CHAPTER 4

GENERAL RESULTS ON TERMINAL WIENER INDEX

4.1 INTRODUCTION

In order to obtain the structure-activity relationships in which theoretical and computational methods are based it is necessary to find appropriate representations of the molecular structure of chemical compounds. These representations are realized through the molecular descriptors. Molecular descriptors are numbers containing structural information derived from the structural representation used for molecules under study (Klein et al 1992).

Gutman et al (2009) introduced the terminal distance matrix or reduced distance matrix of trees. The terminal Wiener index $TW (G)$ of a graph $G$ is the sum of the distances between all pairs of pendant vertices.

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

where $d(v_i, v_j)$ is the distance between pair of pendant vertices in a graph $G$.

In other words, for the tree $T$, $TW (T) = \sum_e p_1(e) p_2(e)$ instead of summing the distances between all pairs of pendant vertices in the tree $T$. Count how many times a particular edge $e$ lies on the path between two pendant vertices, and then add these counts over all edges of the underlying tree. Such shortest paths will start with $p_1 (e)$ pendant vertices those lying on
one side of \( e \) and end at \( p_2 (e) \) pendant vertices those lying on the other side of \( e \).

\[
\begin{align*}
\text{CH}_3 & \quad \text{CH}_3 & \quad \text{CH}_3 \\
\text{CH}_3 & \quad \text{CH} & \quad C & \quad \text{CH} & \quad \text{CH}_2 & \quad \text{CH}_3 \\
\text{CH}_3 & \quad & & \\
\end{align*}
\]

**Figure 4.1(a) The chemical compound \((2,4)\)-methyl-(3,3)-dimethyl hexane**

\[
\begin{align*}
v_1 & \quad e_1 & \quad v_2 & \quad e_2 & \quad e_7 & \quad v_3 & \quad e_3 & \quad v_4 & \quad e_4 & \quad e_9 & \quad v_5 \\
v_7 & \quad v_8 & \quad v_9 & \quad v_{10} & \\
v_6 &
\end{align*}
\]

**Figure 4.1(b) The Tree \( T \) representing the chemical compound \((2,4)\)-methyl-(3,3)-dimethyl hexane**

In Figure 4.1(b) \( v_1, v_2, v_3, v_4, v_5, v_6 \) are pendant vertices and \( v_7, v_8, v_9, v_{10} \) are non pendant vertices.

For the Tree \( T \) in Figure 4.1(b).

\[
W (T) = \sum_e n_1 (e) n_2 (e)
\]
\[ \begin{align*}
W(T) &= n_1(e_1)n_2(e_1) + n_1(e_2)n_2(e_2) + n_1(e_3)n_2(e_3) \\
&\quad + n_1(e_4)n_2(e_4) + n_1(e_5)n_2(e_5) + n_1(e_6)n_2(e_6) \\
&\quad + n_1(e_7)n_2(e_7) + n_1(e_8)n_2(e_8) + n_1(e_9)n_2(e_9) \\
&= (1)(9) + (1)(9) + (1)(9) + (1)(9) + (1)(9) + (1)(9) \\
&\quad + (3)(7) + (6)(4) + (8)(2) \\
&= 115
\end{align*} \]

\[ TW(T) = \sum_e p_1(e)p_2(e) \]

\[ \begin{align*}
&= p_1(e_1)p_2(e_1) + p_1(e_2)p_2(e_2) + p_1(e_3)p_2(e_3) \\
&\quad + p_1(e_4)p_2(e_4) + p_1(e_5)p_2(e_5) + p_1(e_6)p_2(e_6) \\
&\quad + p_1(e_7)p_2(e_7) + p_1(e_8)p_2(e_8) + p_1(e_9)p_2(e_9) \\
&= (1)(5) + (1)(5) + (1)(5) + (1)(5) + (1)(5) \\
&\quad + (1)(5) + (2)(4) + (5)(1) + (4)(2) \\
&= 51
\end{align*} \]

Consider a graph \( G \), vertices having degree one are called pendant vertices and vertices having more than degree one are called non pendant vertices. We represent the sum of the distances between all the pairs of pendant vertices by \( TW(G) \) and sum of the distances between all pairs of non pendant vertices as \( IW(G) \).

In section 4.2, the terminal Wiener index is calculated for the full binary tree and for some new class of graphs derived from a given connected graph. Also we define some new graphs.
In section 4.3, the terminal Wiener index of generalized caterpillar graph derived from path graph is calculated.

In section 4.4, the terminal Wiener index of detour saturated trees $T_3 \ (n)$, $T_4 \ (n)$ and nanostardendrimer $D_3 \ (n)$ are investigated.

4.2 TERMINAL WIENER INDEX FOR SOME NEW CLASS OF GRAPHS

**Theorem 4.2.1.** The terminal Wiener index of full binary tree $T$ is

$$2^{l-1} \sum_{m=1}^{l} m2^m$$

where $l$ is the level of the tree $T$.

**Proof:** A full binary tree is a binary tree in which each non pendant vertex has exactly two children. If $T$ is full binary tree with $i$ non pendant vertices then $T$ has $i+1$ pendant vertices and it has order $2i+1$. The level of a vertex is the number of edges along the unique path between it and the root. The level of the root is defined as 0. The vertices immediately under the root are said to be in level 1 and so on. The maximum number of vertices on level $m$ in a binary tree is $2^m$. The terminal Wiener index of full binary tree is

$$TW (T) = 2^{l-1} \left(1.2 + 2.2^2 + 3.2^3 + \ldots + l.2^l\right)$$

$$TW (T) = 2^{l-1} \sum_{m=1}^{l} m2^m$$

where $l$ is the level of the tree starting from $0^{th}$ level.

**Theorem 4.2.2.** If $G$ is a connected graph then the terminal Wiener index of $G^+$ is $W\ (G) + n\ (n-1)$.

**Proof:** Let $G$ be a connected graph with $n$ vertices $\{v_1, v_2, \ldots, v_n\}$. The graph $G^+$ is obtained from $G$ by adding a pendant edge to all the vertices of $G$. Let the
vertex set of $G^+$ be \( \{v_1, v_2, \ldots, v_n, v'_1, v'_2, \ldots, v'_n\} \) and edge set be 
\[ E(G) \cup \{v'_1v'_2, v'_2v'_3, \ldots, v'_nv'_n, v'_1v'_2v'_3, \ldots, v'_nv'_n\}. \]

![Graph G+](image)

**Figure 4.2** The graph $G^+$

\[ TW\left(G^+\right) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} d\left(v_i, v'_j\right) \]

\[ = \frac{1}{2} \left\{ d(v_1, v_1) + d(v_1, v_2) + 2 + \ldots + d(v_1, v_n) + 2 \right\} \]

\[ = \frac{1}{2} \left\{ d(v_2, v_1) + 2 + d(v_2, v_2) + \ldots + d(v_2, v_n) + 2 \right\} \]

\[ \ldots \]

\[ = \frac{1}{2} \left\{ d(v_n, v_1) + 2 + d(v_n, v_2) + 2 + \ldots + d(v_n, v_n) \right\} \]

\[ = \frac{1}{2} \left\{ \sum_{i=1}^{n} \sum_{j=1}^{n} d\left(v_i, v_j\right) + 2n(n - 1) \right\} \]

\[ = \frac{1}{2} \{2W(G) + 2n(n - 1)\} \]

\[ TW\left(G^+\right) = W(G) + n(n - 1). \]

**Definition 4.2.3.** The graph $G^x_-$ is obtained from $G^+$ by adding an edge from all the non pendant vertices of $G^+$ to the new vertex $x$. 
Theorem 4.2.4. If $G(p, q)$ is a graph then the terminal Wiener index of $G^+_x$ is $2p^2 - 2p - q$.

Proof: Let $G(p, q)$ be a graph. Let the degree sequence of the graph $G$ be $(d_1, d_2, ..., d_p)$. The graph $G^+$ has $2p$ vertices and $p + q$ edges. The graph $G^+_x$ has $2p + 1$ vertices and $2p + q$ edges. In $G^+$, the distance between pendant vertices is neither one nor two. The shortest distance between pair of vertices in $G^+_x$ is either three or four. The number of pairs of adjacent vertices in $G^+_x$ and distance between those pairs of the vertices is three. Number of pairs of non-adjacent vertices in $G$ is equal to number of pairs of non-adjacent vertices in $G^+_x$ is equal to four.

$$TW(G^+_x) = \frac{1}{2} \left\{ 3(d_1 + d_2 + ... + d_p) + 4\left[ p(p-1) - (d_1 + d_2 + ... + d_p) \right] \right\}$$

$$= \frac{1}{2} \left\{ 3(2q) + 4(p(p-1) - 2q) \right\}$$

$$TW(G^+_x) = 2p^2 - 2p - q.$$ 

Theorem 4.2.5. Let $T(p, q)$ be a tree with $k$ pendant vertices. By joining a pendant edge to all the pendant vertices successively, the terminal Wiener index in the $p^{th}$ stage is $TW(T) + pk(k-1)$.

Proof: By definition $TW(T) = \frac{1}{2} \sum_{i=1}^{k} \sum_{j=1}^{k} d(v_i, v_j)$

In the first stage $TW(T^1) = TW(T) + \frac{1}{2} \left[ (2 + 2 + ... + 2) \right]_{k(k-1) \text{ times}}$
In the second stage $TW\left( T^2 \right) = TW\left( T \right) + \frac{1}{2} \left[ \frac{(2 + 2 + \ldots + 2) + (2 + 2 + \ldots + 2)}{k(k-1) \text{ times}} \right]$

![Figure 4.3 The tree $T^p$](Image)

In the $p^{th}$ stage $TW\left( T^p \right) = TW\left( T \right) + \frac{1}{2} \left[ \frac{(2 + 2 + \ldots + 2) + \ldots + (2 + 2 + \ldots + 2)}{k(k-1) \text{ times}} \right]$

\[ = TW\left( T \right) + \frac{1}{2} \left[ \frac{2k(k-1) + \ldots + 2k(k-1)}{p \text{ times}} \right] \]

\[ TW\left( T^p \right) = TW\left( T \right) + pk(k-1). \]

**Definition 4.2.6.** Let $\overset{\wedge}{T}$ be a tree obtained from $T$ by joining $m$ pendant edges to every $k$ pendant vertices. The tree $\overset{\wedge}{T}$ consists of $p + km$ vertices and $q + km$ edges.
**Theorem 4.2.7.** Let $T(p, q)$ be a tree with $k$ pendant vertices. If $\hat{T}$ is a tree obtained from $T$ by joining $m$ pendant edges to every $k$ pendant vertices, then the terminal Wiener index of $\hat{T}$ is $m^2TW(T) + mk(mk - 1)$.

**Proof:**

![Diagram of a tree $\hat{T}$ with pendant vertices labeled $v_1, v_2, v_3, \ldots, v_{k+1}, \ldots, v_p$.]

$$TW(\hat{T}) = \frac{1}{2} m \left[ \left( \frac{2 + 2 + \ldots + 2}{(m-1) \text{ times}} \right) + \left( \frac{2 + 2 + \ldots + 2}{(m-1) \text{ times}} \right) + \ldots + \left( \frac{2 + 2 + \ldots + 2}{(m-1) \text{ times}} \right) \right]$$

$$+ m \left[ \left( \frac{2TW(T) + 2k(k-1)}{m \text{ times}} \right) + \left( \frac{2TW(T) + 2k(k-1)}{m \text{ times}} \right) + \ldots + \left( \frac{2TW(T) + 2k(k-1)}{m \text{ times}} \right) \right]$$

$$= \frac{1}{2} \left( 2mk(m-1) + 2m^2TW(T) + 2m^2k(k-1) \right)$$
\[ TW\left( \bar{T} \right) = m^2 TW\left( T \right) + mk (mk - 1). \]

**Theorem 4.2.8.** If \( G(p, q) \) is a graph and at least one vertex has degree \( p - 1 \) then \( TW(G) = k(k - 1) \), where \( k \) is the number of pendant vertices in \( G \).

**Proof:** By definition \( TW(G) = \frac{1}{2} \sum_{i=1}^{k} \sum_{j=1}^{k} d(v_i, v_j) \)

\[
= \frac{1}{2} \left[ \left( \sum_{i=1}^{k} d(v_i, v_i) \right) + \left( \sum_{i=1}^{k} d(v_i, v_i) \right) + \cdots + \left( \sum_{i=1}^{k} d(v_i, v_i) \right) \right] \\
= \frac{k}{2} \left[ \left( \sum_{i=1}^{k} d(v_i, v_i) \right) \right] \\
= k(k - 1).
\]

**Theorem 4.2.9.** Let \( T \) be a tree with \( p \) vertices in which there are \( k \) pendant vertices. \( T^p \) be a graph obtained from tree \( T \) by adding a pendant edge to all the non pendant vertices of \( T \). The terminal Wiener index of \( T^p \) is \( TW(T^p) = W(T) + (p - k)(p - 1) \).

**Proof:** Let \( T \) be a tree with \( k \) pendant vertices and \( (p - k) \) non pendant vertices. Let the vertex set of \( T^p \) be \( \{v_1, v_2, \ldots, v_p, v'_1, v'_2, \ldots, v'_{p-k} \} \). Shortest distance between pair of pendant vertices in \( T \) is equal to distance between pair of these pendant vertices in \( T^p \). The distance between pendant vertices to non pendant vertices of \( T \) is equal to the distance between pair of pendant
vertices to new pendant vertices of \( T^* \), increased by one. The distance between pair of non pendant vertices of \( T \) is equal to distance between pair of pendant vertices to new pendant vertices of \( T^* \) increased by distance two.

\[
TW\left( T^* \right) = \text{half of the shortest distance between pendant vertices in } T \\
+ \text{half of the shortest distance between old pendant vertices in } T^* \text{ to new pendant vertices in } T^* \\
+ \text{half of the shortest distance between new pendant vertices in } T^* \text{ to the old pendant vertices in } T^* \\
+ \text{half of the shortest distance between new pendant vertices in } T^*
\]

\[
TW\left( T^* \right) = \frac{1}{2} \left\{ 2TW\left( T \right) + \left[ 2IW\left( T \right) + 2(p-k)(p-k-1) \right] + 2 \left[ W\left( T \right) - IW\left( T \right) - TW\left( T \right) + k(p-k) \right] \right\} \\
= \frac{1}{2} \left\{ 2W(T) + 2(p-k)(p-k-1) - 2k(p-k) \right\}
\]

\[
TW\left( T^* \right) = W(T) - (p-k)(p-1).
\]

**Theorem 4.2.10.** Let \( T(p,q) \) be a tree with \( k \) pendant vertices such that there is at least one vertex \( v \) with degree \( p-1 \). The graph \( T^* \) is obtained by connecting \( m \) copies of \( T \) by adding \( m \) new edges from each \( v \) of \( T \) to a new vertex \( x \). Then \( TW\left( T^* \right) = mk \left[ k(2m-1) - 1 \right] \).
Proof: By definition

\[ TW(T^x) = \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{mk} d(v_i, v_j) \]

\[ = \frac{1}{2} \left[ m \left( \frac{(2 + 2 + \ldots + 2) + \ldots + (2 + 2 + \ldots + 2)}{k-1} \right) \right] \]

\[ + m \left( k \left( \frac{4 + 4 + \ldots + 4}{k} \right) + \ldots + k \left( \frac{4 + 4 + \ldots + 4}{k} \right) \right) \]

\[ = \frac{1}{2} \left\{ 2mk(k-1) + 4k^2m(m-1) \right\} \]

\[ TW(T^x) = mk \left[ k(2m - 1) - 1 \right]. \]

4.3 TERMINAL WIENER INDEX FOR GENERALIZED CATERPILLAR GRAPH

Caterpillar graph is a tree in which all the vertices are within the distance one from the main path. In the main path, let the vertex set be \( v_1, v_2, \ldots, v_n \). Caterpillar tree is isomorphic to certain types of molecular graphs. Consider a saturated hydrocarbon with \( n \) carbon atoms and \( k \) methyl molecules attached in various positions \( i, (2 \leq i \leq n-1) \).

Theorem 4.3.1. Let \( P_n \) be a path graph with \( n \) vertices. Construct a caterpillar \( T \) by joining \( k \) pendant edges at various positions \( i, (2 \leq i \leq n-1) \), then

\[ TW(T) = (k+1)(n+k-1) + \frac{1}{2} \sum_{i} \sum_{j} |i_j - i_k|. \]
**Proof:** Let $T(n,k)$ be a caterpillar graph with $n+k$ vertices. Let $\{v_1,v_2,\ldots,v_n\}$ be the vertices on the main path. The degree sequence of a caterpillar graph is $(d_1,d_2,\ldots,d_n,d_{n+1},d_{n+2},\ldots,d_{n+k})$. The degree sequence on the main path $\{d_i\}_{i=2}^{n-1}$ is either 2 or 3. The elements $d_1,d_n,d_{n+1},d_{n+2},\ldots,d_{n+k}$ are equal to one. The positions of $k$ pendant edges lie on the main path in various positions from $v_2$ to $v_{n-1}$. The terminal Wiener index of a graph is the half of the sum of the distances between $v_1^{th}$ and $v_n^{th}$ vertex, half of the sum of the distance between pairs of $k$ pendant vertices and half of the sum of the distance between $v_1$ and $v_n^{th}$ vertex to $k$ pendant vertices.

$$TW(T) = \frac{1}{2} \left\{ 2(n-1) + \sum_{i,j} |i_j - i_k| + 2k(k - 1) + 2 \sum_{i_j} 1 - i_j \right\} + 2 \sum_{i_j} |n - i_j| + 2(2k) \right\}$$

$$TW(T) = \frac{1}{2} \left\{ 2(n-1) + 2k(k + 1) + \sum_{i_j} \sum_{i_k} |i_j - i_k| + 2 \sum_{i_j} |i_j - 1| + 2 \sum_{i_j} |n - i_j| \right\}$$

$$TW(T) = (n-1) + k(k + 1) + \frac{1}{2} \sum_{i_j} \sum_{i_k} |i_j - i_k| + (nk - k)$$

$$TW(T) = (k + 1)(n + k - 1) + \frac{1}{2} \sum_{i_j} \sum_{i_k} |i_j - i_k|.$$ 

**Example 4.3.2.** Using Theorem 4.3.1, the terminal Wiener index of molecular structure (3,4,6,10) - tetramethyldodecane in Figure 4.5 is
Figure 4.5 Molecular structure of (3,4,6,10)-tetramethyldodecane

\[ TW(T) = (4 + 1)(12 + 4 - 1) \]

\[ \frac{1}{2} \left[ |3 - 4| + |3 - 6| + |3 - 10| + |4 - 3| + |4 - 6| + |4 - 10| \right] \]

\[ |6 - 3| + |6 - 4| + |6 - 10| + |10 - 3| + |10 - 4| + |10 - 6| \]

\[ TW(T) = 98 \]

Table 4.1 Terminal Wiener index for certain chemical compounds

<table>
<thead>
<tr>
<th>S.No</th>
<th>Chemical Compound</th>
<th>( TW(G) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(2,3,4,7), (3,4,5,8), (3,6,7,8), (4,7,8,9), (5,8,9,10), (6,9,10,11) - tetramethyldodecane</td>
<td>91</td>
</tr>
<tr>
<td>2</td>
<td>(2,4,6,7), (3,5,7,8), (4,6,8,9), (5,7,9,10), (6,8,10,11), (2,3,5,7), (3,4,6,8), (4,5,7,9), (5,6,8,10), (6,7,9,11) - tetramethyldodecane</td>
<td>92</td>
</tr>
<tr>
<td>3</td>
<td>(2,3,6,7), (3,4,7,8), (4,5,8,9), (5,6,9,10), (6,7,10,11) - tetramethyldodecane</td>
<td>93</td>
</tr>
<tr>
<td>4</td>
<td>(2,3,4,8), (3,4,5,9), (4,5,6,10), (5,6,7,11), (2,6,7,8), (3,7,8,9), (4,8,9,10), (5,9,10,11), (2,4,5,8), (3,5,6,9), (4,6,7,10), (5,7,8,11), (2,5,6,8), (3,6,7,9), (4,7,8,10), (5,8,9,11) - tetramethyldodecane</td>
<td>94</td>
</tr>
</tbody>
</table>
We have used \((a, b, c, d)\) - tetramethyldodecane in Table 4.1, where \((a,b,c,d)\) denotes the positions of the four methyl molecules varying over the positions from 2 to \(n - 1\) in the straight chain consisting of 12 carbon atoms. We can study that for all molecules, the distance between two extremum methyl molecules as well as the two intermediate methyl molecules have the same distance and have same terminal Wiener index. In the molecular structure of \((3,4,6,10)\)- tetramethyldodecane, the distance between the positions of \((3,10)\) and \((4,6)\) are 7 and 2 respectively. For all the compounds given in eighth row in Table 4.1, the distance between \((a & d)\) and \((b & c)\) all of them have same terminal Wiener index 98.
4.4 TERMINAL WIENER INDEX FOR DETOUR SATURATED TREES AND NANOSTAR DENDRIMER

In this section, we investigate the detour saturated trees $T_3(n)$, $T_4(n)$ and nanostardendrimer $D_3(n)$.

A graph is said to be detour saturated if the addition of any edge results in an increased greatest path length. The characteristic graph of a given benzenoid graph consists of vertices corresponding to hexagonal rings of the graph; two vertices are adjacent if and only if the corresponding rings share an edge. A benzenoid graph is called Cata-condensed if its characteristic graph is a tree. In this chapter we derive Wiener indices for characteristic graphs of benzenoid graphs in the form of hexagonal rings, which are detour-saturated trees (Lowell et al 2005).

The species in the form of polyhexes have traditionally been termed “Per condensed” or “Cata-condensed” according to whether or not they contain vertices common to three hexagons (Gutman 1987). An improved definition proposed by Balaban and Harary make use of the dualist graph, whose vertices are the centers of the hexagons (Yousefi et al 2008 & Andrey et al 2002). Two vertices of a dualist graph are adjacent if the respective hexagons have a common side. (Baskar Babujee & Joshi 2008) In the new definition, Cata-condensed species have dualist graphs, which are detour-saturated trees, while those of Peri-condensed species contain at least one circuit. The dualist graph of Cata-Condensed species is a claw. The claw is the detour- saturated tree $T_3$ in Figure 4.7.

The general detour-saturated tree $T_3(n)$ for odd $n \geq 5$ is obtained from $T_3(n-1)$ by attaching two new leaves at each of the old leaves.
Double claw also can be connected to the species in the form of polyhexes. Double claw is denoted by $T_4(n)$ and can be constructed inductively by adding two new leaves at each of the old leaves of $T_4(n-1)$, $n \geq 6$. 
Figure 4.9 Detour saturated Tree for $T_d(0)$, $T_d(1)$ and $T_d(2)$

**Theorem 4.4.1.** The terminal Wiener index of detour saturated tree $T_d(n)$ is

$$TW\left[ T_d(n) \right] = 3.2^{n-1} \left\{ \sum_{i=1}^{n+1} i2^i + (n+1)2^{n+1} \right\}.$$

**Proof:** If $n = 0$ then $T_d(0)$ is a claw which contains 4 vertices, three of them are leaves. $T_d(1)$ is obtained from $T_d(0)$ by adding two new leaves to the three old leaves in $T_d(0)$. Hence six new leaves are added to $T_d(0)$ to form $T_d(1)$, twelve new leaves are added to $T_d(1)$ to form $T_d(2)$ and so on.

Let $n$ denote the number of steps in the formation of detour-saturated trees. Then the number of pendant vertices in the detour saturated tree $T_d(n)$ is $3.2^n$.

By definition the terminal Wiener index of $TW\left( T_d(n) \right) = \frac{1}{2} \sum_{i=1}^{3.2^n} \sum_{j=1}^{3.2^n} d(v_i, v_j)$.  

$$TW\left[ T_d(0) \right] = \frac{1}{2} \{3[2 + 2]\} = 6$$
\[ TW[T_3(1)] = \frac{1}{2} \cdot 3.2^1 \left[ 2 + (4 + 4) + (4 + 4) \right] \]

\[ TW[T_3(2)] = \frac{1}{2} \cdot 3.2^2 \left[ 2 + (4 + 4) + (6 + 6 + 6 + 6) + (6 + 6 + 6 + 6) \right] \]

\[ TW[T_3(3)] = \frac{1}{2} \cdot 3.2^3 \left[ 2 + (4 + 4) + (6 + 6 + 6 + 6) + \left( \frac{8 + 8 + \ldots + 8}{8 \text{ times}} \right) \right] \]

\[ + \left( \frac{8 + 8 + \ldots + 8}{8 \text{ times}} \right) \]

\[ TW[T_3(4)] = \frac{1}{2} \cdot 3.2^4 \left[ 2 + (4 + 4) + \left( \frac{6 + 6 + 6 + 6}{4 \text{ times}} \right) + \left( \frac{8 + 8 + \ldots + 8}{8 \text{ times}} \right) \right] \]

\[ + \left( \frac{10 + 10 + \ldots + 10}{16 \text{ times}} \right) + \left( \frac{10 + 10 + \ldots + 10}{16 \text{ times}} \right) \]

and so on.

By mathematical induction method,

\[ TW[T_3(0)] = \frac{3.2^0}{2} \left[ 2(2) \right] = 6, \text{ is true for } n=0 \]

\[ TW[T_3(1)] = \frac{3.2^2}{2} \left[ 2 + 2 \left( 2^2 \right) \right] + \frac{3.2^2}{2} \left[ 2 \left( 2^2 \right) \right] = 54, \text{ is true for } n=1 \]

\[ TW[T_3(2)] = \frac{3.2^3}{2} \left[ 2 + 2 \left( 2^2 \right) + 3 \left( 2^3 \right) \right] + \frac{3.2^3}{2} \left[ 3 \left( 2^3 \right) \right] = 276, \text{ is true for } n=2 \]

Assume \( TW[T_3(k - 1)] \) is true for \( n=k-1 \)

\[ TW[T_3(k - 1)] = \frac{3.2^{k-1}}{2} \left[ 2 + 2 \left( 2^2 \right) + 3 \left( 2^3 \right) + \ldots + k2^k \right] + \frac{3.2^{k-1}}{2} \left[ k2^k \right] \]
$$TW \left[ T_3(k-1) \right] = \frac{3.2^{k-1}}{2} \left[ \sum_{i=1}^{k} i 2^i \right] + \frac{3.2^{k-1}}{2} (k) 2^k$$

To prove $TW \left[ T_3(k) \right]$ is true for $n=k$

$$TW \left[ T_3(k) \right] = \frac{3.2^{k-1}}{2} \left[ \sum_{i=1}^{k} i 2^i \right] + \frac{3.2^{k-1}}{2} (k+1) 2^{k-1}$$

$$TW \left[ T_3(k) \right] = \frac{3.2^k}{2} \left[ \sum_{i=1}^{k+1} i 2^i \right] + \frac{3.2^k}{2} (k+1) 2^{k+1}$$

$$TW \left[ T_3(k) \right] = 3.2^{k-1} \left[ \sum_{i=1}^{k+1} i 2^i + (k+1) 2^{k+1} \right]$$

we obtain $TW \left[ T_3(n) \right] = 3.2^{n-1} \left[ \sum_{i=1}^{n+1} i 2^i + (n+1) 2^{n+1} \right]$.

**Theorem 4.4.2.** The terminal Wiener index of detour saturated tree $T_4(n)$ is

$$TW \left[ T_4(n) \right] = 2^{n+1} \left[ \sum_{i=1}^{n+1} i 2^i + (2n-3) 2^{n+1} \right].$$

**Proof:** If $n = 0$ then $T_4(0)$ is a double claw which contains 6 vertices, four of them are leaves. $T_4(1)$ is obtained from $T_4(0)$ by adding two new leaves to the four old leaves in $T_4(0)$. Hence eight new leaves are added to $T_4(0)$ to form $T_4(1)$, sixteen new leaves are added to form $T_4(2)$ and so on. Let $n$ denote the number of steps in the formation of detour-saturated trees. Then the number of pendant vertices in the double-claw of detour saturated tree $T_4(n)$ has $2^{n-2}$ pendant vertices.
By definition $TW[T_4(n)] = \frac{1}{2} \sum_{i=1}^{n^2} \sum_{j=1}^{n^2} d(v_i, v_j)$

$TW[T_4(0)] = \frac{1}{2} \left\{ \left( 4.2^0 \right)^2 + (3 + 3) \right\}$

$TW[T_4(1)] = \frac{1}{2} \left\{ \left( 4.2^1 \right)^2 \left( 2 + (4 + 4) + \left( \frac{5 + 5 + 5 + 5}{4 \text{ times}} \right) \right) \right\}$

$TW[T_4(2)] = \frac{1}{2} \left\{ \left( 4.2^2 \right)^2 \left( 2 + (4 + 4) + \left( \frac{6 + 6 + 6 + 6}{4 \text{ times}} \right) + \left( \frac{7 + 7 + \ldots + 7}{8 \text{ times}} \right) \right) \right\}$

$TW[T_4(3)] = \frac{1}{2} \left\{ \left( 4.2^3 \right)^2 \left( 2 + (4 + 4) + \left( \frac{6 + 6 + 6 + 6}{4 \text{ times}} \right) + \left( \frac{8 + 8 + \ldots + 8}{8 \text{ times}} \right) + \left( \frac{9 + 9 + \ldots + 9}{16 \text{ times}} \right) \right) \right\}$

$TW[T_4(4)] = \frac{1}{2} \left\{ \left( 4.2^4 \right)^2 \left( 2 + (4 + 4) + \left( \frac{6 + 6 + 6 + 6}{4 \text{ times}} \right) + \left( \frac{8 + 8 + \ldots + 8}{8 \text{ times}} \right) + \left( \frac{10 + 10 + \ldots + 10}{16 \text{ times}} \right) + \left( \frac{11 + 11 + \ldots + 11}{32 \text{ times}} \right) \right) \right\}$

and so on.

$TW[T_4(0)] = \frac{1}{2} \left\{ \left( 4.2^0 \right)^2 \left( (2) - (2 + 2) + (1 - 1) \right) \right\}$

$TW[T_4(1)] = \frac{4.2}{2} \left\{ \left( 2 + (4 + 4) + \left( \frac{4 + 4 + 4 + 4}{4 \text{ times}} \right) + \left( 1 + 1 + \ldots + 1 \right) \right) \right\}$

$TW[T_4(2)] = \frac{4.2^2}{2} \left\{ \left( 2 + (4 + 4) + \left( \frac{6 + 6 + 6 + 6}{4 \text{ times}} \right) + \left( \frac{6 + 6 + \ldots + 6}{8 \text{ times}} \right) \right) \right\}$
\[
TW[T_4(3)] = \frac{4.2^3}{2} \left[ 2 + 4 + 4 + \left( \frac{6 + 6 + 6 + 6}{4 \text{ times}} \right) + \left( \frac{8 + 8 + ... + 8}{8 \text{ times}} \right) \right] \\
+ \left( \frac{8 + 8 + ... + 8}{16 \text{ times}} \right) + \left( \frac{1 + 1 + ... + 1}{16 \text{ times}} \right)
\]

\[
TW[T_4(4)] = \frac{4.2^4}{2} \left[ 2 + 4 + 4 + \left( \frac{6 + 6 + 6 + 6}{4 \text{ times}} \right) + \left( \frac{10 + 10 + ... + 10}{16 \text{ times}} \right) \right] \\
+ \left( \frac{10 + 10 + ... + 10}{32 \text{ times}} \right) + \left( \frac{1 + 1 + ... + 1}{32 \text{ times}} \right)
\]

and so on.

By mathematical induction method

\[
TW[T_4(0)] = \frac{(4.2^0)}{2} \left[ 2 \left( 2^0 \right) + 2 + 1 \right] = 16, \text{ is true for } n = 0
\]

\[
TW[T_4(1)] = \frac{(4.2^1)}{2} \left[ 2 + 2(2^2) + 2(2^2) + 2(2^2) + 2(2) \right] = 120, \text{ is true for } n = 1
\]

\[
TW[T_4(2)] = \frac{(4.2^2)}{2} \left[ 2 + 2(2^2) + 3(2^2) + 3(2^2) + 3(2^2) + 2(2^2) \right] = 720, \text{ is true for } n = 2
\]

Assume \( TW[T_4(k - 1)] \) is true for \( n = k - 1 \)
\[ TW[T_4(k-1)] = \frac{4.2^{k-1}}{2} \left\{ \sum_{i=1}^{k} i \left( 2^i \right) + k \left( 2^k \right) + k \left( 2^k \right) + 2^k \right\} \]

\[ TW[T_4(k-1)] = \frac{4.2^{k-1}}{2} \left\{ \sum_{i=1}^{k} i \left( 2^i \right) + k \left( 2^k \right) + k \left( 2^k \right) + 2^k \right\} \]

To prove \( TW[T_4(k)] \) is true for \( n=k \)

\[ TW[T_4(k)] = \frac{4.2^k}{2} \left\{ \sum_{i=1}^{k+1} i \left( 2^i \right) + (k+1)2^{k+1} + (k+1)2^{k+1} + 2^{k+1} \right\} \]

\[ TW[T_4(k)] = 2^{k+1} \left\{ \sum_{i=1}^{k+1} i \left( 2^i \right) - (2k+3)2^{k+1} \right\} \]

we obtain

\[ TW[T_4(n)] = 2^{n+1} \left\{ \sum_{i=1}^{n+1} i \left( 2^i \right) + (2n-3)2^{n+1} \right\} \]

A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. The nanostardendrimer is part of a new group of macromolecules that appear to be photon funnels just like artificial antennas. Dendrimers have gained a wide range of applications in supra-molecular chemistry, particularly in host guest reactions and self-assembly processes. Their applications in chemistry,
biology and nano-science are unlimited. Dendrimers have also been studied from the topological point of view, including vertex and fragment enumeration and calculation of some topological descriptors, such as topological indices, sequences of numbers or polynomials. Dendrimers are recognized as one of the major commercially available nano scale building blocks, large and complex molecules with very well defined chemical structure. From a polymer chemistry point of view, dendrimers are nearly perfect monodisperse macromolecules with a regular and highly branched three dimensional architecture. They consist of three major architectural components: core, branches and end groups. New branches emitting from a central core are added in steps until a tree-like structure is created. In literature, the figures of dendrimers are considered as the shapes of molecular graphs.

![Dendrimer Structure](image)

**Figure 4.10**  
\( D_3(0) \)- primal structure of nanostar dendrimer \( \text{N}^1_1 \), \( \text{N}^1_1 \)-bis (4-aminophenyl) benzene-1,4-diamine

The nanostardendrimer \( \text{N}^1_1 \), \( \text{N}^1_1 \)-bis (4-aminophenyl) benzene-1,4-diamine is a part of a new group of macroparticles that appear to be photon funnels just like artificial antennas. These macromolecules and more precisely those containing phosphorus are used in the formation of nanotubes, micro and macro capsules, nanolatex, coloured glasses, chemical sensors, modified electrodes and so on.
Nanostar dendrimers possess a well defined molecular topology. For every infinite integer $n$, $D_3(n)$ denotes the $n^{th}$ growth of nanostar dendrimer. A kind of $3^{rd}$ growth of dendrimer is given in Figure 4.11

**Theorem 4.4.3.** The terminal Wiener index of nanostar dendrimer $N^1$, $N^1$-bis(4-aminophenyl)benzene-1,4-diamine $D_3(n)$ is

$$TW\left[D_3(n)\right] = 15.2^n \left\{ \sum_{i=1}^{n-1} 2^{i+1} + (n+1)2^n \right\}.$$  

**Proof:** Let $D_3(0)$ be the nanostardendrimer $N^1$, $N^1$-bis (4-aminophenyl)benzene-1,4-diamine. We define an element as in Figure 4.12 by leaf.

![Figure 4.12 Leaf of $D_3(n)$](image)
Every leaf consists of a cycle $C_6$ or a benzene ring. We add a $3(2^n)$ leaves to $D_3(n-1)$. If $n = 0$ then $D_3(0)$ is a nanostardendrimer which contains 3 pendant vertices. In the $n^{th}$ stage nanostardendrimer contains $3.2^n$ pendant vertices. By definition

$$TW[D_3(n)] = \frac{1}{2} \sum_{i=1}^{3} \sum_{j=1}^{2^n} d(v_i, v_j)$$

$$TW[D_3(0)] = \frac{1}{2}\{3[10 + 10]\}$$

$$TW[D_3(1)] = \frac{1}{2}\{(3.2)[(10) + (20 + 20) + (20 + 20)]\}$$

$$TW[D_3(2)] = \frac{1}{2}\{(3.2^2)[(10) + (20 + 20) + \left(\frac{30 + 30 + ... + 30}{4 \text{ times}}\right)]\}$$

$$TW[D_3(3)] = \frac{1}{2}\{(3.2^3)[(10) + (20 + 20) + \left(\frac{30 + 30 + ... + 30}{4 \text{ times}}\right)]\}$$

$$+ \left(\frac{40 + 40 + ... + 40}{8 \text{ times}}\right) + \left(\frac{40 + 40 + ... + 40}{8 \text{ times}}\right)\}$$

$$TW[D_3(4)] = \frac{1}{2}\{(3.2^4)[(10) + (20 + 20) + \left(\frac{30 + 30 + ... + 30}{4 \text{ times}}\right)]\}$$

$$+ \left(\frac{40 + 40 + ... + 40}{8 \text{ times}}\right) + \left(\frac{50 + 50 + ... + 50}{16 \text{ times}}\right) + \left(\frac{50 + 50 + ... + 50}{16 \text{ times}}\right)\}$$

and so on.
By mathematical induction method

\[ TW\left[ D_3(0) \right] = \frac{3.10}{2} \{1 + 1\} = 30, \text{ for } n = 0 \]

\[ TW\left[ D_3(1) \right] = \frac{3.10.2}{2} \{1 + 2(2)\} + \frac{\left(3.10.2\right)}{2} \{2(2)\} = 270, \text{ is true for } n = 1 \]

\[ TW\left[ D_3(2) \right] = \frac{3.10.2^2}{2} \{1 + 2(2) + 3(2^2)\} + \frac{\left(3.10.2^2\right)}{2} \{3(2^2)\} = 1740, \text{ is true for } n = 2 \]

Assume \( TW\left[ D_3(k - 1) \right] \) is true for \( n = k - 1 \)

\[ TW\left[ D_3(k - 1) \right] = \frac{3.10.2^{k-1}}{2} \{1 + 2(2) + 3(2^2) + 4(2^3) + \ldots + k(2^{k-1})\} \]

\[ + \frac{\left(3.10.2^{k-1}\right)}{2} \{k(2^{k-1})\} \]

\[ TW\left[ D_3(k - 1) \right] = \frac{3.10.2^{k-1}}{2} \left\{ \sum_{i=1}^{k} i.2^{i-1} + k.2^{k-1} \right\} \]

To prove \( TW\left[ D_3(k) \right] \) is true for \( n = k \)

\[ TW\left[ D_3(k) \right] = \frac{3.10.2^k}{2} \{1 + 2(2) + 3(2^2) + \ldots + k(2^{k-1}) + (k + 1)2^k\} \]

\[ + \frac{\left(3.10.2^k\right)}{2} \{(k + 1)2^k\} \]

\[ TW\left[ D_3(k) \right] = \frac{3.10.2^k}{2} \left\{ \sum_{i=1}^{k} i.2^{i-1} \right\} + \frac{3.10.2^k}{2} \{(k + 1)2^k\} \]
\[ TW[D_3(k)] = \frac{3 \cdot 10 \cdot 2^k}{2} \left\{ \frac{3}{2} \left( k + 1 \right) 2^k \right\} \]

we obtain

\[ TW[D_3(n)] = 15 \cdot 2^n \left\{ \sum_{i=1}^{n-1} i2^{i-1} + (n+1)2^n \right\}. \]