Terminal Wiener Index of Detour saturated Trees and Nanostar Dendrimers

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Abstract

The Terminal Wiener index $TW(G)$ of a graph G is the sum of the distances between all pairs of pendant vertices. In this paper we find an explicit formula for calculating the terminal wiener index for Detour saturated tree and Nanostar Dendrimers.
Keywords: Graph, distance, degree, vertices, dendrimer, detour saturated trees.
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1 Introduction

In a general sense, molecular descriptors are "terms that characterize a specific aspect of a molecule". In particular, topological indices have been defined as those "numerical values associated with chemical contribution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity". They are derived from a graph-theoretical representation of molecules and can be considered as structure-explicit descriptors [13, 14]. A representation of an object giving information only about the number of elements composing it and their connectivity is named as topological representation of an object. Topological indices are used for development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure. 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 the covalent bonds. These points are named vertices and the lines are named edges in graph theory language.

Let G be an undirected connected graph without loops or multiple edges with n vertices, denoted by $\{v_1, v_2, v_3, \ldots, v_n\}$. 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 [12] defined the Wiener index $W(G)$ as the sum of distances between all vertices of the graph G. $W(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} d(v_i, v_j)$ where $d(v_i, v_j)$ is the distance between the vertices v_i and v_j in a graph [4]. Among all the trees on n vertices, the star $K_{1,n-1}$ has the lowest Wiener number and the path P_n has the largest Wiener number.

In 2009, Gutman, B. Furtula, and M. Petrovic [5] introduced 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.

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

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

A benzenoid graph is called Cata-condensed if its characteristic graph is a tree. Lukovits [6] investigated the use of the detour index [3] in quantitative structure-activity relationship (QSAR) studies. Following the work in [7], Trinajstic et al. [10] analyzed the use of the detour index and compared its application and that of the Wiener index in structure-boiling point modeling, while Rücker et al. [9] also probed the detour index as a descriptor for boiling points of acyclic and cyclic alkanes. It was found that the detour index in combination with the Wiener index is very efficient in structure-boiling point modeling of acyclic and cyclic saturated hydrocarbons. Lukovits and Razinger [7] proposed an algorithm for the detection of the longest path between any two vertices of a graph, which was used to derive analytical formulas for the detour index of fused bicyclic structures. Trinajstic et al. [10] and Rücker [9] proposed computer methods for computing the detour distances [1, 2, 11] and hence for computing the detour index.

Double claw also can be connected to the species in the form of polyhexes see Figure 3 double claw is denoted by T_4 can be constructed inductively by adding two new leaves at each of the old leaves of T_{n-2} and $n \geq 6$.

A dendrimer is an artificially manufactured or synthesized molecule

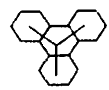

Figure 1: Cata-Condensed and its dualist graph T_0

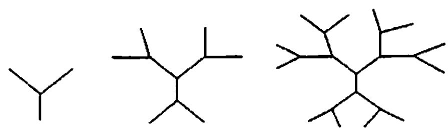

Figure 2: Detour saturated Trees for $T_3(0)$, $T_3(1)$ and $T_3(2)$

built up from branched units called monomers.

The nanostar dendrimer [8] 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. 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 in Figure 6.

In this paper we calculate explicit formula for Detour saturated tree and Nanostar Dendrimers.

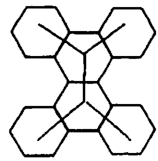

Figure 3: Detour saturated Tree of Double claw

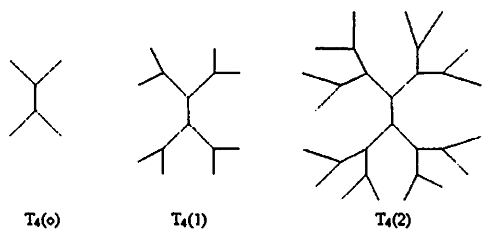

Figure 4: Detour saturated Tree for $T_4(0)$, $T_4(1)$ and $T_4(2)$

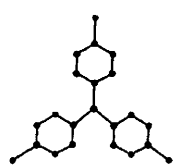

Figure 5: $D_3(0)$ is the primal structure of nanostar dendrimer $D_3(n)$

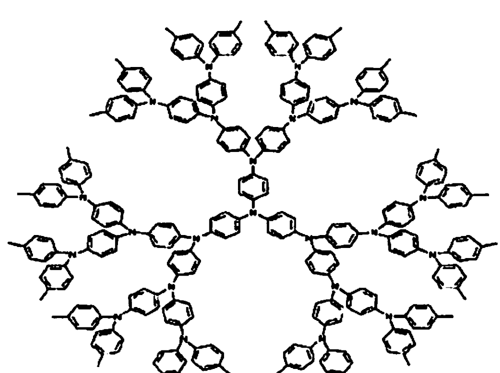

Figure 6: The 2-dimensional of a kind of 3^{rd} growth of dendrimer $D_3(3)$

2 Main Results

Theorem 1. *The Terminal Wiener Index of detour saturated tree $T_3(n)$ is*

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

Proof. If $n = 0$ then $T_3(0)$ is a claw which contains 4 vertices with three leaves. $T_3(1)$ is obtained from $T_3(0)$ by adding two new leaves to the three old leaves in $T_3(0)$. Hence six new leaves are added to $T_3(0)$ to form $T_3(1)$, twelve new leaves are added to form $T_3(2)$ 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 $T_3(n)$ has $3(2^n)$ pendant vertices. The Terminal Wiener Index of $T_3(n) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} d(v_i, v_j)$

$$TW[T_3(0)] = \frac{1}{2}.3[2+2]$$
$$TW[T_3(1)] = \frac{1}{2}.3.2^{i}[2+(4+4)+(4+4)]$$
$$TW[T_3(2)] = \frac{1}{2}.3.2^2[2+(4+4)+(6+6+6+6)+(6+6+6+6)]$$
$$TW[T_3(3)] = \frac{1}{2}.3.2^3\left[2+(4+4)+(6+6+6+6)+\left(\underbrace{8+8+\cdots+8}_{8\ times}\right)+\left(\underbrace{8+8+\cdots+8}_{8\ times}\right)\right]$$
$$TW[T_3(4)] = \frac{1}{2}.3.2^4\left[2+(4+4)+\left(\underbrace{6+6+\cdots+6}_{4\ times}\right)+\left(\underbrace{8+8+\cdots+8}_{8\ times}\right)\left(\underbrace{10+10+\cdots+10}_{16\ times}\right)+\left(\underbrace{10+10+\cdots+10}_{16\ times}\right)\right]$$

and so on.

$$TW[T_3(0)] = \frac{3.2^0}{2}[2(2)]$$

$$TW[T_3(1)] = \frac{3.2}{2}[2+2(2^2)] + \frac{3.2}{2}[2(2^2)]$$

$$TW[T_3(2)] = \frac{3.2^2}{2}[2+2(2^2)+3(2^3)] + \frac{3.2}{2}[3(2^3)]$$

$$TW[T_3(3)] = \frac{3.2^3}{2}[2 + 2(2^2) + 3(2^3) + 4(2^4)] + \frac{3.2^3}{2}[4(2^4)]$$

$$TW[T_3(4)] = \frac{3.2^4}{2}[2 + 2(2^2) + 3(2^3) + 4(2^4) + 5(2^5)] + \frac{3.2^4}{2}[5(2^5)]$$

and so on.

$$TW[T_3(n)] = \frac{3.2^n}{2}[2 + 2(2^2) + 3(2^3) + 4(2^4) + 5(2^5) + \cdots + (n+1)2^{(n+1)}] + \frac{3.2^n}{2}[(n+1)2^{(n+1)}]$$

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

$$TW[T_3(n)] = 3.2^{n-1}\left[\sum_{k=1}^{n+1} k2^k(n+1)2^{(n+1)}\right]. \qquad \square$$

Theorem 2. *The Terminal Wiener Index of detour saturated tree $T_4(n)$ is*

$$TW[T_4(n)] = 2^{n+1}\left\{\sum_{k=1}^{n+1} k2^k + (2n+3)2^{n+1}\right\}$$

Proof. If $n = 0$ then $T_4(0)$ is a double claw which contains 6 vertices with four 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

$$TW[T_4(n)] = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} d(v_i, v_j)$$

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

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

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

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

$$\left.\left.+\left(\underbrace{9+9+\cdots+9}_{16\ times}\right)\right]\right\}$$

$$TW[T_4(4)] = \frac{1}{2}\left\{(4.2^4)\left[2+(4+4)+\left(\underbrace{6+6+6+6}_{4\ times}\right)+\left(\underbrace{8+8+\cdots+8}_{8\ times}\right)\right.\right.$$

$$\left.\left.+\left(\underbrace{10+10+\cdots+10}_{16\ times}\right)+\left(\underbrace{11+11+\cdots+11}_{32\ times}\right)\right]\right\}$$

and so on

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

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

$$TW[T_4(2)] = \frac{4.2^2}{2}\left\{\left[2+(4+4)+\left(\underbrace{6+6+6+6}_{4\ times}\right)+\left(\underbrace{6+6+\cdots+6}_{8\ times}\right)\right]\right.$$

$$\left.+\left(\underbrace{1+1+\cdots+1}_{8\ times}\right)\right\}$$

$$TW[T_4(3)] = \frac{4.2^3}{2}\left\{\left[2+4+4+\left(\underbrace{6+6+6+6}_{4\ times}\right)+\left(\underbrace{8+8+\cdots+8}_{8\ times}\right)\right.\right.$$

$$\left.\left.+\left(\underbrace{8+8+\cdots+8}_{16\ times}\right)\right]+\left(\underbrace{1+1+\cdots+1}_{16\ times}\right)\right\}$$

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

and so on.

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

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

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

$$TW[T_4(3)] = \frac{(4.2^3)}{2}\{[2+2(2^2)+3(2^3)+4(2^4)]+[4(2^4)]+[4(2^4)]+[2(2^3)]\}$$

$$TW[T_4(4)] = \frac{(4.2^4)}{2}\{[2+2(2^2)+3(2^3)+4(2^4)+5(2^5)]+[5(2^5)]+[5(2^5)]$$
$$+[2(2^4)]\}$$

and so on.

$$TW[T_4(n)] = \frac{(4.2^n)}{2}\{[2+2(2^2)+3(2^3)+4(2^4)+5(2^5)+\cdots+(n+1)2^{n+1}]$$
$$+[(n+1)(2^{n+1})]+[(n+1)(2^{n+1})]+[2(2^n)]\}$$

$$TW[T_4(n)] = \frac{(4.2^n)}{2}\left\{\sum_{k=1}^{n+1}k2^k+(n+1)2^{n+1}+(n+1)2^{n+1}+2^{n+1}\right\}$$

$$TW[T_4(n)] = 2^{n+1}\left\{\sum_{k=1}^{n+1}k2^k+(2n+3)2^{n+1}\right\}. \qquad \square$$

Theorem 3. *The Terminal Wiener Index of Nanostar Dendrimer $D_3(n)$ is*

$$TW[D_3(n)] = 15.2^n\left\{\sum_{k=1}^{n+1}k2^{k-1}+(n+1)2^n\right\}$$

Proof. Let $D_3(n)$ be the nanostar dendrimer. We define an element as in figure 7.

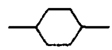

Figure 7: Leaf, is added in each branch of $D_3(n)$

Every leaf consists of a cycle C_6 or Benzene ring. We added a $3(2^n)$ leaves to $D_3(n-1)$. If $n=0$ then $D_3(0)$ is a nanostar dendrimer which contains 3 pendant vertices. In the n^{th} stage nanostar dendrimer contains 3.2^n pendant vertices. The Terminal Wiener Index of Nanostar Demdrimer

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

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

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

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

$$TW[D_3(3)] = \frac{1}{2}\left\{(3.2^3)\left[(10)+(20+20)+\left(\underbrace{30+30+\cdots+30}_{4\ times}\right) + \left(\underbrace{40+40+\cdots+40}_{8\ times}\right) + \left(\underbrace{40+40+\cdots+40}_{8\ times}\right)\right]\right\}$$

$$TW[D_3(4)] = \frac{1}{2}\left\{(3.2^4)\left[(10)+(20+20)+\left(\underbrace{30+30+\cdots+30}_{4\ times}\right) + \left(\underbrace{40+40+\cdots+40}_{8\ times}\right) + \left(\underbrace{50+50+\cdots+50}_{16\ times}\right) + \left(\underbrace{50+50+\cdots+50}_{16\ times}\right)\right]\right\}$$

$$TW[D_3(0)] = \frac{3.10}{2}\{1+1\}$$

$$TW[D_3(1)] = \frac{3.10.2}{2}\{1+2(2)\} + \frac{(3.10.2)}{2}\{2(2)\}$$

$$TW[D_3(2)] = \frac{3.10.2^2}{2}\{1+2(2)+3(2^2)\} + \frac{(3.10.2^2)}{2}\{3(2^2)\}$$

$$TW[D_3(3)] = \frac{3.10.2^3}{2}\{1+2(2)+3(2^2)+4(2^3)\} + \frac{(3.10.2^2)}{2}\{4(2^3)\}$$

$$TW[D_3(4)] = \frac{3.10.2^4}{2}\{1+2(2)+3(2^2)+4(2^3)+5(2^4)\} + \frac{(3.10.2^4)}{2}\{5(2^4)\}$$

and so on.

$$TW[D_3(n)] = \frac{3.10.2^n}{2}\{1+2(2)+3(2^2)+4(2^3)+5(2^4)+\cdots+(n+1)2^n\} + \frac{(3.10.2^n)}{2}\{(n+1)(2^n)\}$$

$$TW[D_3(n)] = \frac{3.10.2^n}{2}\left\{\sum_{k=1}^{n+1} k2^{k-1} + (n+1)2^n\right\}$$

$$TW[D_3(n)] = 15.2^n\left\{\sum_{k=1}^{n+1} k2^{k-1} + (n+1)2^n\right\}$$

□

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