

Wiener Index Of A Graph And Chemical Applications

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Abstract: Wiener index is one of the topological indices which can be used for analyzing intrinsic properties of molecule structure in chemistry. In this paper we evaluate a wiener index of a graph (molecular graph) in two ways: one is new method by using super edge-magic sequence (SEMS) and the other is a different approach for existing method, using Minimal spanning tree at each vertex. By this, we can reduce laborious procedure in existing method by spanning tree algorithms, as many possible. Particularly the studies on wiener index of the molecular graph to analyze the structure of organic molecules like Cyclo alkane, Alkane-n-amine and Alkane-n,n-diamine through the SEMS have been presented in this paper.

Key words: wiener index, super edge-magic sequence, spanning tree.

AMS subject classifications: 05C12, 05C78, 05C05.

Introduction:

1.1. Back ground of wiener Index

In chemistry the Wiener index is one of the most thoroughly studied, best distinguished and most frequently used graph-theory-based molecular-shape descriptors [5 and 14].

Graph theory applied in the study of molecular structures represents an interdisciplinary science, called chemical graph theory or molecular topology. By using tools taken from the graph theory, set theory and statistics it attempts to identify structural features involved in structure-property activity relationships [12 and 13].

The Wiener index W is the first topological index to be used in chemistry [14]. A topological indices are number associated with chemical structures. There is not a one-to-one connection with chemical structures and topological indices, because

several graphs may have the same topological index. Various topological indices usually reflect molecular size and shape.

A topological representation of a molecule is called molecular graph. A molecular graph is a collection of points representing the atoms in the molecule and set of lines representing covalent bonds. These points are named vertices and lines are named edges in graph theory language.

First mathematical definition of Wiener index, based on the concept of graph- theoretical distance as encoded in the distance matrix [11] is due to Hosoya [5] since its initiation the wiener index was used in a numerous structure-property studies [15]. Wiener index was developed by the American Chemist Harold Wiener in 1947 and used it to determine physical properties of types of alkanes known as paraffin [17 and 18]. Alkanes are organic compounds exclusively composed of carbon and hydrogen.

The name Wiener number or Wiener index is nowadays in standard use in chemistry and is sometimes encountered also in the mathematical literature [9 and 10]. It is most studied topological indices both from a theoretical point of view and applications.[1, 4 and 7] The use of modern topological indices in QSPR and QSAR begins with the wiener index.

H.Wiener defined Wiener index $W(G)$ [3 and 8] as the sum of smallest distance 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 .

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

1.2. Outline of the paper

The rest of the paper is organized as follows. In Section 2, we compute wiener index of a graph by the following ways: (i) Through Super edge-magic sequence and

(ii) General method-Minimal Spanning Tree Technique at each vertex. This is a new approach for existing one. It is time consuming method for finding wiener index of a graph having huge number of vertices, because there are so many spanning tree algorithms available.

More than that, method (i) is applicable only for those graphs (molecular graphs) having SEMS. All the molecular graphs can't have SEMS, but it must have wiener index. In that instance we can apply the method (ii).

In Section 3 deals with identification of the chemical compound like

Cyclo alkane, Alkane-n-amine and Alkane-n, n-diamine through the SEMS in addition of studies on wiener index. This is the initial approach to design sequences for chemical compounds by using graph theory. It could be used as a security code in Chemical Research. Finally, concluding remarks are made in Section 4.

2. Super edge-magic sequences and Wiener Index

Various authors have introduced labeling (valuation) concepts. Kotzig and Rosa introduced the concepts of magic valuation [6]. Ringel and

Llado [14] called this type of valuation as edge-magic labeling. Enomoto et. al. [2] restricted the notion of edge-magic labeling of a graph to obtain the definition of super edge-magic labeling.

We introduced the concepts and properties of super edge-magic sequence in [16]. In the same paper we discussed the following theorem:

Theorem: 2.3.1

A graph is a super edge-magic graph if and only if it has super edge-magic sequence.

2.1. Construction of SEMS from a finite set of natural numbers

In the current paper to reach fruitful results in all aspects, we convert any sequence of natural numbers into SEMS as follows. So that molecule structure can be extracted either from natural number sequences or directly from any SEMS if possible.

Conversion of any sequence of natural numbers to super edge-magic sequences achieve by pursuing the following steps.

Step1: Let (x_1, x_2, \dots, x_n) be any sequence of natural numbers whose length is say 'q'.

Step2: Find (y_1, y_2, \dots, y_n) be another sequence of numbers with same length such that $x_i + y_i$ is consecutive with $x_1 + y_1 \dots x_n + y_n$, for $1 \leq i \leq n$.

Step3: Set $L_i = \min \{x_i, y_i\}$ for $1 \leq i \leq n$ and $U_i = \max \{x_i, y_i\}$ for $1 \leq i \leq n$

Now (L_1, L_2, \dots, L_n) denotes the lower end vertices for each $e \in E(G)$ and (U_1, U_2, \dots, U_n) denotes the upper end vertices for each $e \in E(G)$. Then by definition of SEMS (L_1, L_2, \dots, L_n) represents a super edge-magic sequence and the corresponding graph representation is

$$\begin{array}{c} (L_1, L_2, \dots, L_n) \\ \downarrow \quad \downarrow \quad \dots \quad \downarrow \\ (U_1, U_2, \dots, U_n) \end{array}$$

Example 2.1.1: Suppose $(3,4,5,6,1)$ be given any sequence of natural numbers.

According the above steps, $(x_1, x_2, \dots, x_5) = (3,4,5,6,1)$ of length $q=5$.

$(y_1, y_2, \dots, y_5) = (7,5,3,1,5)$ with $6 \ 7 \ 8 \ 9 \ 10$.

$(L_1, L_2, \dots, L_5) = (3,4,3,1,1)$ and $(U_1, U_2, \dots, U_5) = (7,5,5,6,5)$

(3,4,3,1,1)
 $\downarrow \downarrow \downarrow \downarrow \downarrow$
 (7,5,5,6,5) this will produce super edge-magic graph as shown in fig.1 and the corresponding SEMS is (3,4,3,1,1)

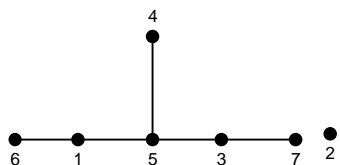


Fig.1

2.2. Calculation of Wiener index using SEMS

Either from the graph (or) sequence, we will get one SEMS. To proceed for further to define the following Bond Matrix.

Definition: 2.2.1. (Bond matrix)

Bond matrix is a matrix which gives relation between every pair among the elements of the set $\{1, 2, 3, \dots, p\}$.

That is, it is an upper triangular(lower triangular) matrix of super edge-magic sequence in which sum of all the entries equal to wiener index of the corresponding graph and is defined as follows:

$$W(G) = [w_{ij}]_{n \times n}, \text{ n-number of vertices of a graph}$$

Where w_{ij} can be defined for $i < j$ and

$$w_{ij} = \begin{cases} 0 & \text{when } v_i \text{ and } v_j \text{ are not related in permutation matrix} \\ k & \text{when min. no of relations in between } v_i, v_j \text{ in the permutation matrix} \end{cases}$$

Where permutation matrix is the sequence representation of a graph mentioned in section 2.1.

Observations of Bond matrix 2.2.2:

Formation of a bond matrix produces complete information about a graph without drawing. Bond matrix is a symmetric matrix.

- Number of one's in a row (column) of a wiener matrix is equal to degree of a vertex.
- Total number of one's in an upper triangular matrix is equal to number of edges of a graph.
- Order of the matrix is equal to number of vertices in a graph. i.e., order of the matrix = $n = \max\{U_i / 1 \leq i \leq n\}$

(iv). In any column (row), If all the entries are zeros then the corresponding vertex is a isolated vertex. Then we say that the corresponding super edge-magic graph has minimum deficiency [16].

(v). In any column (row) has at least one zero then the graph is not connected. We say that it has more than one component.

Concrete Example 2.2.3:

Consider the super edge-magic sequence as in the example 2.1.1.

	1	2	3	4	5	6	7
1	–	0	2	2	1	1	3
2	0	–	0	0	0	0	0
3	2	0	–	2	1	3	1
4	2	0	2	–	1	2	2
5	1	0	1	1	–	2	2
6	1	0	3	2	2	–	4
7	3	0	1	2	2	4	–
	2	4	3	6	10		

Sum of all entries of upper triangular matrix (lower triangular) = $2+4+3+6+10=25$

Using Bond matrix, Wiener index of fig.1 is 25.

2.3. Calculation of Wiener index by Minimal spanning trees

In general, all graphs (molecular graphs) need not have super edge-magic sequences, so wiener index for those graphs are calculated by existing method. But existing method is tedious for those graphs having large number of vertices. So we would like to suggest a new technique based on spanning trees, because many spanning tree algorithms are available. This can be performed by **Minimal spanning tree technique at each vertex** and is as follows.

Procedure:

In the definition of Wiener index, $W(G) = \sum_{i < j} d(V_i, V_j)$. At v_1 , identify a spanning tree from G which is having shortest paths from other vertices to v_1 , from this $\sum_{j > 1} d(V_1, V_j)$ can be calculated and denoted by S_{1j} for $j > 1$. Similarly we identify spanning trees at other vertices of G independently; from them the other component of $W(G)$ can be calculated.

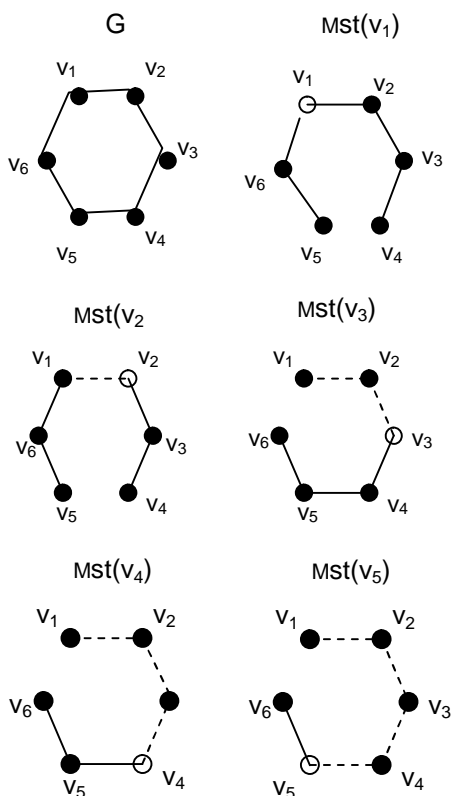
Now we find distance matrix of G using above minimal spanning trees then

$$\begin{bmatrix} s_{11} & s_{12} & s_{13} & s_{14} \\ s_{21} & s_{22} & s_{23} & s_{24} \\ \dots & \dots & \dots & \dots \\ s_{i1} & s_{i2} & s_{i3} & s_{ij} \end{bmatrix} \begin{cases} \sum s_{1j} \text{ for } j > 1 \\ \sum s_{2j} \text{ for } j > 2 \\ \sum s_{3j} \text{ for } j > 3 \\ \sum s_{ij} \text{ for } j > i \end{cases}$$

$$W(G) = \sum_{i < j} s_{ij}$$

Concrete Example 2.3.1:

Choose a graph G which hasn't SEMS. For this, consider a cycle on 6 vertices which doesn't have super edge-magic labeling. That graph is nothing but Hexagon and its minimal spanning trees with respect to its vertices are:



In the above graphs dotted edges for $i < j$, $d(v_i, v_j)$ are not considered. Since they are calculated in the previous spanning trees. The vertices which are marked by white circle indicate that calculation of minimal spanning tree with respect to that vertex. Wiener index of Hexagon is as follows:

$$\begin{matrix} s_{1j} \\ s_{2j} \\ s_{3j} \\ s_{4j} \\ s_{5j} \end{matrix} \begin{bmatrix} - & 1 & 2 & 3 & 2 & 1 \\ - & - & 1 & 2 & 3 & 2 \\ - & - & - & 1 & 2 & 3 \\ - & - & - & - & 1 & 2 \\ - & - & - & - & - & 2 \end{bmatrix} \begin{matrix} 9 \\ 8 \\ 6 \\ 3 \\ 1 \end{matrix}$$

for $i < j$ and $1 \leq j \leq 6; 1 \leq i \leq 5$

$$\text{Sum} = 27$$

Wiener index of Hexagon = 27.

3. Identifying a chemical compound through the super edge-magic sequences:

Each SEMS gives one super edge-magic graph, but all super edge-magic graphs need not represent a chemical compound. So that it is possible to identify some chemical compound through the super edge-magic sequences.

In a graph theory language, the degree of each vertex representing the valency (number of bonds incident on a vertex) of the molecule in molecular graph. Number of covalent Bonds: 4 for carbon; 3 for nitrogen; 2 for oxygen and 1 for hydrogen.

3.1. Rules for Identification

- Suppose $(a_1, a_2, a_3, \dots, a_i, \dots, a_{q-2}, a_{q-1}, a_q)$ represents SEMS for a chemical compound and this sequence has two parts separated by a broken line. Notation and representation of sequences are followed in paper[16]
- First part of the sequence always generates a pendent edge in which vertices are atoms of hydrogen.
- Second part of the sequence generates either a cycle or a chain of a chemical compound depending upon the SEMS.
- Maximum number appeared in the sequence is denoted by total number of atoms and length of the sequence is denoted by total number of bonds of the compound.
- Wiener index of a chemical compound depends upon the second part of the SEMS and it can be calculated by using Bond matrix. Since wiener index are calculated only for Hydrogen suppressed graph.

The compound name corresponding sequence with their property are discussed in Table:3.1.1.

3.2 Results and Discussion

Compound- 1: Cyclo Pentane

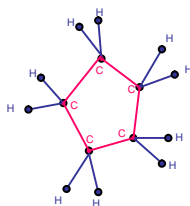
➤ Sequence Representation:

(5, 2, 4, 1, 3, 5, 2, 4, 1, 3, ⋮ 3, 2, 2, 1, 1)

⋮
13 15 12 14 11 8 10 7 9 6 ⋮ 5 5 4 4 3

Maximum number appeared in the above sequence is 15 =Total number of Atoms and Length of the sequence is 15 =Total number of Bonds of Cyclo Pentane.

➤ Structure:



➤ Wiener Index:

$$\begin{matrix} & 1 & 2 & 3 & 4 & 5 \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \begin{bmatrix} - & 2 & 1 & 1 & 2 \\ 2 & - & 2 & 1 & 1 \\ 3 & 1 & 2 & - & 2 & 1 \\ 4 & 1 & 1 & 2 & - & 2 \\ 5 & 2 & 1 & 1 & 2 & - \end{bmatrix} \end{matrix}$$

Using Bond matrix Wiener index of Cyclo Pentane is 15.

Compound-2: Butane-1-amine

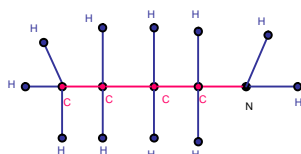
➤ Sequence Representation:

(3, 5, 2, 4, 1, 3, 5, 2, 4, 1, 3, ⋮ 3, 2, 2, 1)

⋮
16 13 15 12 14 11 8 10 7 9 6 ⋮ 5 5 4 4

Maximum number appeared in the above sequence is 16 =Total number of Atoms and Length of the sequence is 15 =Total number of Bonds of Butane-1-amine.

➤ Structure:



➤ Wiener Index:

$$\begin{matrix} & 1 & 2 & 3 & 4 & 5 \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \begin{bmatrix} - & 2 & 4 & 1 & 3 \\ 2 & - & 2 & 1 & 1 \\ 3 & 4 & 2 & - & 3 & 1 \\ 4 & 1 & 1 & 3 & - & 2 \\ 5 & 3 & 1 & 1 & 2 & - \end{bmatrix} \end{matrix}$$

Using Bond matrix Wiener index of Butane-1-amine is 20.

Compound-3: Propane -1, 3- Diamine

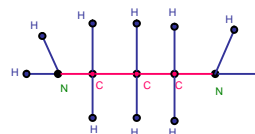
➤ Sequence Representation:

(5, 2, 4, 1, 3, 5, 2, 4, 1, 3, ⋮ 3, 2, 2, 1)

⋮
13 15 12 14 11 8 10 7 9 6 ⋮ 5 5 4 4

Maximum number appeared in the above sequence is 15 =Total number of Atoms and Length of the sequence is 14 =Total number of Bonds.

➤ Structure:



➤ Wiener Index:

$$\begin{matrix} & 1 & 2 & 3 & 4 & 5 \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \begin{bmatrix} - & 2 & 4 & 1 & 3 \\ 2 & - & 2 & 1 & 1 \\ 3 & 4 & 2 & - & 3 & 1 \\ 4 & 1 & 1 & 3 & - & 2 \\ 5 & 3 & 1 & 1 & 2 & - \end{bmatrix} \end{matrix}$$

Wiener index of Propane 1,3- Diamine is 20.

The details of results and discussions of a chemical compound are presented in Table :3.2.1.

4. Conclusion

This paper contained two important mechanisms: one is calculation of wiener index that includes two ways: first is the new method using SEMS and the other method is a new technique for existing one. The other part of the mechanism is the identification of the chemical compound through the SEMS. This approach will help to transmit the chemical formula into sequence.

Table:3.1.1

S.No.	Compound Name	SEMS for a Compound	Property of SEMS in[16]	Particular case for sequence when N=2.
1.	Cyclo Alkane	$((2N+1, N, 2N, N-1, 2N-1, \dots, \dots, 1, N+1)^{(2)}, N+1, N, N, N-1, N-1, \dots, 1, 1)$	$\ast=N+2, \quad q=3(2N+1)$ $p=3(2N+1)$ $p = q$ (unicycle)	$(5, 2, 4, 1, 3, 5, 2, 4, 1, 3, \vdots 3, 2, 2, 1, 1)$ -Cyclo Pentane
2.	Alkane-n-Amine	$(N+1, (2N+1, N, 2N, N-1, 2N-1, \dots, 1, N+1)^{(2)}, N+1, N, N, N-1, N-1, \dots, 1)$	$\ast=N+3$ $q=3(2N+1)$ $p=3(2N+1)+1.$ $p = q+1$ (tree)	$(3, 5, 2, 4, 1, 3, 5, 2, 4, 1, 3, \vdots 3, 2, 2, 1)$ - Butane-1-Amine
3.	Alkane- n, n -Diamine	$((2N+1, N, 2N, N-1, 2N-1, \dots, 1, N+1)^{(2)}, N+1, N, N, N-1, N-1, \dots, 1)$	$\ast=N+3$ $q=3(2N+1)-1$ $p=3(2N+1).$ $p = q+1$ (tree)	$(5, 2, 4, 1, 3, 5, 2, 4, 1, 3, \vdots 3, 2, 2, 1)$ - Propane-1, 3- Diamine

Table : 3.2.1.

S. No.	Results for chemical compound	Compound - 1		Compound - 2		Compound - 3	
		General case	Specific case for N=2	General case	Specific case for N=2	General case	Specific case for N=2
1.	Number of Atoms	$3(2N+1)$	15	$3(2N+1)+1$	16	$3(2N+1)$	15
2.	Number of Bonds	$3(2N+1)$	15	$3(2N+1)$	15	$3(2N+1)-1$	14
3.	Cyclomatic number	1	1	0	0	0	0
4.	Number of atoms in the cycle/ chain	$2N+1$	5	$2N+1$	5	$2N+1$	5
5.	Number of bonds in the cycle /chain	$2N+1$	5	$2N$	4	$2N$	4
6.	Chemical formula for a compound	$C_{2N+1}H_{2(2N+1)}$	C_5H_{10}	$C_{2N}H_{(2(2N)+3)}N$	$C_4H_{11}N$	$NH_2-(CH_2)_{2N-1}-NH_2$	$NH_2-CH_2)_3-NH_2$
7.	IUPAC Name	Cyclo Alkanes	Cyclo Pentane	Alkane-n-amine	Butane-1-amine	Alkane-n,n -diamine	Propane-1, 3- Diamine
8.	Wiener index	calculated by bond matrix using the cycle C_{2N+1}	15	calculated by bond matrix using the chain C_{2N}	20	calculated by bond matrix using the chain C_{2N}	20

References:

1. Andrey A. Dobrynin, Ivan Gutman, Sandi Klavzar and Petra Zigert, wiener Index of hexagonal systems, *Acta Applicandae mathematicae*, 72, 247-294, (2002).
2. H. Enomoto, A. Llado, T. Nakamigawa, and G. Ringel, Super edge magic-graphs, *SUT J Math.* 34(1998), 105-109.
3. A.Graovac, and T.Pisanski, On the wiener index of a graph, *J. Math. Chem.* 8, 53- 62 (1991).
4. I.Gutman, Y.N.Yeh, S.L.Lee, and Y.L.Luo, some recent results in the theory of the wiener number, *Indian J. Chem.*, 32A, 651-661, (1993) .
5. H.Hosoya, A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. soc. Japan*, 44, 2332-2339, (1971).
6. A. Kotzig, and A. Rosa, Magic valuations of finite graphs, *Canad. Math. Bull.* 13(1970), 451-461.
7. S.Klavzar, I.Gutman and B.Mohar, Labeling of benzenoid system which reflects the vertex-distance relations, *J.chem. Inf. Comput. Sci.* 35 (1995) 590-593.
8. Sandi Klavzar, Ivan Gutman, Wiener number of vertex-weighted graphs and a chemical application, *Discrete Appl. Math.*, 80 (1997) 73-81.
9. R.Merris, An edge version of the matrix-tree theorem and the wiener index, *Lin. Multilin. Algebra* 25 (1988) 291-296.
10. R.Merris, Laplacian matrices of graphs: A survey, *Lin. Algrbra Appl.* 197/198 (1994), 143-176.
11. Z.Mihalic, D.Veljan, D.Amic, S.Nilkolic, D.Plavsic, N.Trianjstic, The distance matrix in chemistry, *J. Math. Chem.*, 11, 223-258 (1992).
12. B.Mohar, and T.Pisanski, How to compute the wiener index of a graph, *Journal of mathematical Chemistry*, 2 (1988) 267-277.
13. S.Nikolic, N.Trianjstic and Z.Mihalic, The Wiener Index: Developments and applications, *Croat. Chem. Acta.*, 68(1995) 105-129.
14. G.Ringel and A.Llado, Another tree conjecture, *Bull.Inst. Combin. Appl.* 18(1996), 83-85.
15. N.Trianjstic, ed., mathematics and computational concepts in chemistry, Horewood/Wiley, New York, 1986.
16. A.Vijayabarathi, Dr.G.S.G.N.Anjaneyulu, Novel Sign of Super Edge-Magic Graphs, *International Journal of Pure and Applied Mathematics-Accepted*.
17. H.Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* 69 (1947) 17-20.
18. H.Wiener, *J. Chem. Phys.* 15 (1947) 766.
