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SECOND ORDER AND THIRD ORDER CONNECTIVITY INDICES OF A POLYPHENYLENE DENDRIMER

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The *m*-order connectivity index ${}^{m}\chi(G)$ of a graph G is $(d_{i_1}d_{i_2}...d_{i_{m+1}})^{-1/2}$, where $d_{i_1}d_{i_2}...d_{i_{m+1}}$ runs over all paths of length *m* in G and d_i denotes the degree of vertex v_i. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this paper, we compute 2- and 3-order connectivity index of an infinite family of polyphenylene dendrimer.

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1. Introduction

A simple graph *G* = (*V*,*E*) is a finite nonempty set *V*(*G*) of objects called vertices together with a (possibly empty) set *E*(*G*) of unordered pairs of distinct vertices of *G* called edges. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds.

A single number which characterizes the graph of a molecular is called a graph theoretical invariant or topological index. Among the many topological indices considered in chemical graph, only a few have been found noteworthy in practical application, connectivity index is one of them. The connectivity index is one of the most popular molecular-graph. This index has been used in a wide spectrum of applications ranging from predicting physicochemical properties such as boiling point and solubility partition. The molecular connectivity index χ provides a quantitative assessment of branching of molecules. Randic (1975) first addressed the problem of relating the physical properties of alkanes to the degree of branching across an isomeric series [6]. The degree of branching of a molecule was quantified using a branching index which subsequently became known as first- order molecular connectivity index χ. Kier and Hall (1986) extended this to higher orders and introduced modifications to account for heteroatoms [4].

Molecular connectivity indices are the most popular class of indices (Trinajastic, 1992). They have been used in a wide spectrum of applications ranging from predicting physicochemical properties such as boiling point, solubility partition, coefficient etc, (Murray et al., 1975; Kier and Hall, 1976) for predicting biological activities such as antifungal effect, an esthetic effect, enzyme inhibition etc, (Kier et al., 1975; Kier and Murray, 1975) [4].

Let G be a simple connected graph of order *n*. For an integer $m \geq 1$, the *m*-order connectivity index of an organic molecule whose molecule graph G is defined as

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$$^{m}\chi(G)=\sum_{i_1\ldots i_{m+1}}\frac{1}{\sqrt{d_{i_1}\ldots d_{i_{m+1}}}},$$

where $i_1 \ldots i_{m+1}$ runs over all paths of length m in G and d_i denote the degree of vertex v_i. In particular, 2-order connectivity index and 3-order connectivity index are defined as follows:

$$^{2}\chi(G)=\sum_{i_1 i_2 i_3}\frac{1}{\sqrt{d_{i_1}d_{i_2}d_{i_3}}},\qquad ^{3}\chi(G)=\sum_{i_1 i_2 i_3 i_4}\frac{1}{\sqrt{d_{i_1}d_{i_2}d_{i_3}d_{i_4}}}.$$

Dendrimers are hyper-branched macromolecules, with a rigorously tailored architecture. They can be synthesized, in a controlled manner, either by a divergent or a convergent procedure. 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. Recently, some researchers investigated *m*-order connectivity indices of some dendrimer nanostars, where $m = 2$ and 3 (see [1,2,3,7]). In this paper, we shall study the 2- and 3-order connectivity index of an infinite family of polyphenylene dendrimers.

2. Second-order and third-order connectivity index of dendrimer

In this section, we shall study the 2-order and 3-order connectivity index of a dendrimer. We consider polyphenylene dendrimer by construction of generations G_n with *n* growth stages. We denote this graph by $D_4[n]$. Figure 1 shows the generations G_2 with 2 growth stages.

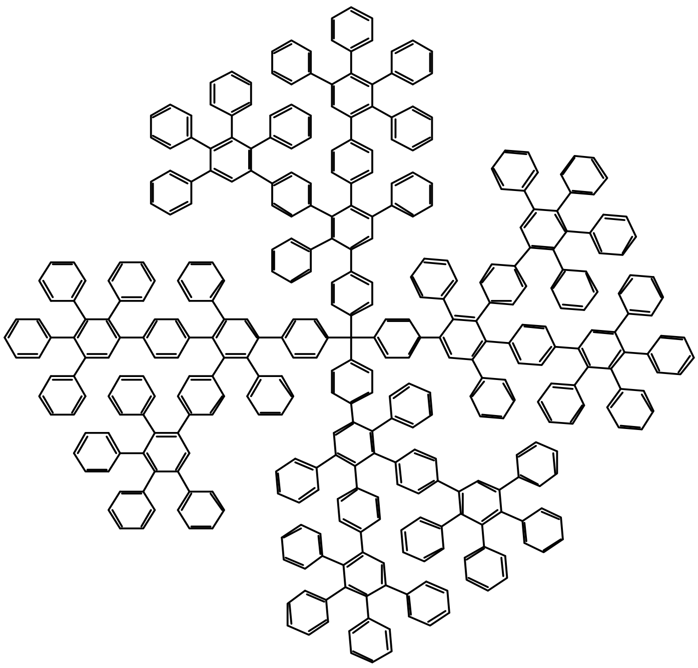

Fig. 1. Polyphenylene dendrimer of generations G_n with 2 growth stages.

The following theorem gives the 2-order connectivity index of polyphenylene dendrimer.

Theorem 1. Let $n \in$ N. Then, the 2-order connectivity index of $D_4[n]$ is given by

$$^{2}\chi(D_4[n])=\frac{1}{9}(198\sqrt{2}+152\sqrt{3}+6\sqrt{6}+9)+(\frac{19\sqrt{2}}{2}+\frac{67\sqrt{3}}{9})(2^{n+1}-4).$$

Proof. First we compute ${}^2\chi(D_4[1])$. Let $d_{i_1i_2i_3}$ denote the number of 2-paths whose three consecutive vertices are of degree i_1, i_2, i_3, respectively. In the same way, we use $d^{(n)}_{i_1i_2i_3}$ to mean $d_{i_1i_2i_3}$ in $n-th$ stages. Particularly, $d^{(n)}_{i_1i_2i_3} = d^{(n)}_{i_3i_2i_1}$.
We can see that

$$d^{(1)}_{222} = 48,\ d^{(1)}_{223} = 48,\ d^{(1)}_{232} = 24,\ d^{(1)}_{233} = 56,\ d^{(1)}_{323} = 4,\ d^{(1)}_{333} = 44,\ d^{(1)}_{234} = 8,\ d^{(1)}_{343} = 6.$$

Therefore, we have

$$\begin{aligned}{}^2\chi(D_4[1]) &= \frac{48}{\sqrt{2\times2\times2}} + \frac{48}{\sqrt{2\times2\times3}} + \frac{24}{\sqrt{2\times3\times2}} + \frac{56}{\sqrt{2\times3\times3}} \\ &+ \frac{4}{\sqrt{3\times2\times3}} + \frac{44}{\sqrt{3\times3\times3}} + \frac{8}{\sqrt{2\times3\times4}} + \frac{6}{\sqrt{3\times4\times3}} \\ &= \frac{1}{9}(198\sqrt{2} + 152\sqrt{3} + 6\sqrt{6} + 9).\end{aligned}$$

Now, we construct the relation between ${}^2\chi(D_4[n])$ and ${}^2\chi(D_4[n-1])$ for $n \geq 2$.
By simple reduction, we have

$$d^{(n)}_{222} = d^{(n-1)}_{222} + 18\times2^n,\ d^{(n)}_{223} = d^{(n-1)}_{223} + 20\times2^n,\ d^{(n)}_{232} = d^{(n-1)}_{232} + 10\times2^n,\ d^{(n)}_{233} = d^{(n-1)}_{233} + 28\times2^n,$$
$$d^{(n)}_{323} = d^{(n-1)}_{323} + 2\times2^n,\ d^{(n)}_{333} = d^{(n-1)}_{333} + 22\times2^n,$$

and for any $(i_1i_2i_3) \neq (222),(223),(232),(233),(323),(333),(234),(343)$, we have $d^{(n)}_{i_1i_2i_3} = 0.$
Therefore

$$\begin{aligned}{}^2\chi(D_4[n]) &= {}^2\chi(D_4[n-1]) + \frac{18\times2^n}{\sqrt{2\times2\times2}} + \frac{20\times2^n}{\sqrt{2\times2\times3}} + \frac{10\times2^n}{\sqrt{2\times3\times2}} + \frac{28\times2^n}{\sqrt{2\times3\times3}} + \\ &+ \frac{2\times2^n}{\sqrt{3\times2\times3}} + \frac{22\times2^n}{\sqrt{3\times3\times3}} \\ &= {}^2\chi(D_4[n-1]) + (\frac{19\sqrt{2}}{2} + \frac{67\sqrt{3}}{9})\times2^n.\end{aligned}$$

From above recursion formula, we have

$$\begin{aligned}{}^2\chi(D_4[n]) &= {}^2\chi(D_4[n-1]) + (\frac{19\sqrt{2}}{2} + \frac{67\sqrt{3}}{9})\times2^n \\ &= {}^2\chi(D_4[n-2]) + (\frac{19\sqrt{2}}{2} + \frac{67\sqrt{3}}{9})(2^n + 2^{n-1}) \\ &\vdots \\ &= {}^2\chi(D_4[1]) + (\frac{19\sqrt{2}}{2} + \frac{67\sqrt{3}}{9})(2^n + 2^{n-1} + \ldots + 2^2)\end{aligned}$$

$${}^2\chi(D_4[n]) = \frac{1}{9}(198\sqrt{2} + 152\sqrt{3} + 6\sqrt{6} + 9) + (\frac{19\sqrt{2}}{2} + \frac{67\sqrt{3}}{9})(2^{n+1} - 4).$$

The proof is now complete. ■

The following theorem gives the 3-order connectivity index of polyphenylene dendrimer.

Theorem 2. Let $n \in$ N. Then, the 3-order connectivity index of $D_4[n]$ is given by

$${}^3\chi(D_4[n]) = \frac{1}{9}(216 + 104\sqrt{6} + 6\sqrt{3} + 18\sqrt{2}) + \frac{1}{9}(99 + 46\sqrt{6})(2^{n+1} - 4).$$

Proof. Let $d_{i_1i_2i_3i_4}$ denote the number of 3-paths whose four consecutive vertices are of degree i_1, i_2, i_3, i_4, respectively. With the same way, we use $d^{(n)}_{i_1i_2i_3i_4}$ to mean $d_{i_1i_2i_3i_4}$ in $n-th$ stages. It is clear that $d^{(n)}_{i_1i_2i_3i_4} = d^{(n)}_{i_4i_3i_2i_1}$.

Similar to Theorem 1, we first compute ${}^3\chi(D_4[1])$. We can see that

$d^{(1)}_{2222} = 32$, $d^{(1)}_{2223} = 32$, $d^{(1)}_{2232} = 48$, $d^{(1)}_{2233} = 40$, $d^{(1)}_{2332} = 16$, $d^{(1)}_{2333} = 72$, $d^{(1)}_{3233} = 16$, , $d^{(1)}_{3223} = 8$,

$d^{(1)}_{3333} = 48$, $d^{(1)}_{2234} = 8$, $d^{(1)}_{2343} = 24$.

Thus,

$$
\begin{aligned}
{}^3\chi(G_4[1]) = &\frac{32}{\sqrt{2\times2\times2\times2}} + \frac{32}{\sqrt{2\times2\times2\times3}} + \frac{48}{\sqrt{2\times2\times3\times2}} + \frac{40}{\sqrt{2\times2\times3\times3}} + \\
&\frac{16}{\sqrt{2\times3\times3\times2}} + \frac{72}{\sqrt{2\times3\times3\times3}} + \frac{16}{\sqrt{3\times2\times3\times3}} + \frac{8}{\sqrt{3\times2\times2\times3}} + \\
&\frac{48}{\sqrt{3\times3\times3\times3}} + \frac{8}{\sqrt{2\times2\times3\times4}} + \frac{24}{\sqrt{2\times3\times4\times3}} \\
= &\frac{1}{9}(216 + 104\sqrt{6} + 6\sqrt{3} + 18\sqrt{2}).
\end{aligned}
$$

Now, we compute ${}^3\chi(D_4[n])$.

The relations between $d^{(n)}_{i_1i_2i_3i_4}$ and $d^{(n-1)}_{i_1i_2i_3i_4}$ for $n \geq 2$ are

$d^{(n)}_{2222} = d^{(n-1)}_{2222} + 12\times2^n$, $d^{(n)}_{2223} = d^{(n-1)}_{2223} + 12\times2^n$, $d^{(n)}_{2232} = d^{(n-1)}_{2232} + 20\times2^n$, $d^{(n)}_{2233} = d^{(n-1)}_{2233} + 20\times2^n$,

$d^{(n)}_{2332} = d^{(n-1)}_{2332} + 8\times2^n$, $d^{(n)}_{2333} = d^{(n-1)}_{2333} + 36\times2^n$, $d^{(n)}_{3233} = d^{(n-1)}_{3233} + 8\times2^n$, $d^{(n)}_{3223} = d^{(n-1)}_{3223} + 4\times2^n$,

$d^{(n)}_{3333} = d^{(n-1)}_{3333} + 24\times2^n$,

and for any $(i_1i_2i_3i_4) \neq (2222),(2223),(2232),(2233),(2332),(2333),(3233)$ $,(3223),(3333),(2234),(2343),$ we have $d^{(n)}_{i_1i_2i_3i_4} = 0$.

Therefore,

$$
\begin{aligned}
{}^3\chi(D_4[n]) = {}^3\chi(D_4[n-1]) &+ \frac{12\times2^n}{\sqrt{2\times2\times2\times2}} + \frac{12\times2^n}{\sqrt{2\times2\times2\times3}} + \frac{20\times2^n}{\sqrt{2\times2\times3\times2}} \\
+ \frac{20\times2^n}{\sqrt{2\times2\times3\times3}} + \frac{8\times2^n}{\sqrt{2\times3\times3\times2}} &+ \frac{36\times2^n}{\sqrt{2\times3\times3\times3}} + \frac{8\times2^n}{\sqrt{3\times2\times3\times3}} + \frac{4\times2^n}{\sqrt{3\times2\times2\times3}} + \frac{24\times2^n}{\sqrt{3\times3\times3\times3}}
\end{aligned}
$$

$$
\begin{aligned}
&= {}^3\chi(D_4[n-1]) + \frac{1}{9}(99 + 46\sqrt{6})\times2^n \\
&= {}^3\chi(D_4[n-2]) + \frac{1}{9}(99 + 44\sqrt{6})(2^n + 2^{n-1}) \\
&\quad\vdots \\
&= {}^3\chi(D_4[1]) + \frac{1}{9}(99 + 44\sqrt{6})(2^n + 2^{n-1} ... + 2^2)
\end{aligned}
$$

So,

$$^{3}\chi(D_4[n]) = \frac{1}{9}(216 + 104\sqrt{6} + 6\sqrt{3} + 18\sqrt{2}) + \frac{1}{9}(99 + 46\sqrt{6})(2^{n+1} - 4).$$

The proof is now complete. ■

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