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Second-Order and Third-Order Connectivity Indices of an Infinite Family of Dendrimer Nanostars

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Abstract

The m-order connectivity index ${}^m\chi(G)$ of a molecular graph G is the sum of the weights $(d_{i_1}d_{i_2}\cdots d_{i_{m+1}})^{-\frac{1}{2}}$, where $d_{i_1}d_{i_2}\cdots d_{i_{m+1}}$ runs over all paths of length m in G and d_i denotes the degree of vertex v_i. Dendrimer is a polimer molecule with a distinctive structure that resembles the crown of a tree. In this paper we compute second-order and third-order connectivity indices of an infinite family of dendrimer nanostars.

Mathematics Subject Classification: 05C05, 05C12

Keywords: Connectivity index, second-order connectivity index, third-order connectivity index, dendrimer nanostar

1 Introduction

In 1975, Randić introduced a molecular structure-descriptor in his study of alkanes[1] which he called *the branching index*, and is now called the *the Randić index* or *the connectivity index* . The Randić index has been closely correlated with many chemical properties (see [2]). Let $G = (V, E)$ be a simple graph with vertex set $\{v_1, v_2, \cdots, v_n\}$. For any two vertices $v_i, v_j \in V(G)$ with $i < j$, we will use the symbol ij to denote the edge $e = v_iv_j$. For $v_i \in V$, the degree of v_i, written by d_i, is the number of edges incident with v_i. For an integer $m \geq 1$, the $m-$order connectivity index of a graph G is defined as

$$ {}^m\chi(G) = \sum_{i_1i_2\cdots i_{m+1}} \frac{1}{\sqrt{d_{i_1}d_{i_2}\cdots d_{i_{m+1}}}} \quad (1) $$

where $i_1 i_2 \cdots i_{m+1}$ runs over all paths(that is $i_s \neq i_t$ for $1 \leq s < t \leq m+1$) of length m of G.

The higher order connectivity indices are of great interest in molecular graph theory ([3-4]) and some of their mathematical properties have been reported in [5-7].

In particular, the second order(or simply write as 2-order) connectivity and the third order(or simply write as 3-order) connectivity indices are defined as

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

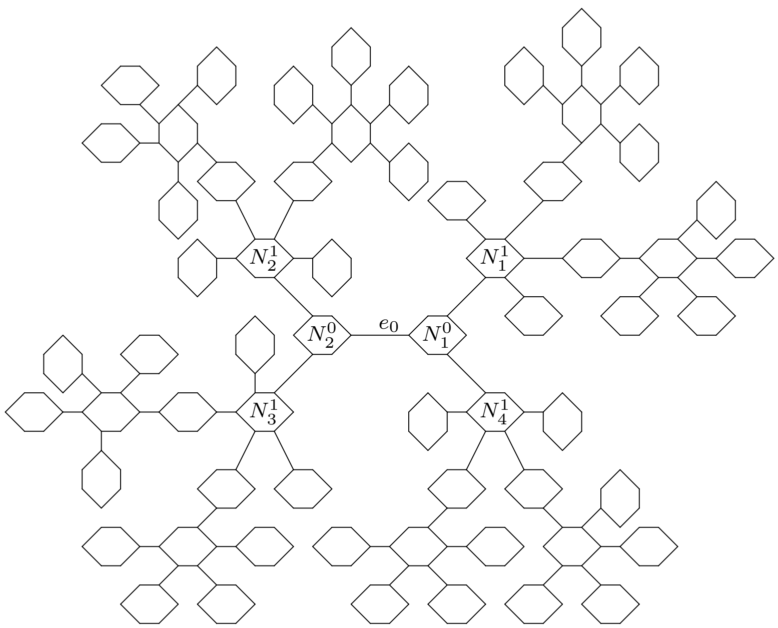

Figure 1. The nanostar dendrimer $NS[2]$

Dendrimer is a synthetic 3-dimentional macromolecule that is prepared in a step-wise fashion from simple branched monomer units. The nanostar dendrimer is part of a new group of macromolecules that appear to be photon funnels just like artificial antennas[8-10].

During the past several years, there are many papers dealing with the topological indices of dendrimer nanostars, the readers may consult [10-14] and references cited therein.

We shall consider the 2-order connectivity index and 3-order connectivity indices of an infinite family of dendrimer nanostars $NS[n]$ described in Figure 1[14].

2 The 2-order and 3-order connectivity indices of $NS[n]$

In the following, we shall compute the 2-order connectivity index and 3-order connectivity index for the dendrimer nanostar $NS[n]$ as shown in Figure 1.

Theorem 2.1 *Let $NS[n]$ be the dendrimer nanostar as shown in Figure 1. Then*

$$^2\chi(NS[n]) = \frac{1}{9}\Big(213\sqrt{2}+113\sqrt{3}\Big) + \Big(\frac{19\sqrt{2}}{2}+\frac{70\sqrt{3}}{9}\Big)\Big(2^{n+1}-4\Big)$$

Proof. Firstly, we compute $^2\chi(NS[1])$.

Let d_{ijk} denotes the number of 2-path whose three consecutive vertices are of degree i, j, k, *resp.* Similarly, we use $d_{ijk}^{(s)}$ to mean d_{ijk} in $s-th$ stage. Particularly, $d_{ijk}^{(s)} = d_{kji}^{(s)}$.

It is ease to see that

$$d_{222}^{(1)} = 48, d_{223}^{(1)} = 32, d_{232}^{(1)} = 22, d_{233}^{(1)} = 60, d_{323}^{(1)} = 10, d_{333}^{(1)} = 44.$$

Therefore, we have that

$$\begin{aligned} ^2\chi(NS[1]) &= \frac{48}{\sqrt{2\times2\times2}} + \frac{32}{\sqrt{2\times2\times3}} + \frac{22}{\sqrt{2\times3\times2}} + \frac{60}{\sqrt{2\times3\times3}} + \frac{10}{\sqrt{3\times2\times3}} + \frac{44}{\sqrt{3\times3\times3}} \\ &= \frac{1}{9}(213\sqrt{2}+125\sqrt{3}) \end{aligned}$$

Secondly, we establish the relation between $^2\chi(NS[s])$ and $^2\chi(NS[s-1])$ for $s \geq 2$.

By simple reduction, we are ready to have,

$$\begin{aligned} d_{222}^{(s)} &= d_{222}^{(s-1)} + 18\cdot 2^s, \\ d_{223}^{(s)} &= d_{223}^{(s-1)} + 20\cdot 2^s, \\ d_{232}^{(s)} &= d_{232}^{(s-1)} + 12\cdot 2^s, \\ d_{233}^{(s)} &= d_{233}^{(s-1)} + 28\cdot 2^s, \\ d_{323}^{(s)} &= d_{323}^{(s-1)} + 2\cdot 2^s \\ d_{333}^{(s)} &= d_{323}^{(s-1)} + 22\cdot 2^s. \end{aligned}$$

and for any $(i,j,k) \neq (222),(223),(232),(233),(323),(333)$ we have $d_{ijk}^{(s)} = 0$ or $d_{ijk}^{(s)} = d_{rst}^{(s-1)} = \cdots = d_{ijk}^{(1)}$ for $s = 2,3,4,\cdots,n$. Thus,

$$\begin{aligned} ^2\chi(NS[n]) &= {}^2\chi(NS[n-1]) + \frac{18\times2^n}{\sqrt{2\times2\times2}} + \frac{20\times2^n}{\sqrt{2\times2\times3}} + \frac{12\times2^n}{\sqrt{2\times3\times2}} + \frac{28\times2^n}{\sqrt{2\times3\times3}} \\ &\quad + \frac{2\times2^n}{\sqrt{3\times2\times3}} + \frac{22\times2^n}{\sqrt{3\times3\times3}} \\ &= {}^2\chi(NS[n-1]) + (\frac{19\sqrt{2}}{2}+\frac{70\sqrt{3}}{9})2^n \end{aligned}$$

From above recursion formula, we have

$$\begin{aligned}
{}^2\chi(NS[n]) &= {}^2\chi(NS[n-1]) + (\tfrac{43\sqrt{2}}{6} + \tfrac{46\sqrt{3}}{9})2^n \\
&= {}^2\chi(NS[n-2]) + (\tfrac{43\sqrt{2}}{6} + \tfrac{46\sqrt{3}}{9})(2^n + 2^{n-1}) \\
&\vdots \\
&= {}^2\chi(NS[1]) + (\tfrac{19\sqrt{2}}{2} + \tfrac{70\sqrt{3}}{9})\Big(2^n + 2^{n-1} + \cdots + 2^2\Big) \\
&= \tfrac{1}{9}\Big(213\sqrt{2} + 125\sqrt{3}\Big) + \Big(\tfrac{19\sqrt{2}}{2} + \tfrac{70\sqrt{3}}{9}\Big)\Big(2^{n+1} - 4\Big)
\end{aligned}$$

This completes the proof.

Theorem 2.2 *Let $NS[n]$ be the dendrimer nanostar as shown in Figure 1. Then*

$$^3\chi(NS[n]) = \tfrac{1}{9}\Big(222 + 94\sqrt{6}\Big) + \tfrac{1}{9}\Big(99 + 44\sqrt{6}\Big)\Big(2^{n+1} - 4\Big)$$

Proof. Let d_{ijkl} denotes the number of 3-paths whose three consecutive vertices are of degree i, j, k, l, *resp.* At the same time, we use $d^{(s)}_{ijkl}$ to mean d_{ijkl} in $s-th$ stage. Obviously, $d^{(s)}_{ijkl} = d^{(s)}_{lkji}$.

Similar to the discussion way in Theorem 2.1, at the first, we compute $^3\chi(NS[1])$. It is easy to see that

$d^{(1)}_{2222} = 32, d^{(1)}_{2223} = 32, d^{(1)}_{2232} = 32, d^{(1)}_{2233} = 32, d^{(1)}_{2323} = 12, d^{(1)}_{2332} = 24, d^{(1)}_{2333} = 64, d^{(1)}_{3232} = 12, d^{(1)}_{3233} = 28, d^{(1)}_{3333} = 48.$

Thus,

$$\begin{aligned}
{}^3\chi(NS[1]) &= \tfrac{32}{\sqrt{2\times2\times2\times2}} + \tfrac{32}{\sqrt{2\times2\times2\times3}} + \tfrac{32}{\sqrt{2\times2\times3\times2}} + \tfrac{32}{\sqrt{2\times2\times3\times3}} + \tfrac{24}{\sqrt{2\times3\times3\times2}} \\
&\quad + \tfrac{64}{\sqrt{2\times3\times3\times3}} + \tfrac{12}{\sqrt{3\times2\times3\times2}} + \tfrac{28}{\sqrt{3\times2\times3\times3}} + \tfrac{48}{\sqrt{3\times3\times3\times3}} \\
&= \tfrac{1}{9}(222 + 94\sqrt{6})
\end{aligned}$$

Secondly, we compute $^3\chi(NS[n])$.

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

$$\begin{aligned}
d^{(s)}_{2222} &= d^{(s-1)}_{2222} + 12 \times 2^s, \\
d^{(s)}_{2223} &= d^{(s-1)}_{2223} + 12 \times 2^s, \\
d^{(s)}_{2232} &= d^{(s-1)}_{2232} + 20 \times 2^s, \\
d^{(s)}_{2233} &= d^{(s-1)}_{2233} + 20 \times 2^s, \\
d^{(s)}_{2332} &= d^{(s-1)}_{2332} + 8 \times 2^s, \\
d^{(s)}_{2333} &= d^{(s-1)}_{3233} + 32 \times 2^s \\
d^{(s)}_{3233} &= d^{(s-1)}_{3233} + 4 \times 2^s \\
d^{(s)}_{3333} &= d^{(s-1)}_{3233} + 24 \times 2^s.
\end{aligned}$$

For any $(i, j, k, l) \neq (2222), (2223), (2232), (2233), (2332), (2333), (3233), (3333)$, $d^{(s)}_{ijkl} = 0$ or $d^{(s)}_{ijkl} = d^{(s-1)}_{ijkl} = \cdots = d^{(1)}_{ijkl}$ for $s = 2, 3, 4, \cdots, n$.

Thus,

$$\begin{aligned}
{}^3\chi(NS[n]) &= {}^3\chi(NS[n-1]) + \tfrac{12\times 2^n}{4} + \tfrac{12\times 2^n}{2\sqrt{6}} + \tfrac{20\times 2^n}{2\sqrt{6}} + \tfrac{20\times 2^n}{6} + \tfrac{8\times 2^n}{6} \\
&\quad + \tfrac{32\times 2^n}{3\sqrt{6}} + \tfrac{4\times 2^n}{6} + \tfrac{8\times 2^n}{3\sqrt{6}} + \tfrac{24\times 2^n}{9} \\
&= {}^3\chi(NS[n-2]) + \tfrac{2^n}{9}(99 + 44\sqrt{6}) \\
&\ \vdots \\
&= {}^3\chi(NS[1]) + \tfrac{1}{9}(99 + 44\sqrt{6})\left(2^n + 2^{n-1} + \cdots + 2^2\right) \\
&= \tfrac{1}{9}\left(222 + 94\sqrt{6}\right) + \tfrac{1}{9}\left(99 + 44\sqrt{6}\right)\left(2^{n+1} - 4\right)
\end{aligned}$$

This completes the proof.

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