International Journal of Research in Advent Technology, Vol.7, No.1, January 2019
E-ISSN: 2321-9637
Available online at www.ijrat.org

Schultz Polynomial, Modified Schultz Polynomial and Indices of Molecular Graph of Anthracene Based On Domination

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Abstract: Consider a Graph G with vertex set V= V (G) and edge set E=E (G) .Here in the Molecular Graph, vertices represent atoms and edges represent bonds. In this paper, Schultz Polynomial, Modified Schultz Polynomial of the molecular graph of Anthracene are obtained by using Minimum Dominating Distance Matrix and also their Indices is calculated.

Keywords: Dominating set, Minimum Dominating Distance matrix, Schultz Polynomial, Modified Schultz Polynomial, Schultz Index, Modified Schultz Index.

1. INTRODUCTION

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 (Damir vukicevic, Nenad Trinajstic, 2004).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. 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(S. Klavzar, I. Gutman,1996). 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 (NisreenBukhary,2010).

2. PRELIMINARIES

2.1 Graph (Arumugam.S 2014):

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

2.2 Dominating Set

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.

2.3 Minimum Dominating Set

Any dominating set with minimum cardinality is called a minimum dominating set.

2.4 Adjacency Matrix (Qian-Nan Hu, Yi-Zeng Liang and Kai-Tai Fang, 2003)

The adjacency matrix of a molecular graph having N vertices is a square N x N symmetric matrix which is defined as

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

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

2.5 Distance Matrix

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.

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

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

2.6 Minimum Dominating Distance Matrix (S.Vijayalakshmi, M.Raji and G.Jayalalitha ,2018**)**

Let D be a minimum dominating set of a graph G. The minimum dominating distance matrix of G is N x N matrix defined by

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

2.7 Molecular Graph Of Anthracene

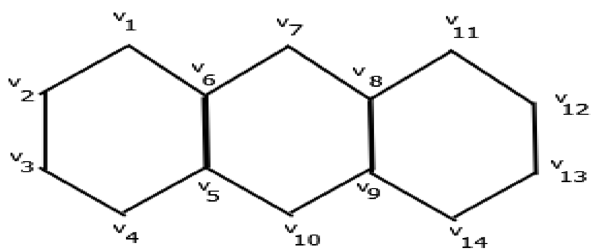


Figure 1.Molecular Graph of Anthracene

2.8 Schultz Polynomial (S. Klavzar, I. Gutman 1996, 1997**,** H.P. Schultz1989**,** Mohammad Reza Farahani, Hosoya, 2013)**:**

Schultz Polynomial is defined as

$$S_C\,(G, X) = \sum_{u,v \in V(G)} (du + dv)\, x^{d(u,v)} \qquad (1)$$

Where du, dv are degree of vertex u and v for the vertex set V (G) respectively.

2.9 Schultz Index

Harry P. Schultz introduced Schultz index in 1989 and Schultz Index is defined by

$$S_C G = \sum_{u,v \in V(G)} (du + dv)\, d(u, v) \qquad (2)$$

Where du, dv are degree of vertex u and v for the vertex set V(G) respectively.

2.10 Modified Schultz Polynomial

Modified Schultz Polynomial is defined as

$$\boldsymbol{S^*}_{\boldsymbol{C}}(G, X) = \sum_{u,v \in V(G)} (du.\,dv)\, x^{d(u,v)} \qquad (3)$$

Where du, dv are degree of vertex u and v for the vertex set V (G) respectively.

2.11 Modified Schultz Index

S. Klavžar and I. Gutman in 1997 introduced the Modified Schultz Index of G is defined as:

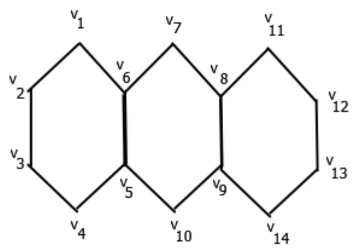
$$\boldsymbol{S}^{*}{}_{\boldsymbol{C}}\mathrm{G} = \sum_{u,v\in V(G)}(du.dv)\, d(u,v) \tag{4}$$

Where du, dv are degree of vertex u and v for the vertex set V (G) respectively.

3. MAIN RESULTS

In Section 3.1explains Based on the Molecular Graph of Anthracene(2.7),it finds the degree of each vertex for the Molecular Graph of Anthracene (Table 1), and also in Section 3.2. Based on definition of Minimum Dominating Distance Matrix (2.6), it finds Minimum Dominating Distance Matrix of Anthracene, and also in Section 3.3. Based on the distance d(u,v) , $\sum_{\boldsymbol{u},\boldsymbol{v}\in\boldsymbol{V}(\boldsymbol{G})}(\boldsymbol{du}+\boldsymbol{dv})$, $\sum_{\boldsymbol{u},\boldsymbol{v}\in\boldsymbol{V}(\boldsymbol{G})}(\boldsymbol{du}.\boldsymbol{dv})$ for every vertex u and v for the vertex set V(G) respectively of the molecular graph of Anthracene and in Section 3.4. Based on Minimum Dominating Distance Matrix of Anthracene, it finds Schultz Polynomial, Modified Schultz Polynomial and their Indices of the molecular graph of Anthracene.

In the molecular graph of Anthracene, from 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}} and V-D ={ v_1,v_2, v_4,v_5, v_7,v_8, ,v_{10},v_{11},v_{13},v_{14}}.

3.1 Table 1 gives the degree of each vertex for the Molecular Graph of Anthracene.

Table 1. Degree of Molecular Graph

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	2	2	3	3	2	3	3	2	2	2	2	2

3.2 Minimum Dominating Distance Matrix of Anthracene.

$$
\begin{array}{c}
 \\ V_1 \\ V_2 \\ V_3 \\ V_4 \\ V_5 \\ V_6 \\ V_7 \\ V_8 \\ V_9 \\ V_{10} \\ V_{11} \\ V_{12} \\ V_{13} \\ V_{14}
\end{array}
\begin{array}{c}
\begin{array}{cccccccccccccc} V_1 & V_2 & V_3 & V_4 & V_5 & V_6 & V_7 & V_8 & V_9 & V_{10} & V_{11} & V_{12} & V_{13} & V_{14} \end{array} \\
\left(\begin{array}{cccccccccccccc}
0 & 1 & 2 & 3 & 2 & 1 & 2 & 3 & 4 & 3 & 4 & 5 & 6 & 5 \\
1 & 0 & 1 & 2 & 3 & 2 & 3 & 4 & 5 & 4 & 5 & 6 & 7 & 6 \\
2 & 1 & 1 & 1 & 2 & 3 & 4 & 5 & 4 & 3 & 6 & 7 & 6 & 5 \\
3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 3 & 2 & 5 & 6 & 5 & 4 \\
2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 1 & 4 & 5 & 4 & 3 \\
1 & 2 & 3 & 2 & 1 & 1 & 1 & 2 & 3 & 2 & 3 & 4 & 5 & 4 \\
2 & 3 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 3 & 4 & 3 \\
3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 1 & 2 & 3 & 2 \\
4 & 5 & 4 & 3 & 2 & 3 & 2 & 1 & 1 & 1 & 2 & 3 & 2 & 1 \\
3 & 4 & 3 & 2 & 1 & 2 & 3 & 2 & 1 & 0 & 3 & 4 & 3 & 2 \\
4 & 5 & 6 & 5 & 4 & 3 & 2 & 1 & 2 & 3 & 0 & 1 & 2 & 3 \\
5 & 6 & 7 & 6 & 5 & 4 & 3 & 2 & 3 & 4 & 1 & 1 & 1 & 2 \\
6 & 7 & 6 & 5 & 4 & 5 & 4 & 3 & 2 & 3 & 2 & 1 & 0 & 1 \\
5 & 6 & 5 & 4 & 3 & 4 & 3 & 2 & 1 & 2 & 3 & 2 & 1 & 0
\end{array}\right)
\end{array}
$$

3.3 Table 2 gives the distance *d(u,v)* , $\sum_{u,v\in V(G)}(du+dv)$, $\sum_{u,v\in V(G)}(du.dv)$

For every vertex u and v for the vertex set *V(G)* respectively of the Molecular Graph of Anthracene,

TABLE 2.Distance of Molecular Graph

The distance d(u , v)	1	2	3	4	5	6	7
$\sum_{u,v\in V(G)}(du+dv)$	172	208	192	128	88	48	16
$\sum_{u,v\in V(G)}(du.dv)$	206	244	220	144	96	48	16

3.4 Schultz Polynomial, Modified Schultz Polynomial and their Indices of the Molecular Graph of Anthracene

From Equation (1), Schultz Polynomial of Anthracene of Minimum Dominating Distance Matrix

$$S_C\ (G, X) = 86X + 104X^2 + 96X^3 + 64X^4 + 44X^5 + 24X^6 + 8X^7 .$$

From Equation (3), Schultz Index of Anthracene of Minimum Dominating Distance Matrix

$$S_C G = 86 + 104\,(2) + 96\,(3) + 64\,(4) + 44\,(5) + 24\,(6) + 8\,(7) = 1266.$$

From Equation (2), Modified Schultz Polynomial of Anthracene of Minimum Dominating Distance Matrix

$$S^*_C(G, X) = 103X + 122\,X^2 + 110\,X^3 + 72\,X^4 + 48\,X^5 + 24\,X^6 + 8\,X^7\ .$$

From Equation (4), Modified Schultz Index of Anthracene of Minimum Dominating Distance Matrix

$$S^*_C G = 103 + 122\,(2) + 110\,(3) + 72\,(4) + 48\,(5) + 24\,(6) + 8\,(7) = 1405.$$

4. CONCLUSION

This Paper obtained Minimum Dominating Distance Matrix Of Anthracene, Schultz Polynomial, Modified Schultz Polynomial and their Indices of the Molecular graph of Anthracene.

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