THE K-CONNECTIVITY INDEX OF AN INfINITE CLASS OFDENDRIMER NANOSTARS

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The k-connectivity index ${}^k\chi(G)$ of a molecular graph G is the sum of the weights $(d_{v_1}d_{v_2}\cdots d_{v_{k+1}})^{-1/2}$, where $v_1v_2\cdots v_{k+1}$ runs over all paths of length k in G and d_{v_i} denotes the degree of vertex v_i . In this paper, we give the explicitly formula of the k-connectivity index of a finite class of dendrimer s, which generalized Ahmadiand Sadeghimehr's result [Second-order connectivity index of an infinite class of dendrimer nanostars, Dig. J. Nanomater Bios., 2009].

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1 Introduction

A dendrimer is generally described as a macromolecule, which is characterized by its highly branched 3D structure that provides a high degree of surface functionality and versatility. It is constructed through a set of repeating chemical synthesis procedures that build up from the molecular level to the nanoscale region under the condition that is easily performed in a standard organic chemistry laboratory.

Dendrimers have often been referred to as the "Polymers of the 21st century". Dendrimer chemistry was first introduced in 1978 by Buhleier, Wehner, and Vogtle [3], and in 1985, Tomalia et al [14] synthesized the first family of dendrimers. In 1990, a convergent synthetic approach was introduced by Hawker and Frechet [4]. Dendrimer popularity then greatly increased, resulting in a large number of scientific papers and patents.

Let G be a simple connected graph of order n. In 1975, Randic [10] introduced the connectivity index (now called also Randic index) as $\chi(G) = \sum_{uv} \sqrt{\frac{1}{d_u d_v}}$, where uv runs over all edges of G. This index has been successfully related to chemical properties, namely if G is the molecular graph of an alkane, then $\chi(G)$ has a strong correlation with the boiling point and the stability of the compound [8, 9, 12].

The k-connectivity index of an organic molecule whose molecule graph is G is defined

As

$$^{1}\chi(G) = \sum_{\nu_{1}\nu_{2}\cdots\nu_{k+1}} \left(d_{\nu_{1}}d_{\nu_{2}}\dots d_{\nu_{k+1}}\right)^{-\frac{1}{2}}$$

where $v_1v_2\cdots v_{k+1}$ runs over all paths of length k in G and d_{vi} denotes the degree of vertex v_i . The higher connectivity indices are of great interest in molecular graph theory, one can refer [6] and [13] for more details, and some of their mathematical properties have been reported in [2, 5, 7, 11].

In [1], Ahmadi and Sadeghimehr determined the 2-connectivity index of an infinite class of dendrimer nanostars. In this paper, we give the exact value of the k-connectivity index of such dendrimers for a nonnegative integer k, which generalize Ahmadi and Sadeghimehr's result.

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2. Main results

Let D[n] denote a type of dendrimer with n growth stages, D[2], D[3] and D[5] are shown in Fig.1. The dendrimer D[n] can be constructed recursively: set $D[1] := K_{1,4}$ the star with four leaves (vertices of degree one), and D[n + 1] is obtained from D[n] by adding two new independent vertices adjacent to each of the leaves of D[n]. The unique vertex of degree four in D[n] is called the center of D[n].

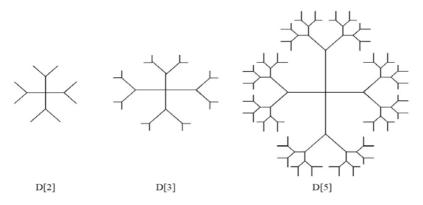


Fig. 1

For a given positive integer k, let P⁽ⁿ⁾_{i1 i2 ···ik+1} denote the number of paths composed by k+1 consecutive vertices of degree i_1 , i_2 ,..., i_{k+1} , respectively in D[n]. Since D[n] is undirected, $P_{i_1}^{(n)}$ $_{i2\,\cdots ik+1}\!=P^{(n)}_{ik+1\,ik\,\cdots i1}$.

We compute $P_{i_1i_2\cdots i_{k+1}}$ according to the choices of $i_1i_2\cdots i_{k+1}$.

I.
$$i_1 i_2 \cdots i_{k+1} = 1 \underbrace{3 \cdots 3}_{k-1}$$
 the paths exist if and only if k is even and $2 \le k \le 2n-2$.

Such a path must start from a leaf, then k/2 steps toward to the center and k/2 steps away from the center. There are $4 \cdot 2n1$ ways to choose an end of such a path (as there are $4 \cdot 2n1$ leaves). Then the following k/2 consecutive vertices are uniquely determined (toward the center). Since the next step must toward the reverse direction, this vertex again is determined uniquely. For each of the remaining k-1 vertices, there are two choices, so there are totally $2^{k/2-1}$ ways to choose them. By the symmetry, each path is calculated twice. Hence

$$P^{(n)}_{13\cdots 31} = 4 \cdot 2^{n-1} \cdot 2^{\frac{k}{2}-1} \cdot \frac{1}{2} = 2^{\frac{k}{2}+n-1}, 2 \le k \le 2n-2$$
II. Such paths exist if and only if k = n.
$$i_1 i_2 \cdots i_{k+1} = 13 \cdots 34$$

Such a path is uniquely determined by the end of degree one. So

III.
$$P^{(n)} = \underbrace{1}_{\text{Such}} \underbrace{1}_{\text{paths}} \underbrace{2}_{\text{exist}} \underbrace{1}_{\text{if}} \underbrace{2}_{\text{and}} \underbrace{1}_{\text{only}} \underbrace{1}_{i_1 i_2} \underbrace{1}_{i_2 i_3} \underbrace{1}_{i_{k+1}} \underbrace{1}_{i_1 i_2 i_3} \underbrace{1}_{i_2 i_3 i_4} \underbrace{1}_{i_1 i_2 i_4} \underbrace{1}_{i_1 i_4 i_4$$

By the recursion of D[n], such a path can be seen as a path in D[k] of type $13 \cdots 34$. Hence, by II,

$$P^{(n)}_{33\cdots 34} = P^{(k)}_{13\cdots 34} = 2^{k+1}, 1 \le k \le n-1$$

= 13...343..($\frac{k}{4} + k_2 = k-2$). Such paths exist if and only if $k_1 = k_2 = n-1$

 $P^{(n)}_{33\cdots 34} = P^{(k)}_{13\cdots 34} = 2^{k+1}, 1 \le k \le n-1$ $i_1 i_2 \cdots i_{k+1} = 1 \underbrace{3 \cdots 3}_{k} 4 \underbrace{3 \cdots (k - 1)}_{k} + k_2 = k-2). \text{ Such paths exist if and only if } k_1 = k_2 = n-1 \text{ and } k$ IV. Such a path is composed by two symmetric segments of length $k_2 = n$, each segment can be

considered as a path from the center to a vertex of degree one. There are choices for the first vertex adjacent to the center of the two segments. For each of the remaining k-2 vertices in the two segments, there are two choices to take them. Hence

$$P^{(n)}_{13\cdots 4\cdots 31} = {4 \choose 2} \cdot 2^{k-2} = 3 \cdot 2^{k-1}, k = 2n$$

V. $i_1 i_2 \cdots i_{k+1} = 1 \underbrace{3 \cdots 3}_{k_1} 4 \underbrace{3 \cdots 3}_{k_2}$ ($k_2 \ge 1$, $k_1 + k_2 = k-1$). Such paths exist if and only if $k_1 = n-1$, $k_2 = n-1$

 $k-n, n+1 \le k \le 2n-1$

Such a path is composed by two segments of length k₁ + 1 and k₂, respectively, each of which starts from the center. The difference between the case from case IV is that the two segments are not symmetric. So, by a similar reason as in IV,

$$P^{(n)}_{13\cdots 4\cdots 3} = 4 \cdot 3 \cdot 2^{k-2} = 3 \cdot 2^k, n+1 \le k \le 2n-1$$
$$i_1 i_2 \cdots i_{k+1} = 1 \underbrace{3 \cdots 3}_{k_1} 4 \underbrace{3 \cdots 3}_{k_2}$$

VI.

(VI.1) k is even and $1 \le k \le n-1$.

Such a path must start from a vertex of degree one to a vertex of degree three with k/2+1 steps toward to the center, then k/2-1 steps toward or away from the center. There are $4 \cdot 2^{n-1}$ choices for the vertex of degree one, and the first k/2+2 vertices are uniquely determined once the starting vertex of degree one has been chosen. For each of the remaining k/2-1 vertices, there are two choices. So

(VI.2) k is even and
$$R \le k \le 2n = 4 \cdot 2^{n-1} \cdot 2^{\frac{k}{2}-1} = 2^{\frac{k}{2}+n}$$

Such a path must start from a vertex of degree one to a vertex of degree three with i steps with $k/2+1 \le i \le n-1$ toward the center, then k-i steps away from the center. There are 4.2n-1 ways to choose the vertex of degree one, and the first i+2 vertices (including the first vertex chosen for the reverse direction) are uniquely determined once the starting vertex of degree one has been chosen. For each of the remaining k-i-1 vertices, there are two choices. So,

$$P^{(n)}_{13\cdots 33} = 4 \cdot 2^{n-1} \cdot \sum_{i=k/2+1}^{n-1} 2^{k-i-1} = 2^{\frac{k}{2}+n} - 2^{k+1}$$

With a similar discussion as in (VI.1) and (VI.2), respectively, we have the following two formulas when k is odd.

(VI.3) k is odd and $1 \le k \le n - 1$

$$P^{(n)}_{13\cdots 33} = 4 \cdot 2^{n-1} \cdot 2^{\frac{k-1}{2}} = 2^{\frac{k+1}{2}+n}$$

(VI.4) k is odd and $n \le k \le 2n - 3$

$$P^{(n)}_{13\cdots 33} = 4 \cdot 2^{n-1} \cdot \sum_{i=(k+1)/2}^{n-1} 2^{k-i-1} = 2^{\frac{k+1}{2}+n} - 2^{k+1}$$

$$i_1 i_2 \cdots i_{k+1} = \underbrace{3 \cdots 3}_{k+1}$$

VII.

$$i_1 i_2 \cdots i_{k+1} = \underbrace{3 \cdots 3}_{k+1}$$

(VII.1) k is even. Such a path exists if and only if $k \le 2n-4$, that is $n \ge k+4$

If k = 2n-4, i.e. n = (k+4)/2, by the recursion of D[n], such a path corresponds to a path of type 13...31 of length k in D[n-1]. Hence, by **I**

$$P^{(n)}_{13\cdots 33} = P^{(\frac{k+4}{2})}_{33\cdots 33} = P^{(\frac{k+4}{2}-1)}_{13\cdots 31} = 2^{\frac{k}{2} + \frac{k+4}{2} - 1 - 1} = 2^k, (k = 2n - 4)$$

If k < 2n-4, i. e. n > (k+4)/2, by the recursion of D[n], a 3···3 path in D[n] is either a 3···3 path in D[n-1], or a 13...31 path in D[n-1], or a 13...3 path in D[n-1]. So,

$$P^{(n+1)}_{33\cdots 33} = P^{(n)}_{33\cdots 33} + P^{(n)}_{13\cdots 31} + P^{(n)}_{13\cdots 33}$$
 (1)

Using (1) recursively, and by I and VI, we have

$$P^{(n)}_{33\cdots 33} = P^{(\frac{k+4}{2})}_{33\cdots 33} + \sum_{i=\frac{k+4}{2}}^{n-1} (P^{(i)}_{13\cdots 31} + P^{(i)}_{13\cdots 33})$$

$$= \begin{cases} 2^{k} + \sum_{i=\frac{k+4}{2}}^{n-1} (3 \cdot 2^{\frac{k}{2}+i-1} - 2^{k+1}), k \ge n \\ 2^{k} + \sum_{i=\frac{k+4}{2}}^{k} (3 \cdot 2^{\frac{k}{2}+i-1} - 2^{k+1}) + \sum_{i=k+1}^{n-1} 3 \cdot 2^{\frac{k}{2}+i-1}, k \le n-1 \end{cases}$$

$$= \begin{cases} 3 \cdot 2^{n+\frac{k}{2}-1} - (2n+1-k) \cdot 2^{k}, n \le k \le 2n-4 \\ 3 \cdot 2^{n+\frac{k}{2}-1} - (3+k) \cdot 2^{k}, k \le n-1 \end{cases}$$

(VII.2) k is odd. Such paths exist if and only if $k \le 2n-5$, that is $n \ge (k+5)/2$. If k = 2n-5 and $k \ge 3$, such a path can be considered as a path of type 13…3 of length k in D[n-1]. So, by (VI.4),

$$P^{(n)}_{3\cdots 3} = P^{(\frac{k+5}{2})}_{3\cdots 3} = P^{(\frac{k+5}{2}-1)}_{13\cdots 3} = 2^{\frac{k+1}{2} + \frac{k+5}{2} - 1} - 2^{k+1} = 2^{k+1}$$

If $3 \le k < 2n - 5$ i.e. $n \ge (k+5)/2 + 1 \ge 5$, such a path corresponds to either a path of type 3···3 in D[n-1] or a path of type 13···3 in D[n-1]. So

$$P^{(n)}_{3\cdots 3} = P^{(n-1)}_{3\cdots 3} + P^{(n-1)}_{13\cdots 3}$$
 (2)

Applying (2) recursively and by VI

$$P^{(n)}_{3\cdots 3} = P^{(\frac{k+5}{2})}_{3\cdots 3} + \sum_{i=\frac{k+5}{2}}^{n-1} P^{(i)}_{13\cdots 3}$$

$$= \begin{cases} 2^{k+1} + \sum_{i=\frac{k+5}{2}}^{n-1} (2^{\frac{k+1}{2}+i} - 2^{k+1}), n \le k \le 2n - 5 \\ 2^{k+1} + \sum_{i=\frac{k+5}{2}}^{k} (2^{\frac{k+1}{2}+i} - 2^{k+1}) + \sum_{i=k+1}^{n-1} 2^{\frac{k+1}{2}+i}, 3 \le k \le n - 1 \end{cases}$$

$$= \begin{cases} 2^{n+\frac{k+1}{2}} - (2n+1-k) \cdot 2^k, n \le k \le 2n - 5 \\ 2^{n+\frac{k+1}{2}} - (3+k) \cdot 2^k, 3 \le k \le n - 1 \end{cases}$$

If k = 1 and n = 3, such a path can be considered as a path of type 13 in D[2]. By (VI.3),

Applying (2) recursively and again by **VI**,

$$P^{(3)}_{33} = 2^3$$

$$P^{(n)}_{33} = P^{(3)}_{33} + \sum_{i=1}^{n-1} P^{(i)}_{13}$$

$$=\begin{cases} 2^{n+1}-8, n \ge 3\\ 2^{0}, n \ge 1, 2 + 2^{n} \end{cases}$$

Therefore, we have

$$P_{3\cdots 3}^{(n)} = \begin{cases} 2^{n + \frac{k+1}{2}} - (2n+1-k) \cdot 2^k, n \le k \le 2n-5 \\ 2^{n + \frac{k+1}{2}} - (3+k) \cdot 2^k, 1 \le k \le n-1 \end{cases}$$

VIII.
$$i_1i_2\cdots i_{k+1}=\underbrace{3\cdots 3}_{k_1}\underbrace{43\cdots 3}_{k_2}$$
, where $k_1+k_2=k,\,k_1\geq 1,\,k_2\geq 1$ By the symmetry of k_1 and k_2 , we may assume $k_1\geq k_2$.

(VIII.1) k is even

If $k_1 = k_2 = k/2$, such a path can be seen as a path of type $13 \cdot \cdot \cdot 343 \cdot \cdot \cdot 31$ in D[k/2].

By IV,

$$P^{(n)}_{3\cdots 343\cdots 3} = P^{(k/2)}_{13\cdots 343\cdots 3} = 3 \cdot 2^{k-1}$$

If $k_1 > k_2$, that is $k_1 \ge k/2 + 1$, such a path can be seen as a path of type 13...343...3 in D[k_1]. By **V**,

If $k \le n$, then

$$P_{3\dots343\dots3}^{(n)} = P_{13\dots343\dots3}^{(k_1)} = 3 \cdot 2^k$$

$$P^{(n)}_{3\cdots 343\cdots 3} = P^{(k/2)}_{13\cdots 343\cdot k\cdot 31} + \sum_{k_1=k/2+1}^{k-1} P^{(k_1)}_{13\cdots 343\cdots 3}$$

= $3 \cdot 2^{k-1} + \sum_{k_1=k/2+1}^{k-1} 3^{k-2} 2^{k_2+1}$
= $3(k-1)2^{k-1}$

If $n+1 \le k \le 2n-2$, then

$$P_{3\dots343\dots3}^{(n)} = P_{13\dots343\cdot n\cdot31}^{(k/2)} + \sum_{k_1=k/2+1}^{n-1} P_{13\dots343\cdot n\cdot31}^{(k_1)} + \sum_{k_2=k/2+1}^{n-1} P_{13\dots343\cdot n\cdot3}^{(k_1)}$$

$$= 3(2n-k-1)2^{k-1}$$

(VIII.2) k is odd

Similarly as in (VIII.1) (the only difference is $k_1 \neq k_2$ in this case), we have

$$P^{(n)}_{3\dots343\dots3} = \sum_{\substack{k_1 = (k+1)/2 \\ = 3(k-1)2^{k-1}}}^{k-1} P^{(k_1)}_{13\dots343\dots3} = \sum_{\substack{k_1 = (k+1)/2 \\ = k+1}}^{k-1} 3 \cdot 2^{k_1}$$

and

$$P^{(n)}_{3\cdots 343\cdots 3} = \sum_{k_1 = (k+1)/2}^{n-1} P^{(k_1)}_{13\cdots 343\cdots 3} = \sum_{k_1 = (k+1)/2}^{n-1} 3 \cdot 2^{k_1}$$

Based on the above computations, we can get the formula of the k-connected index of D[n] for any nonnegative integer k.

Theorem 2.1 Given a positive integer n, the k-connected index of D[n] for any nonnegative integer k are listed in Table 1.

Proof: If k=0, let ni denote the number of vertices of degree i in D[n], then $n_1=2^{n+1}$, $n_3=2^2+\cdots+2^n=2^{n+1}-4$, and $n_4=1$ from the definition of D[n]. Hence

$$^{0}\chi(D[n]) = \frac{2^{n+1}}{\sqrt{1}} + \frac{2^{n+1}-4}{\sqrt{3}} + \frac{1}{\sqrt{4}} = 3^{-\frac{1}{2}}(2^{n+1}-4) + 2^{n+1} + 2^{-1}$$

If $1 \le k \le n - 1$ and k is even, then the possible types of all paths of length k in D[n] are 13...31, 3...34, 13...3, 3...3 and 3...343...3. By **I, III, (VI.1), (VII.1)** and (**VIII.1**),

$$P^{(n)}_{13\cdots 31} = 2^{\frac{k}{2}+n-1}, P^{(n)}_{33\cdots 34} = 2^{k+1}, P^{(n)}_{33\cdots 33} = 3 \cdot 2^{\frac{k}{2}+n-1} - (3+k) \cdot 2^k, P^{(n)}_{13\cdots 33} = 2^{\frac{k}{2}+n}$$
 and
$$P^{(n)}_{3\cdots 4\cdots 3} = 3(k-1) \cdot 2^{k-1}, \text{ respectively. So,}$$

$${}^{k}\chi(D[n]) = 2^{n+\frac{k}{2}-1} \frac{1}{\sqrt{3^{k-1}}} + 2^{n+\frac{k}{2}} \frac{1}{\sqrt{3^{k}}} + 2^{k+1} \frac{1}{\sqrt{4 \cdot 3^{k}}}$$

$$+ [3 \cdot 2^{n+\frac{k}{2}-1} - (3+k) \cdot 2^{k}] \frac{1}{\sqrt{3^{k+1}}} + 3(k-1) \cdot 2^{k-1} \frac{1}{\sqrt{4 \cdot 3^{k}}}$$

$$= \frac{\sqrt{3}+1}{\sqrt{3^{k}}} 2^{n+\frac{k}{2}} + \frac{(3\sqrt{3}-4)k + (\sqrt{3}-12)}{\sqrt{3^{k+1}}} 2^{k-2}$$

If $1 \le k \le n-1$ and k is odd, then the possible types of all paths of length k in D[n] are $3\cdots 34,13\cdots 3$, $3\cdots 3$ and $3\cdots 343\cdots 3$ By III, (VI.3), (VII.2) and (VIII.2), $P^{(n)}_{33\cdots 34} = 2^{k+1}$,

$$P_{13\cdots 33}^{(n)} = 2^{\frac{k+1}{2}+n}, P_{33\cdots 33}^{(n)} = 2^{\frac{k+1}{2}+n} - (3+k)\cdot 2^k$$
 and $P_{3\cdots 4\cdots 3}^{(n)} = 3(k-1)\cdot 2^{k-1}$, respectively. So,

$${}^{k}\chi(D[n]) = 2^{k+1} \frac{1}{\sqrt{4 \cdot 3^{k}}} + 2^{n+\frac{k+1}{2}} \frac{1}{\sqrt{3^{k}}} +$$

$$+ [2^{n+\frac{k+1}{2}} - (3+k) \cdot 2^{k}] \frac{1}{\sqrt{3^{k+1}}} + 3(k-1) \cdot 2^{k-1} \frac{1}{\sqrt{4 \cdot 3^{k}}}$$

$$= \frac{\sqrt{3} + 1}{\sqrt{3^{k+1}}} 2^{n+\frac{k+1}{2}} + \frac{(3\sqrt{3} - 4)k + (\sqrt{3} - 12)}{\sqrt{3^{k+1}}} 2^{k-2}$$

The other formulas can be verified similarly.

Table 1: formula of k-connected index of D[n]

k		$^{^{k}}\chi(D[n])$
k = 0		$\frac{\sqrt{3}+1}{\sqrt{3}}2^{n+1}+\frac{\sqrt{3}-8}{2\sqrt{3}}$
$1 \le k \le n-1$	odd	$\frac{\sqrt{3}+1}{\sqrt{3^{k+1}}}2^{n+\frac{k+1}{2}} + \frac{(3\sqrt{3}-4)k + (\sqrt{3}-12)}{\sqrt{3^{k+1}}}2^{k-2}$
	even	$\frac{\sqrt{3}+1}{\sqrt{3^k}}2^{n+\frac{k}{2}} + \frac{(3\sqrt{3}-4)k + (\sqrt{3}-12)}{\sqrt{3^{k+1}}}2^{k-2}$
k = n	odd	$\frac{\sqrt{3}+1}{\sqrt{3^{k+1}}}2^{\frac{3k+1}{2}} + \frac{(3\sqrt{3}-4)k + (8-11\sqrt{3})}{\sqrt{3^{k+1}}}2^{k-2}$
	even	$\frac{\sqrt{3}+1}{\sqrt{3^k}}2^{\frac{3}{2}^k} + \frac{(3\sqrt{3}-4)k + (8-11\sqrt{3})}{\sqrt{3^{k+1}}}2^{k-2}$
$n+1 \le k \le 2n-4$	odd	$\frac{\sqrt{3}+1}{\sqrt{3^{k+1}}} 2^{n+\frac{k+1}{2}} + \frac{(6\sqrt{3}-8)n - (4-3\sqrt{3})k + (14-11\sqrt{3})}{\sqrt{3^{k+1}}} 2^{k-2}$

	even	$\frac{\sqrt{3}+1}{\sqrt{3^k}}2^{n+\frac{k}{2}} + \frac{(6\sqrt{3}-8)n - (4-3\sqrt{3})k + (14-11\sqrt{3})}{\sqrt{3^{k+1}}}2^{k-2}$
k = 2n - 3		$\frac{3\sqrt{3}+7}{\sqrt{3^k}}2^{k-1}$
k = 2n - 2		$\frac{3\sqrt{3}+10}{\sqrt{3^{k-1}}}2^{k-2}$
k = 2n - 1		$\frac{1}{\sqrt{3^{k-3}}} 2^{k-1}$
k = 2n		$\frac{1}{\sqrt{3^{k-4}}} 2^{k-2}$
k > 2n		0

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