Wiener Index For Detour Saturated Trees

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Abstract

In order to establish the mathematical basis for connections between molecular structures and physicochemical properties of chemical compounds, some topological indices have been put forward. Among them, the Wiener index is one of the most important topological indices. The sum of distances of all pairs of vertices in a connected graph is known as Wiener index or Wiener number. All structural formulas of chemical compounds are molecular graphs where vertices represent the set of atoms and edges represent chemical bonds. 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 bezenoid graph is called Cata-condensed if its characteristic graph is a tree. In this paper we derive Wiener indices for characteristic graphs of bezenoid graphs in the form of hexagonal rings, which are detour-saturated trees.
Key words : molecular graphs, trees, polyhexes, wiener number.

1 Introduction

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. An improved definition proposed by Balaban and Harary [2] makes use of the dualist graph whose vertices are the centers of the hexagons. Two vertices of a dualist graph are adjacent if the respective hexagons have a common side. 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 sees Figure 1. The general detour-saturated tree T_n for odd n_5 is obtained from T_{n-2} by attaching two new leaves at each of the old leaves.

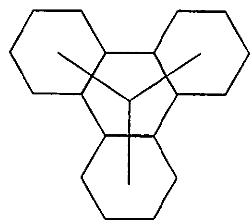

Figure 1: Cata-Condensed and its dualist graph T_3

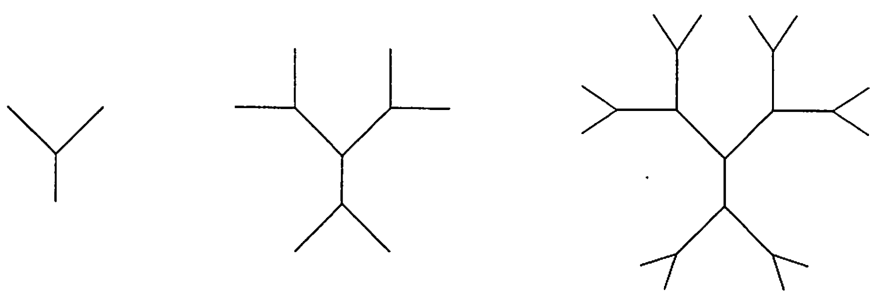

Figure 2:

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

2 Main Results

Result 2.1 *The number of vertices N in T_{2n+1} is $N = 3.2^n - 2$ and in $T_{2(n+1)}$ is $N = 2^{n+2} - 2$.*

Proof : If $n = 3$ then T_3 is a claw which contains 4 vertices with leaves. T_5 is obtained from T_3 by adding two new leaves to the three old leaves in T_3. Hence six new leaves are added to T_3 to form T_5, twelve new leaves are added to form T_7 and so on.

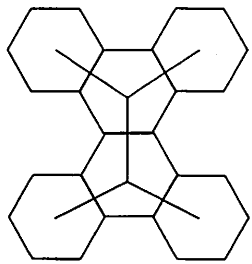

Figure 3: Double Claw

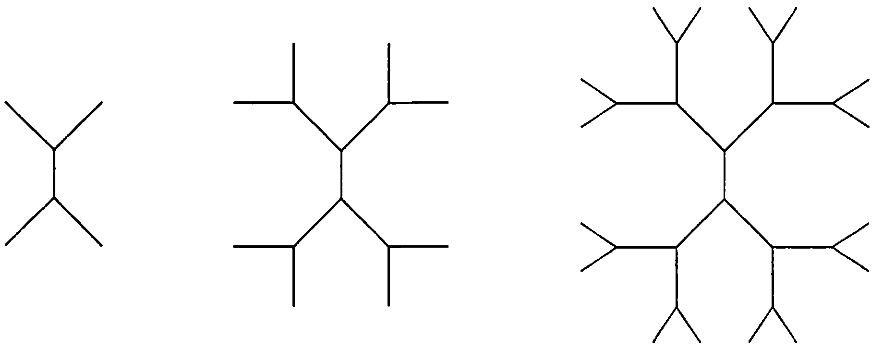

Figure 4:

Let n denote the number of steps in the formation of detour-saturated trees. Then Number of vertices in

$$\begin{aligned} T_{2n+1} &= 4+6+12+24+48+\cdots \\ &= 4+6(1+2+2^2+2^3+\cdots+2^{n-2}) \\ &= 3.2^n-2 \end{aligned}$$

If $n=4$ then T_4 is a double claw with six vertices with four leaves. T_6 is obtained from T_4 by adding two leaves to each old leaf; hence there are eight new leaves in T_6, sixteen new leaves in T_8 and so on.

$$\begin{aligned} \text{Number of vertices in } T_{2(n+1)} &= 2+2^2+2^3+2^4+\cdots+2^{n+1} \\ N(T_{2(n+1)}) &= 2^{n+2}-2 \end{aligned}$$

Result 2.2 *The Wiener index for the detour saturated tree* T_{2n+1},

$n = 1, 2, 3, \ldots$ *is*

$$W(T_{2n+1}) = \frac{1}{2}\left[3 + 6\sum_{k=2}^{n} k2^{k-2} + \sum_{r=2}^{n+1} 3 * 2^{r-2} \left\{ \begin{array}{l} 3\left[\sum_{k=r}^{n} 2^{k-r}(k-r+1)\right] + (n-r+2)2^{n-r+1} + \\ \sum_{k=1}^{r-2}\left[(2(n-r+1)+(4k+1))2^{n-(r-1)+k}\right] + \\ (n+(r-1)2^{n} \end{array} \right\}\right]$$

Proof : The centroid of the detour-saturated tree T_{2n+1} has one vertex. The sum of distances from the centre to all other $3(2^n) - 3$ vertices will be

$$3 + 6 * 2 + 12 * 3 + 24 * 4 + \cdots = 3 + 6\sum_{k=2}^{n}(2^{k-2})k$$

The sum of distances from adjacent vertices of a vertex in centroid to all the other $3 * 2^n - 3$ vertices is $3[3 + 6(2) + 12(3) + 24(4) + 16(5) + 32(6) + \cdots]$.

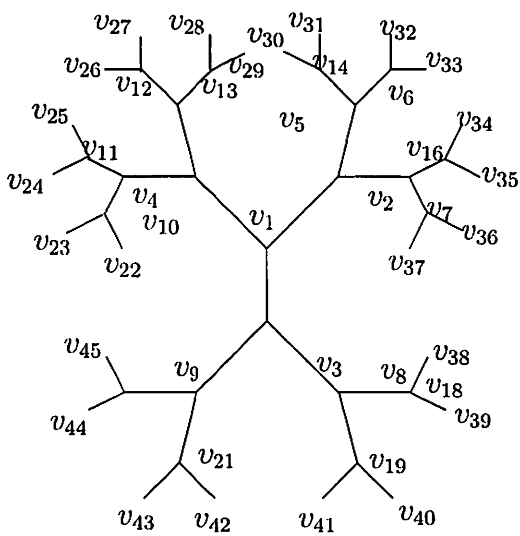

Figure 5:

The sum of distances from adjacent vertices of distance two from centroid to all the other $3 * 2^n - 3$ vertices is

$$6[1 + 2(2) + 2(3) + 4(4)] \text{ when } n = 2$$
$$6[3 + 2(2) + 4(3) + 4(4) + 8(5) + \cdots] \text{ when } n > 2$$
$$12[1 + 2(2) + 2(3) + 4(4) + 4(5) + 8(6)] \text{ when } n = 3$$
$$12[3 + 2(2) + 2(3) + 4(4) + 8(5) + 8(6) + 16(7)] \text{ when } n > 3$$

Proceeding in this way we get the following general terms

$$3\left[3\sum_{k=1}^{n}(n-1) + 2^{n-1}(n) + 2^n(n+1)\right] n \geq 1$$
$$6\left[3\sum_{k=1}^{n}2^{n-3}(n-2) + 2^{n-2}(n-1) + 2^{n-1}(n) + 2^n(n+2)\right] n \geq 2$$
$$12\left[3\sum_{k=1}^{n}2^{n-4}(n-3) + 2^{n-3}(n-2) + 2^{n-2}(n-1) + 2^{n-2}(n) + 2^{n-1}(n+1) + 2^{n-1}(n+2) + 2^n(n+3)\right] n \geq 3$$

The sum of distances between all the other vertices are also calculated in this way and the sum is

$$\sum_{r=2}^{n+1} 3{*}2^{r-2} \left\{ \begin{array}{l} 3\left[\sum_{k=r}^{n} 2^{k-r}(k-r+1)\right] + (n-r+2)2^{n-r+2} + \\ \sum_{k=1}^{r-2}(2(n-r+1) + (4k+1))2^{n-(r-1)+k} + (n + (r-1)2^n) \end{array} \right\}$$

The wiener index for the detour-saturated tree of odd order is

$$W(T_{2n+1}) = \frac{1}{2}\left[3 + 6\sum_{k=2}^{n} k2^{k-2} + \sum_{r=2}^{n+1} 3 * 2^{r-2} \left\{ \begin{array}{l} 3\left[\sum_{k=r}^{n} 2^{k-r}(k-r+1)\right] + (n-r+2)2^{n-r+1} + \\ \sum_{k=1}^{r-2}\left[(2(n-r+1) + (4k+1))2^{n-(r-1)+k}\right] + \\ (n + (r-1)2^n \end{array} \right\}\right]$$

Table 1 shows the number of vertices and the Wiener Index of T_{2n+1} for $n = 1, 2, 3, \ldots$.

Result 2.3 *The Wiener index for the detour-saturated tree* $T_{2(n+1)}$

n	N	$W(T_{2n+1})$
1	4	9
2	10	117
3	22	909
4	46	5661
5	94	31293
6	190	160893
7	382	788733
8	766	3740157
9	1534	17310717
10	3070	78661629

Table 1:

$n = 1, 2, 3 \ldots$ *is*

$$W(T_{2(n+1)}) = \frac{1}{2}\left[\sum_{r=1}^{n+1} 2^r \left(\begin{array}{c} \left\{3\sum_{k=r}^{n} 2^{k-r}(k-r+1)\right\} + 2^{n-r+1}(n-r+2)+ \\ 2^{n-r+1}\sum_{k=1}^{r-1}[2(n-r+1)+(4k+1)]\,2^k \end{array}\right)\right]$$

Proof : The centroid of the detour-saturated tree $T_{2(n+1)}$ has 2 vertices. The distance between the vertices to all other vertices in the tree is

$$2[3(1) + 2(2) + 2^2(2) + 2^3(3) + \cdots + 2^{n-1}(n) + 2^n(n+1)]$$

In general term is $2\left[\sum_{k=1}^{n} 3\left(2^{k-1}(k) + 2^n(n+1)\right)\right]$.
The distance between four vertices to all the other vertices is
$2^2\left[\sum_{k=2}^{n} 3\left(2^{k-2}(k-1)\right) + 2^{n-1}\left(2^0(n) + 2(2n+3)\right)\right]$.
The distance between eight vertices to all other vertices is
$2^3\left[\sum_{k=3}^{n} 3\left(2^{k-3}(k-2)\right) + 2^{n-2}\left(2^0(n-1) + 2(2n+1) + 2^2(2n+3)\right)\right]$ and so on. Therefore the Wiener Index for the detour-saturated tree of even order is

$$W(T_{2(n+1)}) = \frac{1}{2}\left[\sum_{r=1}^{n+1} 2^r \left(\begin{array}{c} \left\{3\sum_{k=r}^{n} 2^{k-r}(k-r+1)\right\} + 2^{n-r+1}(n-r+2)+ \\ 2^{n-r+1}\sum_{k=1}^{r-1}[2(n-r+1)+(4k+1)]\,2^k \end{array}\right)\right]$$

Table 2 shows the number of vertices and the Wiener Index of $T_{2(n+1)}$ for $n = 1, 2, 3, \ldots$.

n	N	$W(T_{2(n+1)})$
1	6	29
2	14	314
3	30	2295
4	62	13940
5	126	76145
6	254	388974
7	510	1899371
8	1022	8983400
9	2046	41501541
10	4094	188326754

Table 2:

3 Conclusion

Hexagonal rings of a benzenoid graph may be angularly or linearly connected. In this paper we considered only angularly connected benzenoid graphs. The growing characteristic graph (detour-saturated tree) may give the new chemical compound. The physicochemical property of this new compound can be analyzed using the Wiener index of the detour-saturated tree.

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