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WIENER INDEX OF PHYSIO-CHEMICAL LABELED GRAPH

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Abstract

In this paper by the term Wiener Lower sum we mean the Wiener index. Mathematically, the Wiener index of a graph is defined as the sum of distances between all pairs of vertices in a connected graph. Here we obtain the Wiener index of the Diamond Silicate Snake.

Keywords: Wiener Index, Diamond Silicate Snake

MSC Code: 05C78, 05C12

1. INTRODUCTION

Distance properties of molecular graphs form an important topic in chemical graph theory. To justify this statement just recall the famous Wiener index is also known as the Wiener number. This index is the first but also one of the most important topological indices of chemical graphs. The research in this field is still very active; many methods and algorithms for computing the Wiener index of a graph are proposed in the chemical literature. A new approach to the study of distance properties of molecular graphs was proposed by Klavzjar, Gutman, and Mohar. Molecules and molecular compounds are often modeled by molecular graphs. The Wiener index named after the chemist Harold Wiener is one of the most widely known topological descriptor [2]. The Wiener Index has been well studied over the last quarter of a century and it correlates well with many physico chemical properties of organic compounds [3]. The Wiener Index of a graph is defined as the sum of the distances between all vertex pairs in a connected graph.

In mathematical terms a graph is represented as G = (V, E) where V is the set of vertices and E is the set of edges. Let G be an undirected connected graph without loops or multiple edges with n vertices, denoted by 1, 2, . . . , n. The topological distance between a pair of vertices i and j, which is denoted by $d(v_i , v_j)$, is the number of edges of the shortest path joining i and j. In 1947 Harold Wiener [1] defined the Wiener index W(G) as the sum of distances between all vertices of the graph G.

$$W(G) = \sum_{i<j} d(v_i, v_j)$$

The Wiener index W(G) of a graph G is defined as the sum of the half of the distances between every pair of vertices of G.

$$W(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} d(v_i, v_j)$$

2. PRELIMINARIES

Definition: 2.1

Let G = (V(G), E(G)) be a connected undirected graph. For any two vertices u, v of V(G), δ(u, v) denotes the minimum distance between u and v[4][5]. Then the Wiener Lower Sum $W^L(G)$ of the graph is defined by

$$W^L(G) = \frac{1}{2}\sum_{u,v\in V(G)} \delta(u,v) \text{ where } \delta(u, v) = \min d(u,v)$$

Definition: 2.2

If diamond silicates are arranged linearly the diamond silicate snake is obtained [6]. Let vertices labeled as O_1, O_2, O_3 be the oxygen ions and s_1 be the silicon ion of first diamond silicate (Fig.(i)).

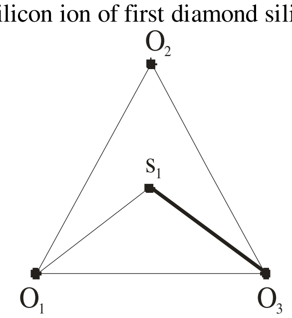

Fig. (i)

Definition: 2.3

The Distance Matrix (DM) is a lower or upper triangular matrix whose elements are d(u,v)[7].

Definition: 2.4

Let D(u,v) denote the shortest distance between two vertices u,v ∈ V(G). The Wiener index of a graph G with q edges is denoted by $W(G{:}q) = \sum q^{D(u,v)}$. The sum is given by $D(u,v) = \Sigma W'(G{:}1)$ where W′ denotes the derivative of W[G:q] with respect to q.

3. CONSTRUCTION OF DIAMOND SILICATE SNAKE (DSS)

If diamond silicates are arranged linearly the diamond silicate snake is obtained. Let O_1, O_2, O_3 be the oxygen ions and s_1 be the silicon ion of first diamond silicate Fig(i). Let O_4, O_5, O_6 and s_2 be respectively the oxygen ions and the silicon ion of second diamond silicate Fig. (ii). The oxygen ions O_3 and O_4 are merged to get the diamond silicate snake of 2 dimension Fig(iii). The oxygen ion O_5 of DSS_2 and O_7 of third diamond silicate are merged to get DSS_3. The DSS_n is shown in Fig(iv).

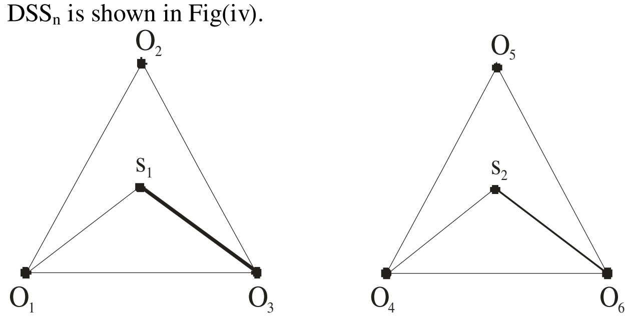

Fig. (iia) **Fig. (iib)**

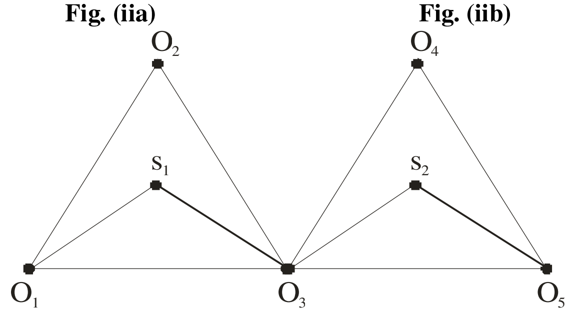

Fig. (iii): DSS$_2$

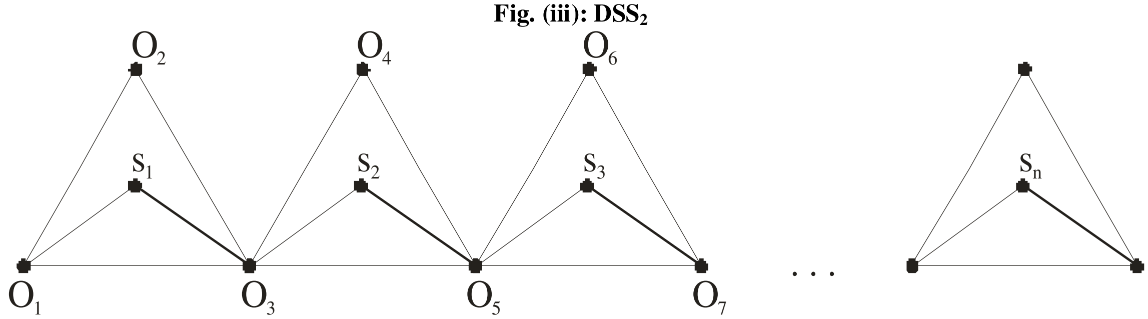

Fig. (iv): DSS$_n$

4. WIENER INDEX OF DSS$_n$

Theorem: 4.1

The Wiener index of diamond silicate snake (DSS) of dimension n ≥ 2 is a positive integer such that $W(n) = \dfrac{n(3n^2 + 9n + 2)}{2}$.

Proof: Let G = DSS$_n$, n ≥ 2. Let V(G) = {$O_1, O_2, O_3, O_4, O_5, \ldots, O_n, s_1, s_2, \ldots, s_n$}and E(G) = {$O_iO_{i+1}$; 1 ≤ i ≤ 2n} ∪ {$O_{2i-1}O_{2i+1}$; 1 ≤ i ≤ n} ∪{$O_{2i-1}s_i$; 1 ≤ i ≤ n} ∪ {s_iO_{2i+1} ; 1≤i≤n} be respectively the vertex set and edge set of G.

The Graph of DSS$_2$ is given in Fig. (iii).
Consider the distance matrix of DSS$_2$

DM =

	O_1	O_2	S_1	O_3	O_5	S_2	O_6
O_1	0	1	1	1	2	2	2
O_2	-	0	2	1	2	2	2
S_1	-	-	0	1	2	2	2
O_3	-	-	-	0	1	1	1
O_5	-	-	-	-	0	2	1
S_2	-	-	-	-	-	0	1
O_6	-	-	-	-	-	-	0

$W(G{:}q) = 10q^1 + 11q^2$, where G = DSS$_2$
Similarly,
$W(G{:}q) = 15q^1 + 21q^2 + 9q^3$, where G = DSS$_3$
$W(G{:}q) = 20q^1 + 31q^2 + 18q^3 + 9q^4$, where G = DSS$_4$
$W(G{:}q) = 25q^1 + 41q^2 + 27q^3 + 18q^4 + 9q^5$, where G = DSS$_5$
$W(G{:}q) = 30q^1 + 51q^2 + 36q^3 + 27q^4 + 18q^5 + 9q^6$, where G = DSS$_6$
…
…
$W(DSS_n : q) = 5nq^1 + (10n - 9)q^2 + 9(n - 2)q^3 + 9(n - 3)q^4 + 9(n - 4)q^5 + \ldots$where the coefficients are positive and n ≥ 2.
Wiener Sum = *W(1)* = 7,
W(2) = 32, ….

$$W(k) = \frac{k(3k^2 + 9k + 2)}{2}$$

$$W(k+1) = \frac{(k+1)[3(k+1)^2 + 9(k+1) + 2]}{2}$$

$$= W(1) + 9\frac{(k+1)(k+2)}{2} - 2$$

$$= \frac{3k^3 + 9k^2 + 2k + 9k^2 + 27k + 18 - 4}{2}$$

$$= \frac{3k^3 + 18k^2 + 29k + 14}{2}$$

$$W(k+1) = \frac{(k+1)[3(k+1)^2 + 9(k+1) + 2]}{2}$$

By the principle of mathematical induction we conclude that

$$W(n) = \frac{n(3n^2 + 9n + 2)}{2}$$

5. CONCLUSION

In this paper the distance matrices are used in order to find lower bounds of diamond silicate snake. These bounds are very useful for radar tracking, remote control, radio-astronomy, communication networks, etc. As it is well known that the valence of the carbon atom is four and vertex with more than degree four is not agreeable in reality, it is in the interest of the chemists to use this work and study the stability of the compounds and the existence of the molecule with the properties with which have analyzed the Wiener index.

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