On the Wiener indices of molecular graphs

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Abstract: The Wiener index of a graph $G$ is denoted by $W(G)$ and defined as the sum of distances between all pairs of vertices in simple connected graph. Wiener index is used for modeling the shape of organic molecules and for calculating several of their physicochemical properties. In this paper comparison and inequalities for Wiener index, hyper-Wiener index, reverse Wiener index, revised version of Wiener index, degree-distance index, reciprocal degree-distance, Gutman index, complementary Wiener index, multiple version of Wiener index, modified Wiener index and average distance $\mu(G)$ in isomers of octane are investigated.

Keywords: Topological indices, degree-distance, isomers of octane, distance matrix, inequality.

I. INTRODUCTION

Let $G = (V(G), E(G))$ be a simple connected graph of order $n$ and size $m$. The degree of any vertex is the number of first neighbor of $v$ is denoted by $\text{deg}(v)$. Let the maximum and minimum of all the vertices of $G$ are respectively, denoted by $\Delta$ and $\delta$. The distance of between any two vertices $u$ and $v$ of graph is defined as the length of the shortest path connecting $u$, $v$ is $d(u, v)$. A topological index is a number related to molecular graph invariant under automorphism of $G$. Simplest topological indices of graph $G$ are the number of vertices, edges, degree of vertex $v$ and distance between vertices $u, v \in V(G)$, are denoted by $n$, $m$, $d_v$ and $d(u,v)$ respectively [1]. Topological indices are particularly suitable if properties like shape or degree of branching are expected to have an influence on the property predicted. Calculation is often based on the distance matrix of molecular graph. A disadvantage of topological indices is that they are unrelated to observable physical properties.

The Wiener index $W(G)$ of connected graph $G$ is the sum of distances between all pairs of vertices in $G$ [2]. Equivalently, $W(G)$ is obtained by the first derivative of $H(G,x)$ at $x = 1$, i.e.

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$$

$$= H'(G,x) \bigg|_{x=1}$$

And modified Wiener index is

$$W_\lambda(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)^\lambda$$

Where $\lambda$ is some real number and $\lambda \neq 0$

The Wiener index is a good foundation for determining if there is correlation between molecule’s structure and properties because it takes into account distances between atoms, more specifically their electron clouds, so when the distance increases the Wiener index increases [3].

Our notations are standard and mainly taken from standard books of graph theory [4-7]. All graphs considered here are simple and connected. There are 18 isomers of octane as $n$-octane, 2-methylheptane, 3-methylheptane, 4-methylheptane, 3-ethyl-hexane, 2,2-dimethylhexane, 2,3-dimethylhexane, 2,4-dimethylhexane, 2,5-dimethylhexane, 3,3-dimethylhexane, 3,4-dimethylhexane, 3,2-
ethyl-methyl-pentane, 3,3-ethyl-methyl-pentane, 2,2,3-trimethyl-pentane, 2,2,4-trimethyl-pentane, 2,3,3-trimethyl-pentane, 2,3,4-trimethyl-pentane, 2,2,3,3-tetramethyl-butane.

In this paper comparative and inequality study of Wiener index, hyper-Wiener index, reverse Wiener index, modified Wiener index $W_\lambda(G)$, revised version of reverse Wiener index, degree-distance index, Gutman index, multiplicative version of the Wiener index, complementary Wiener index, and a related quantity average distance $\mu(G)$ for isomers of octane are investigated. For definitions and formulae used to study types of Wiener indices refer [8-13].

II. RESULTS AND DISCUSSION

2.1 Molecular graph and distance matrix

Let $G$ be a simple graph with $n$-vertices and $m$-edges. For vertices $u, v \in V(G)$ the distance between $u$ and $v$ in $G$ is denoted by $d(u, v)$, is the length of a shortest path in $G$. The eccentricity $e_G(v)$ of a vertex $v$ is defined as the distance between $v$ and vertex furthest from $v$. The largest of the eccentricities of vertices of graph $G$ is diameter, denoted by $\text{dia}(G)$. The radius of $G$, $\text{rad}(G)$, is the smallest of the eccentricities of vertices. Let $p$, $\Delta$ and $\delta_1$ denote the number of pendent vertices, maximum vertex degree and minimum non-pendent degree of $G$, respectively. The distance is an important tool in studying the structure of graph, and plays also dominant role in the applications of graph theory in computer science, chemistry and in variety of other fields.

The isomers of octane are n-octane, 2-methyl-heptane, 3-methyl-heptane, 4-methyl heptane, 3-ethyl–hexane, 2,2-dimethyl-hexane, 2,3-dimethyl-hexane, 2,4-dimethyl-hexane, 2,5-dimethyl-hexane, 3,3–dimethyl hexane, 3,4–dimethyl-hexane, 3,2-ethyl-methyl-pentane, 3,3-ethyl-methyl-pentane, 2,2,3-trimethyl-pentane, 2,2,4-trimethyl-pentane, 2,3,3-trimethyl-pentane, 2,3,4-trimethyl-pentane, 2,2,3,3-tetramethyl-butane. The molecular graph of 2,3-dimethyl-hexane is shown in figure (1). The distance matrix is $|V| \times |V|$ matrix. The types of Wiener indices computed from distance matrices which are defined as

\[
D_{i,j} = \begin{cases} 
0 & i = j \\
 d_{ij} & i \neq j 
\end{cases} \tag{4}
\]

Where $d_{i,j}$ is the length of the shortest path from $i$ to $j$. The distance matrix for 2, 3-dimethyl-hexane is represented in figure (2), from such matrices the respective Wiener indices are computed.

![Fig (1): Molecular graph G of 2, 3-dimethyl hexane](image-url)
2.2 Types of Wiener Indices:

In this section, comparison and some inequalities for Wiener index, hyper-Wiener index, reverse-Wiener index, revised version of Wiener index, degree-distance, reciprocal degree-distance, Gutman index, multiplicative version of Wiener index, complementary Wiener index and average distance $\mu(G)$ are studied in isomers of octane. The values of Wiener index, hyper-Wiener index and reciprocal degree distance are given in table (1) for isomers of octane [14-16]. The values of $\text{dia}(G)$, $\text{rad}(G)$, $p$, $\Delta$, $\delta_1$ considered from respective molecular graph of isomers of octane and are used to compute reverse Wiener index, revised version of Wiener index, degree-distance, Gutman index, multiplicative version of Wiener index, complementary Wiener index and average distance $\mu(G)$. The diameter $\text{dia}(G)$ for isomers of octane is in the range 3 to 7. As number of vertices are 8, then $\text{rad}(G) \leq n/2$, the radius is 1 in each case of molecular graph. The reverse Wiener indices for all octane has unequal values except 4-M-heptane, 2,3-MM-hexane, 2,4-MM-hexane. In 2,3-MM-hexane, 2,4-MM-hexane RRD(G) is same due to having 7 and 8 carbon vertices at downside of chain. In 2, 2, 3, 3-tetramethyl butane topological indices follows order

$\Delta(G) < W(G) < WW(G)$ due to both sides branching of the vertices. From molecular graphs of each octane $p$, $n\Delta$ and $\delta_1$ computed and employed in inequality study of Wiener indices. In 2,3,4-MMMM-pentane,2,2,3,3-MMMM-butane,$\Delta$, $\delta_1$ are equal, having values 3 and 4 respectively due to particular ramification.

### Table (1): $W(G)$, $WW(G)$ and $RRD(G)$ for isomers of octane (M-methyl, E-ethyl).

<table>
<thead>
<tr>
<th>Sr.no.</th>
<th>Octane</th>
<th>$W(G)$</th>
<th>$WW(G)$</th>
<th>$RRD(G)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>n-octane</td>
<td>84</td>
<td>210</td>
<td>99.57</td>
</tr>
<tr>
<td>2</td>
<td>2-M-heptane</td>
<td>79</td>
<td>185</td>
<td>104.33</td>
</tr>
<tr>
<td>3</td>
<td>3-M-heptane</td>
<td>76</td>
<td>170</td>
<td>106.2</td>
</tr>
<tr>
<td>4</td>
<td>4-M-heptane</td>
<td>75</td>
<td>165</td>
<td>112.27</td>
</tr>
<tr>
<td>5</td>
<td>3-E-hexane</td>
<td>72</td>
<td>150</td>
<td>108.6</td>
</tr>
<tr>
<td>6</td>
<td>2,2-MM-hexane</td>
<td>71</td>
<td>149</td>
<td>113.4</td>
</tr>
<tr>
<td>7</td>
<td>2,3-MM-hexane</td>
<td>70</td>
<td>143</td>
<td>112.27</td>
</tr>
<tr>
<td>8</td>
<td>2,4-MM-hexane</td>
<td>71</td>
<td>147</td>
<td>112.27</td>
</tr>
<tr>
<td>9</td>
<td>2,5-MM-hexane</td>
<td>74</td>
<td>161</td>
<td>109.2</td>
</tr>
</tbody>
</table>
The types of Wiener indices computed on molecular graphs using the formulae [8-13] for octane in $\Lambda(G)$, $W(CD, G)$, $\Lambda'(G)$, $\Pi$-index, $\mu(G)$. 

The star graph is the unique graph having minimum $\Pi$-index and path is unique graph with maximum $\Pi$-index. The 2, 2, 3, 3-tetramethyl butane has minimum value for $\Pi$-index value and n-octane has maximum $\Pi$-index agreeing well with Gutman [10]. The topological indices 

$W(CD, G)$ and $\mu(G)$ have highest value in n-octane as 54 due to linear structure and lowest value 2.0714 in 2, 2, 3, 3-tetramethyl butane being a star graph. The n-octane with linear structure has maximum value for $\Lambda(G)$ as 87.5 whereas minimum value 15.5 in 2, 2, 3, 3-tetramethyl butane. Among $rDD(G)$ and $DD(G)$, $rDD$ shows maximum value in n-octane due to path structure, $rDD$ and $DD$ has same value in 2, 2, 3 trimethyl pentane. The inequality in topological indices $rDD \leq DD$ in 3,2,EM-pentane and 2,2,3-trimethyl pentane is because of symmetrical ramifications in molecular graphs but this is not the case in 2,3,3-trimethyl pentane as it has diameter $\text{Dia}(G) = 4$.

$$D'(G) = 4 \ W(G) - n (n-1)$$

Where $D'(G)$ is the degree distance, thus there is no need to study the degree-distance for trees because this is equivalent to the Wiener index. The mean Wiener index is calculated by dividing the Wiener index by number of topological distances in the molecular graph. Wiener index reaches maximum value $n(n^3 - n)/6$ in path graph, where $n$ is the number of vertex. Using the same formula we can normalize the Wiener index as $W_0(G) = 6 \ W(G)/(n^3 - n)$ giving $W_0(G) \in [0,1]$ which is followed in the n-octane, as has $W(G) = 84$ [17]. The relationship between TI’s in isomers of octane is $W(W(G)) > rRD(G) > W(G)$.

### 2.3 Inequality

In this section some of the inequalities are discussed for isomers of octane. The vertex-degree based topological indices such as $X(G), H(G), M_1(G), M_2(G), GA_1(G), GA_4(G)$ and $ABC(G)$, if are replaced by distance based types of Wiener indices the inequalities between them appear to be as follows:

1) With $n \geq 2$, $0 \leq \Lambda(G) \leq n (n-1) (n-2)/3$  

Here $n = 8$, $\Lambda(G) = 112$, this is observed only for $G = P_n$ in n-octane, for all other isomers of octane $\Lambda(G) < 112$ [18].

2) $H(G) > 2m^2 / M_1(G)$, If $H(G)$ is replaced by $W(G)$ and $M_1(G)$ by $\Lambda(G)$ then the inequality applicable for all isomers of octane.

3) In $H(G) \geq X(G)$  

If $H(G)$ is replaced by $W(CD, G)$, and $\Lambda(G)$ by $X(G)$, then $W(CD, G) \geq \Lambda(G)$ is valid for octane as $W(CD, G)$ values are greater in $\Lambda(G)$.
4) In G A₁ (G) ≥ 2m / n, 
G A₄ (G) ≥ 2m/n
If GA₁(G),GA₄(G) are replaced by W(G), A (G), A (G) , rDD, DD, W(CD,G) in types of Wiener indices then, the inequality has to be rewritten to suit the types of Wiener indices as  ≥m / n.
5) The inequality between first and second Zagreb indices,
M₁ (G)/n ≤ M₂ (G) / m, can be modified in types of Wiener indices as
W (G)/n ≤WW (G)/m
Numerically this inequality valid in all isomers of octane. Similarly many inequalities between degree-based topological indices, the types of Wiener indices can be studied. For G a simple graph, the graph is called good if Zagreb indices inequality holds. The same concept can be extended to the molecular graphs of isomers of octane [19].
(6)The inequality
m / n-1≤ W(G) ≤ m, where n is number of vertices and m is number of edges. As Wiener indices have larger values this inequality does not apply for other types of Wiener indices.

III. CONCLUSION
The types of Wiener indices computed from distance matrices of molecular graphs. Many inequalities between vertex-degree based topological indices are valid for distance based types of Wiener indices in isomers of octane. The topological indices are used to study quantitative structure relationships–property / activity (QSAR/QSAR).

REFERENCES
4. F.Harary, Graph theory, Addison, Wesley, Reading MA, 1971.
5. C.Vasdev, Graph theory with applications, New Age, International publishers, New Delhi, 2006.