.17	0.2	5.98
V_4	0.33	0.5	1	0	1	0.5	0.3	0.25	0.3	0.5	0.2	0.17	0.2	0.25	5.5
V_5	0.5	0.3	0.5	1	0	1	0.5	0.3	0.5	1	0.25	0.2	0.25	0.3	6.6
V_6	1	0.5	0.3	0.5	1	1	1	0.5	0.3	0.5	0.3	0.25	0.2	0.25	7.6
V_7	0.5	0.3	0.25	0.3	0.5	1	0	1	0.5	0.3	0.5	0.3	0.25	0.3	5.5
V_8	0.3	0.25	0.2	0.25	0.3	0.5	1	0	1	0.5	1	0.5	0.3	0.5	6.6
V_9	0.25	0.2	0.25	0.3	0.5	0.3	0.5	1	1	1	0.5	0.3	0.5	1	7.6
V_{10}	0.3	0.25	0.3	0.5	1	0.5	0.3	0.5	1	0	0.3	0.25	0.3	0.5	6
V_{11}	0.25	0.2	0.17	0.2	0.25	0.3	0.5	1	0.5	0.3	0	1	0.5	0.3	5.47
V_{12}	0.2	0.17	0.14	0.17	0.2	0.25	0.3	0.5	0.3	0.25	1	1	1	05	5.98
V_{13}	0.17	0.14	0.17	0.2	0.25	0.2	0.25	0.3	0.5	0.3	0.5	1	0	1	4.98
V_{14}	0.2	0.17	0.2	0.25	0.3	0.25	0.3	0.5	1	0.5	0.3	0.5	1	0	5.47
														GRAND TOTAL	83.73

Harary Index of Anthracene using Reciprocal Minimum Dominating Distance Matrix = $\frac{1}{2}$(83.73)

= 41.865

= 42(approximately)

Proposition

If there are at most four vertices that belongs to a Minimum Dominating set D_A of Chemical Graph of Anthracene G_A and these four vertices has length 3 of the shortest path between them, then these paths are both vertex disjoint paths and edge disjoint paths.

Proof

Given G_A is the Chemical graph of Anthracene with 14 vertices and 16 edges.

Let V_A = { 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} }.

Here 10 vertices are of degree two and 4 vertices are of degree three.

Taking a minimum dominating set which has 2 vertices of degree three and 2 vertex of degree two.

Consider a set of vertices of Minimum Dominating set as an ordered pair.

(i) Suppose Minimum Dominating set $D_A = \{v_3, v_6, v_9, v_{12}\}$.

It is to be calculated the length of the shortest paths between (v_3, v_6), (v_6, v_9), (v_9, v_{12}).

a. There are two ways to reach vertex v_3 to v_6 by Shortest Paths.
   i. $v_3 \rightarrow v_2 \rightarrow v_1 \rightarrow v_6$.
   ii. $v_3 \rightarrow v_2 \rightarrow v_1 \rightarrow v_6$.
b. There are two ways to reach vertex v_6 to v_9 by Shortest Paths.
   i. $v_6 \rightarrow v_7 \rightarrow v_8 \rightarrow v_9$.
   ii. $v_6 \rightarrow v_5 \rightarrow v_{10} \rightarrow v_9$.
c. There are two ways to reach vertex v_9 to v_{12} by Shortest Paths.
   i. $v_9 \rightarrow v_8 \rightarrow v_{11} \rightarrow v_{12}$.
   ii. $v_9 \rightarrow v_{14} \rightarrow v_{13} \rightarrow v_9$.

From this, there is no common vertex and no common edge in the above shorest paths. Hence these shortest paths are both vertex disjoint and edge disjoint paths.

(ii) Suppose Dominating set $D_A = \{v_2, v_5, v_8, v_{13}\}$.

a. There are two ways to reach vertex v_2 to v_5 by Shortest Paths.
   i. $v_2 \rightarrow v_1 \rightarrow v_6 \rightarrow v_5$.
   ii. $v_2 \rightarrow v_3 \rightarrow v_4 \rightarrow v_5$.
b. There are two ways to reach vertex v_5 to v_8 by Shortest Paths.
   i. $v_5 \rightarrow v_6 \rightarrow v_7 \rightarrow v_8$.
   ii. $v_5 \rightarrow v_{10} \rightarrow v_9 \rightarrow v_8$.
c. There are two ways to reach vertex v_8 to v_{13} by Shortest Paths.
   i. $v_8 \rightarrow v_{11} \rightarrow v_{12} \rightarrow v_{13}$.
   ii. $v_8 \rightarrow v_9 \rightarrow v_{14} \rightarrow v_{13}$.

Here there is no common vertex and no common edge in the above shortest paths.
Hence these shortest paths are both vertex disjoint and edge disjoint paths.
Therefore, It can be concluded that length of the shortest paths of Minimum Dominating set D_A of Chemical Graph Of Anthracene G_A are both vertex disjoint paths and edge disjoint paths.

The Proof is complete.

Conclusion

This Paper obtained Harary Index for the Chemical Graph of Anthracene G_A= **42** using Reciprocal Minimum Dominating Distance Matrix and a proposition about Minimum Dominating set of it.

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