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SECOND-ORDER CONNECTIVITY INDEX OF AN INFINITE CLASS OF DENDRIMER NANOSTARS

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Dendrimer is a polimer molecule with a distinctive structure that resembles the crown of a tree. Dendrimers are key molecules in nanotechnology and can be put to good use e.g. in medicine as carrier molecules for drugs or contrast agents. In this paper we compute 2-connectivity index of an infinite family of dendimers.

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1. Introduction

Molecular connectivity indices are identified as components of the molecular accessibility. The first- and second-order connectivity indices represent molecular accessibility areas and volumes, respectively, whereas higher order indices represent magnitudes in higher dimensional spaces. In identifying accessibility perimeters, we recognized the atom degrees as a measure of the accessibility perimeter of the corresponding atom. The Randić and connectivity indices are identified as the two components of the molecular accessibility area.

Let G be a simple connected graph of order n. The m-connectivity index of an organic molecule whose molecule graph is G is defined as

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

where $i_1 i_2 \ldots i_{m+1}$ runs over all paths of length m in G and d_i denotes the degree of the vertex i. In particular, 2-connectivity index is defined as follows:

$$^{2}\chi(G) = \sum_{i_1 i_2 i_3} \frac{1}{\sqrt{d_{i_1} d_{i_2} d_{i_3}}}$$

In this paper, we focus our attention to achieve 2-connectivity index of infinite family of dendrimers .
Consider the modecular graph dendrimer $D[n]$, where n is steps of growth in the type of dendrimer [fig. 1].

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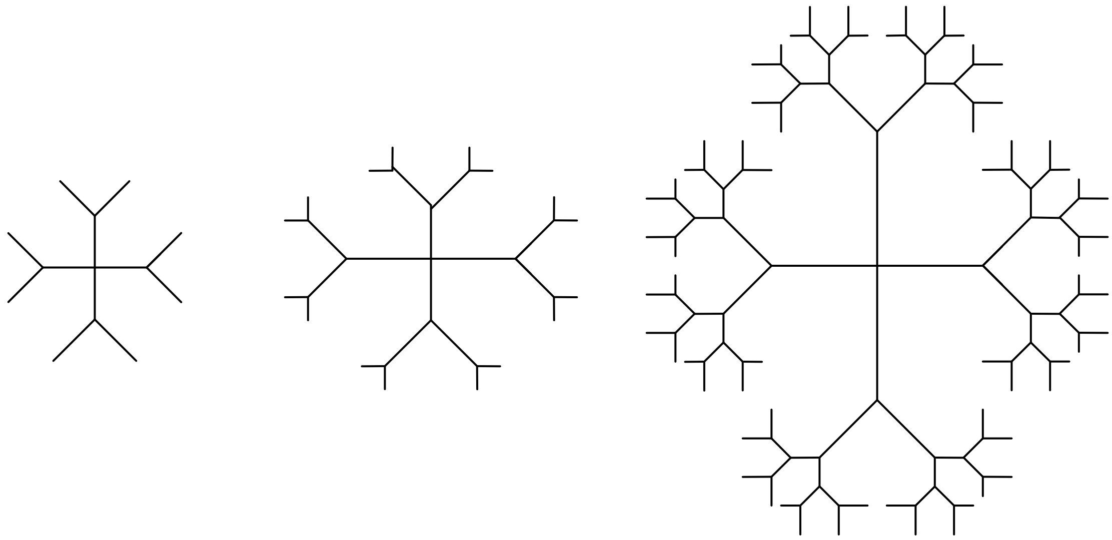

D[2] D[3] D[5]

fig 1: structures of the dendrimers used in this study

2. Main results and discussion

Define d_{ijk} as a number of 2-edges paths with 3 vertices of degree i, j and k respectively. Also $d_{ijk}^{(n)}$ means d_{ijk} for n^{th} stage. It is clear that $d_{ijk}^{(n)} = d_{kji}^{(n)}$.
It is obvious that, in $D[1]$,

$$d_{141}^{(1)} = 6, d_{ijk}^{(1)} = 0 \ , ijk \neq 141 \ . \qquad (1)$$

Thus $${}^{2}\chi(D[1]) = \frac{6}{\sqrt{1\times 4\times 1}} = 3.$$

In $D[2]$, we have

$$d_{131}^{(2)} = 4 \ , \ d_{134}^{(2)} = 8, d_{343}^{(2)} = 6 \qquad (2)$$

$$d_{ijk}^{(2)} = 0, \qquad ijk \neq \{131,134,343\}, \qquad (3)$$

Therefore

$${}^{2}\chi(D[2]) = \frac{4}{\sqrt{1\times 3\times 1}} + \frac{8}{\sqrt{1\times 3\times 4}} + \frac{6}{\sqrt{3\times 4\times 3}} = \frac{8\sqrt{3}}{3} + 1 = 5.618802 \quad (6D).$$

For $n = 3$ and $n = 4$, we have

$$p_{ijk}^{(3)} = \begin{cases} 8 & ijk = 131 \\ 16 & ijk = 133 \\ 4 & ijk = 333 \\ 8 & ijk = 334 \\ 6 & ijk = 343 \\ 0 & otherwise \end{cases} \quad (4)$$

$$p_{ijk}^{(4)} = \begin{cases} 16 & ijk = 131 \\ 32 & ijk = 133 \\ 28 & ijk = 333 \\ 8 & ijk = 334 \\ 6 & ijk = 343 \\ 0 & otherwise \end{cases} \quad (5)$$

In $D[n]$, for $n \geq 3$, the value of $p_{334}^{(n)}$ and $p_{343}^{(n)}$ are constants, and $p_{334}^{(n)} = 8, p_{343}^{(n)} = 6$. Thus we have

$$\frac{p_{334}^{(n)}}{\sqrt{3\times 3\times 4}} + \frac{p_{343}^{(n)}}{\sqrt{3\times 4\times 3}} = \frac{8}{6} + 1 = \frac{7}{3}, \quad n \geq 3 \quad (6)$$

From (4) and (6), we obtain

$$^{2}\chi(D[3]) = \frac{8}{\sqrt{1\times 3\times 1}} + \frac{16}{\sqrt{1\times 3\times 3}} + \frac{4}{\sqrt{3\times 3\times 3}} + \frac{7}{3} = \frac{28\sqrt{3}}{9} + \frac{23}{3} = 13.055269 \quad (6D).$$

A simple calculation shows that for $n \geq 4$

$$p_{ijk}^{(n)} = \begin{cases} 2^{n} & ijk = 131 \\ 2^{n+1} & ijk = 133 \\ \sum_{i=2}^{n} 2^{i} & ijk = 333 \\ 8 & ijk = 334 \\ 6 & ijk = 343 \\ 0 & otherwise \end{cases} \quad (7)$$

Theorem 1 : The 2-conneciviy index of $D[n]$ is computed as follows:

$$^{2}\chi(D[n]) = 1.628917\times 2^{n} + 1.563533 \quad \text{for } n \geq 4$$

Proof: At first, by induction we show that

$$^{2}\chi(D[n]) = \frac{2^{n}}{\sqrt{1\times 3\times 1}} + \frac{2^{n+1}}{\sqrt{1\times 3\times 3}} + \frac{\sum_{i=2}^{n} 2^{i}}{\sqrt{3\times 3\times 3}} + \frac{7}{3} \quad \text{for } n \geq 4. \quad (8)$$

For $n = 4$ from (5) we have

$$^{2}\chi(D[4])=\frac{16}{\sqrt{1\times3\times1}}+\frac{32}{\sqrt{1\times3\times3}}+\frac{28}{\sqrt{3\times3\times3}}+\frac{7}{3}$$
$$=\frac{2^4}{\sqrt{1\times3\times1}}+\frac{2^5}{\sqrt{1\times3\times3}}+\frac{2^2+2^3+2^4}{\sqrt{3\times3\times3}}+\frac{7}{3}.$$

Thus for $n=4$, relation (8) is true. Now suppose (8) is true for $n=k$, i.e.,

$$^{2}\chi(D[k])=\frac{2^k}{\sqrt{1\times3\times1}}+\frac{2^{k+1}}{\sqrt{1\times3\times3}}+\frac{\sum_{i=2}^{k}2^i}{\sqrt{3\times3\times3}}+\frac{7}{3}.$$

We show that (8) is true for $n=k+1$.
According to the structure of $D[n]$, in stage k $(k\geq4)$, we have $p_{131}^{(k)}=2^k, p_{133}^{(k)}=2^{k+1}$ and $p_{333}^{(k)}=\sum_{i=2}^{k}2^i$, and in stage $k+1$, $p_{131}^{(k+1)}=2^{k+1}, p_{133}^{(k+1)}=2^{k+2}$. Also the nodes with degree 1 in stage k have degree 3 in stage $k+1$, therefore

$$p_{333}^{(k+1)}=p_{333}^{(k)}+2^{k+1}=\sum_{i=2}^{k}2^i+2^{k+1}=\sum_{i=2}^{k+1}2^i.$$

Thus

$$^{2}\chi(D[k+1])=\frac{2^{k+1}}{\sqrt{1\times3\times1}}+\frac{2^{k+2}}{\sqrt{1\times3\times3}}+\frac{\sum_{i=2}^{k+1}2^i}{\sqrt{3\times3\times3}}+\frac{7}{3}.$$

Therefore (8) is true for $n=k+1$.
Since $\sum_{i=2}^{n}2^i=2^{n+1}-4$, we can simplify (8) as follows:

$$^{2}\chi(D[n])=\frac{2^n}{\sqrt{3}}+\frac{2^{n+1}}{3}+\frac{2^{n+1}-4}{3\sqrt{3}}+\frac{7}{3}$$
$$=\frac{2^n(5+2\sqrt{3})+7\sqrt{3}-4}{3\sqrt{3}}$$

$=1.628917\times2^n+1.563533$ (6D).
The proof is now complete.
We can summarize the given results for 2-connectivity index of $D[n]$ as follows:

$$^{2}\chi(D[n])=\begin{cases}3 & n=1\\ 5.618802 & n=2\\ 13.055269 & n=3\\ 1.628917\times2^n+1.563533 & n\geq4\end{cases}$$

In table 1, the 2-connectivity index of $D[n]$ is computed for $n=1,\ldots,15$.

Table 1. Computing 2-connectivity Index for dendrimer D[n].

N	The Number of Vertices	2-connectivity Index
1	5	3
2	13	5.618802
3	29	13.055269
4	61	27.626207
5	125	53.688881
6	253	105.814229
7	509	210.064924
8	1021	418.566316
9	2045	835.569098
10	4093	1669.574664
11	8189	3337.585795
12	16381	6673.608056
13	32765	13345.652580
14	65533	26689.741627
15	131069	53377.919721

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