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(RECOMMENDED CITATION)

THE CONNECTIVITY INDEX OF PAMAM DENDRIMERS

NABEEL E. ARIF[a], ROSLAN HASNI[b]

ABSTRACT. The *m*-order connectivity index is an extension of the Randic (simple) connectivity index that counts the connectivity of all paths of length *m inG.* A dendrimer is ahyperbranchedmolecule built up from branched units called monomers. In this paper, the 2-order, 3-order and 4-order connectivity indices of an infinite family of PAMAM dendrimers are computed.

Keywords: *Randic connectivity index, Graph, Dendrimer*

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 represent the atoms of the molecule and the edges represent the chemical bonds.

A single number that characterizes the molecular graph is called a graph theoretical invariant or topological index. Among the many topological indices considered in chemical graph theory, only a few have been found noteworthy in practical applications, connectivity index being one of them. 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 [1]. Kier and Hall (1986) extended χ index to higher orders and introduced modifications to account for heteroatoms [2].

Molecular connectivity indices are the most popular class of indices (Trinajastic [3]). They have been used in a wide spectrum of correlating applications, including physicochemical properties (e.g. boiling point, solubility, partition coefficient etc.) and biological (activities such as antifungal effect, an esthetic effect, enzyme inhibition etc.) (Murray et al. [4], Kier and Hall [5]).

[a] *School of Mathematical Sciences, UniversitiSains Malaysia, 11800 USM, Penang, Malaysia*
[b] *Department of Mathematics, Faculty of Science and Technology Universiti Malaysia Terengganu, 21030 Kuala Terengganu, Terengganu, Malaysia, hroslan@umt.edu.my*

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

$$^{m}\chi(G) = \sum_{i_1 \dots i_{m+1}} \frac{1}{\sqrt{d_1 \dots d_{m+1}}},$$

where $i_1 \dots i_{m+1}$ runs over all paths of length m in G and d_i denote the degree of vertex v_i, and in particular, 2-, 3- and 4-order connectivity indices are defined as follows:

$$^{2}\chi(G) = \sum_{i_1 i_2 i_3} \frac{1}{\sqrt{d_1 d_2 d_3}} \qquad ^{3}\chi(G) = \sum_{i_1 i_2 i_3 i_4} \frac{1}{\sqrt{d_1 d_2 d_3 d_4}}$$

and $$^{4}\chi(G) = \sum_{i_1 i_2 i_3 i_4 i_5} \frac{1}{\sqrt{d_1 d_2 d_3 d_4 d_5}}.$$

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 nanoscience are unlimited.

Recently, some researchers investigated the *m*-order connectivity index and *m*-sum connectivity index for some families of dendrimers, where *m* = 2 and 3 (see [6-12]).

Note that one of the first studies on the topology of dendrimers was performed by Diudea and Katona [13].

In this paper, we will study the 2-order, 3-orderand 4-order connectivity indices of an infinite family of PAMAM dendrimers.

RESULTS AND DISCUSSIONS

In this section, we shall compute 2-order, 3-orderand 4-order connectivity indices of a class of dendrimers, namely, PAMAM dendrimers by construction of dendrimer generations G_n which has grown n stages. We denote simply this graph by $PD_1[n]$. Figure 1 shows generations G_3 has grown 3 stages.

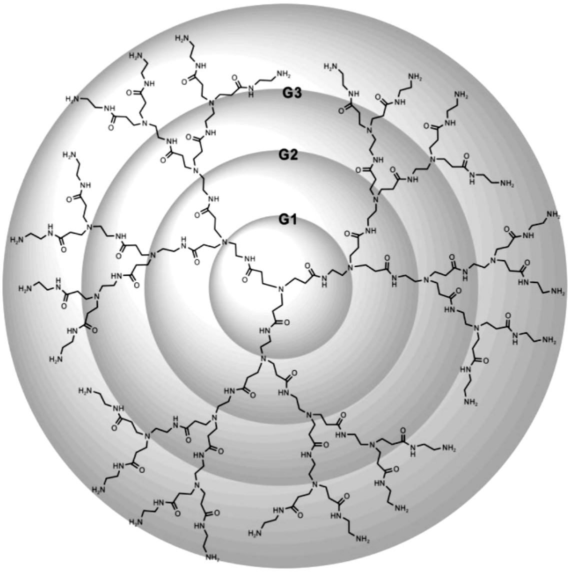

Figure 1. PAMAM dendrimer of generation G_n has grown 3 stages, denoted by $PD_1[n]$

Below we give our main results.

Theorem 1. Let $n \in \mathrm{N}_0$. The second-order connectivity index of $PD_1[n]$ is computed as follows

$$^2\chi(PD_1[n]) = \frac{1}{4}[(3\sqrt{2} + 10\sqrt{3} + 4\sqrt{6} + 6) + (3\sqrt{2} + 12\sqrt{3} + 4\sqrt{6} + 3)(2^{n+1} - 2)]$$

Proof. For this structure, the core means that the number of stages equal to zero. Firstly, we compute $^2\chi(PD_1[0])$. Let $d_{i_1 i_2 i_3}$ denote the number of 2-paths whose three consecutive vertices are of degree $i_1, i_2, i_3,$ respectively. By the same way, we use $d^{(n)}_{i_1 i_2 i_3}$ to mean $d_{i_1 i_2 i_3}$ in $n-th$ stages. Particularly, $d^{(n)}_{i_1 i_2 i_3} = d^{(n)}_{i_3 i_2 i_1}$. By Figure 2, one can verify that

$$d^{(0)}_{122} = 3\,,\; d^{(0)}_{222} = 3\,,\; d^{(0)}_{223} = 9,\; d^{(0)}_{232} = 6\,,\; d^{(0)}_{231} = 6\,.$$

It is easy to see that in the core of this structure as vertices are labeled in Figure 2, we have $d^{(0)}_{122} = 3$ which is $d^{(0)}_{i_9 i_8 i_7} = 3$, $d^{(0)}_{222} = 3$ which is $d^{(0)}_{i_6 i_7 i_8} = 3$, $d^{(0)}_{223} = 9$, which are ($d^{(0)}_{i_3 i_2 i_1} = 3$ + $d^{(0)}_{i_2 i_3 i_4} = 3$ + $d^{(0)}_{i_7 i_6 i_5} = 3$), $d^{(0)}_{232} = 6$ which are ($d^{(0)}_{i_2 i_1 i_2} = 3$ + $d^{(0)}_{i_3 i_4 i_6} = 3$) and $d^{(0)}_{231} = 6$ which are ($d^{(0)}_{i_3 i_4 i_5} = 3$ + $d^{(0)}_{i_6 i_4 i_5} = 3$).

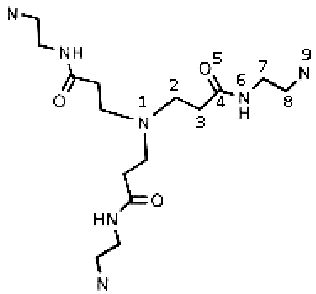

Figure 2. The core of PAMAM dendrimer $PD_1[0]$

Therefore, we have that

$$^{2}\chi(PD_1[0]) = \frac{3}{\sqrt{1\times 2\times 2}} + \frac{3}{\sqrt{2\times 2\times 2}} + \frac{9}{\sqrt{2\times 2\times 3}} + \frac{6}{\sqrt{2\times 3\times 2}} + \frac{6}{\sqrt{2\times 3\times 1}}$$
$$= \frac{1}{4}[(3\sqrt{2} + 10\sqrt{3} + 4\sqrt{6} + 6)$$

Secondly, we construct the relation between $^{2}\chi(PD_1[n])$ and $^{2}\chi(PD_1[n-1])$ for n ≥ 1.

By simple reduction, we have

$$d_{122}^{(n)} = d_{122}^{(n-1)} + 3\times 2^{n-1},\ d_{222}^{(n)} = d_{222}^{(n-1)} + 6\times 2^{n-1},$$
$$d_{223}^{(n)} = d_{223}^{(n-1)} + 21\times 2^{n-1},\ d_{232}^{(n)} = d_{232}^{(n-1)} + 15\times 2^{n-1},$$
$$d_{231}^{(n)} = d_{231}^{(n-1)} + 12\times 2^{n-1},$$

and for any $(i_1i_2i_3) \neq (122),(222),(223),(232),(231)$, we have $d_{i_1i_2i_3}^{(n)} = 0.$

Therefore,

$$^{2}\chi(PD_1[n]) = {}^{2}\chi(PD_1[n-1]) + (\frac{3}{\sqrt{1\times 2\times 2}} + \frac{6}{\sqrt{2\times 2\times 2}}$$
$$+ \frac{21}{\sqrt{2\times 2\times 3}} + \frac{15}{\sqrt{2\times 3\times 2}} + \frac{12}{\sqrt{2\times 3\times 1}}) \times 2^{n-1}$$
$$= {}^{2}\chi(PD_1[n-1]) + \frac{1}{4}(3\sqrt{2} + 12\sqrt{3} + 4\sqrt{6} + 3)\times 2^{n}\cdot$$

From above recursion formula, we have

$$^{2}\chi(PD_1[n]) = {}^{2}\chi(PD_1[n-1]) + \frac{1}{4}(3\sqrt{2} + 12\sqrt{3} + 4\sqrt{6} + 3)\times 2^{n}$$
$$= {}^{2}\chi(PD_1[n-2]) + \frac{1}{4}(3\sqrt{2} + 12\sqrt{3} + 4\sqrt{6} + 3)(2^{n} + 2^{n-1})$$

$$\vdots$$

$$= {}^{2}\chi(PD_1[0]) + \frac{1}{4}(3\sqrt{2} + 12\sqrt{3} + 4\sqrt{6} + 3)(2^n + 2^{n-1} + \ldots + 2^2 + 2)$$

Hence,

$${}^{2}\chi(PD_1[n]) = \frac{1}{4}[(3\sqrt{2} + 10\sqrt{3} + 4\sqrt{6} + 6) + (3\sqrt{2} + 12\sqrt{3} + 4\sqrt{6} + 3)(2^{n+1} - 2)]$$

The proof is now complete.

Theorem 2. Let $n \in \mathrm{N}_0$. The third-order connectivity index of $PD_1[n]$ is computed as follows

$${}^{3}\chi(PD_1[n]) = \frac{1}{4}[(3\sqrt{2} + 4\sqrt{3} + 5\sqrt{6} + 2) + (3\sqrt{2} + 8\sqrt{3} + 12\sqrt{6} + 4)(2^n - 1)]$$

Proof. We compute ${}^{3}\chi(PD_1[0])$ and let $d_{i_1 i_2 i_3 i_4}$ denote the number of m3-paths whose four consecutive vertices are of degree i_1, i_2, i_3, i_4, respectively. By the same way, we use $d^{(n)}_{i_1 i_2 i_3 i_4}$ to mean $d_{i_1 i_2 i_3 i_4}$ in $n-th$ stages. Particularly, $d^{(n)}_{i_1 i_2 i_3 i_4} = d^{(n)}_{i_4 i_3 i_2 i_1}$.

In Figure 2, one can verify that

$$d^{(0)}_{1222} = 3\,,\ d^{(0)}_{2223} = 3\,,\ d^{(0)}_{2231} = 6\,,\ d^{(0)}_{2232} = 12\,,\ d^{(0)}_{3223} = 3\,.$$

We can see that in the core of this structure as vertices are labeled in Figure 2, we have $d^{(0)}_{1222} = 3$ which is $d^{(0)}_{i_9 i_8 i_7 i_6} = 3$, $d^{(0)}_{2223} = 3$ which is $d^{(0)}_{i_8 i_7 i_6 i_4} = 3$, $d^{(0)}_{2231} = 6$ which are ($d^{(0)}_{i_7 i_6 i_4 i_5} = 3$ + $d^{(0)}_{i_2 i_3 i_4 i_5} = 3$), $d^{(0)}_{2232} = 12$ which are ($d^{(0)}_{i_2 i_1 i_2 i_3} = 6$ + $d^{(0)}_{i_2 i_3 i_4 i_6} = 3 + d^{(0)}_{i_7 i_6 i_4 i_3} = 3$) and $d^{(0)}_{3223} = 3$ which is $d^{(0)}_{i_1 i_2 i_3 i_4} = 3$.

Therefore, we have that

$${}^{3}\chi(PD_1[0]) = \frac{3}{\sqrt{1 \times 2 \times 2 \times 2}} + \frac{3}{\sqrt{2 \times 2 \times 2 \times 3}} + \frac{6}{\sqrt{2 \times 2 \times 3 \times 1}} + \frac{12}{\sqrt{2 \times 2 \times 3 \times 2}} + \frac{3}{\sqrt{3 \times 2 \times 2 \times 3}}$$

$$= \frac{1}{4}(3\sqrt{2} + 4\sqrt{3} + 5\sqrt{6} + 2)$$

Now, we construct the relation between ${}^{3}\chi(PD_1[n])$ and ${}^{3}\chi(PD_1[n-1])$ for $n \geq 1$

By simple reduction, we have

$$d_{1222}^{(n)} = d_{1222}^{(n-1)} + 3\times 2^{n-1},\ d_{2223}^{(n)} = d_{2223}^{(n-1)} + 6\times 2^{n-1},$$
$$d_{2231}^{(n)} = d_{2231}^{(n-1)} + 12\times 2^{n-1},\ d_{2232}^{(n)} = d_{2232}^{(n-1)} + 30\times 2^{n-1},$$
$$d_{3223}^{(n)} = d_{3223}^{(n-1)} + 6\times 2^{n-1}$$

and for any $(i_1i_2i_3i_4) \neq (1222),(2223),(2231),(2232),(3223)$ we have $d_{i_1i_2i_3i_4}^{(n)} = 0.$

Thus,

$$\begin{aligned}{}^3\chi(PD_1[n]) &= {}^3\chi(PD_1[n-1]) + \Big(\frac{3}{\sqrt{1\times 2\times 2\times 2}} + \frac{6}{\sqrt{2\times 2\times 2\times 3}} \\ &+ \frac{12}{\sqrt{2\times 2\times 3\times 1}} + \frac{30}{\sqrt{2\times 2\times 3\times 2}} + \frac{6}{\sqrt{3\times 2\times 2\times 3}}\Big)\times 2^{n-1} \\ &= {}^3\chi(PD_1[n-1]) + \frac{1}{8}(3\sqrt{2} + 8\sqrt{3} + 12\sqrt{6} + 4)\times 2^n \\ &= {}^3\chi(PD_1[n-2]) + \frac{1}{8}(3\sqrt{2} + 8\sqrt{3} + 12\sqrt{6} + 4)(2^n + 2^{n-1}) \\ &\vdots \\ &= {}^3\chi(PD_1[0]) + \frac{1}{8}(3\sqrt{2} + 8\sqrt{3} + 12\sqrt{6} + 4)(2^n + 2^{n-1} + \ldots + 2^2 + 2)\end{aligned}$$

Hence,

$${}^3\chi(PD_1[n]) = \frac{1}{4}[(3\sqrt{2} + 4\sqrt{3} + 5\sqrt{6} + 2) + (3\sqrt{2} + 8\sqrt{3} + 12\sqrt{6} + 4)(2^n - 1)]$$

The proof is now complete.

Theorem 3. Let $n \in \mathrm{N}_0$. The fourth-order connectivity index of $PD_1[n]$ is computed as follows

$${}^4\chi(PD_1[n]) = \frac{1}{4}[(3\sqrt{2} + 3\sqrt{3} + 2\sqrt{6} + 2) + (5\sqrt{2} + 9\sqrt{3} + 3\sqrt{6} + 4)(2^n - 1)]$$

Proof. Similar to that of Theorems 1 and 2, we compute ${}^4\chi(PD_1[0])$ and let $d_{i_1i_2i_3i_4i_5}$ denote the number of 4-paths whose five consecutive vertices are of degree i_1, i_2, i_3, i_4, i_5, respectively. We use $d_{i_1i_2i_3i_4i_5}^{(n)}$ to mean $d_{i_1i_2i_3i_4i_5}$ in $n-th$ stages. Particularly, $d_{i_1i_2i_3i_4i_5}^{(n)} = d_{i_5i_4i_3i_2i_1}^{(n)}$. By Figure 2, one can verify that

$$d_{12223}^{(0)} = 3,\ d_{22231}^{(0)} = 3,\ d_{22232}^{(0)} = 3,\ d_{22322}^{(0)} = 6,\ d_{23223}^{(0)} = 9,\ d_{13223}^{(0)} = 3,\ d_{32223}^{(0)} = 0.$$

Also we can see that in the core of this structure as vertices are labeled in Figure 2, we have $d^{(0)}_{12223}=3$ which is $d^{(0)}_{i_9 i_8 i_7 i_6 i_4}=3$, $d^{(0)}_{22231}=3$ which is $d^{(0)}_{i_8 i_7 i_6 i_4 i_5}=3$, $d^{(0)}_{22232}=3$ which is $d^{(0)}_{i_8 i_7 i_6 i_4 i_3}=3$, $d^{(0)}_{22322}=6$ which are ($d^{(0)}_{i_3 i_2 i_1 i_2 i_3}=3$ + $d^{(0)}_{i_2 i_3 i_4 i_6 i_7}=3$), $d^{(0)}_{23223}=9$ which are ($d^{(0)}_{i_2 i_1 i_2 i_3 i_4}=6$ + $d^{(0)}_{i_6 i_4 i_3 i_2 i_1}=3$) and $d^{(0)}_{13223}=3$ which is $d^{(0)}_{i_5 i_4 i_3 i_2 i_1}=3$.

Therefore,

$$
\begin{aligned}
{}^4\chi(PD_1[0]) &= \frac{3}{\sqrt{1\times 2\times 2\times 2\times 3}}+\frac{3}{\sqrt{2\times 2\times 2\times 3\times 1}}+\\
&\frac{3}{\sqrt{2\times 2\times 2\times 3\times 2}}+\frac{6}{\sqrt{2\times 2\times 3\times 2\times 2}}\\
&+\frac{9}{\sqrt{2\times 3\times 2\times 2\times 3}}+\frac{3}{\sqrt{1\times 3\times 2\times 2\times 3}}\\
&=\frac{1}{4}[(3\sqrt{2}+3\sqrt{3}+2\sqrt{6}+2)\cdot
\end{aligned}
$$

We now study the relation between ${}^4\chi(PD_1[n])$ and ${}^4\chi(PD_1[n-1])$ for $n \geq 1$, that is

$$
\begin{aligned}
&d^{(n)}_{12223}=d^{(n-1)}_{12223}+3\times 2^{n-1},\ d^{(n)}_{22231}=d^{(n-1)}_{22231}+6\times 2^{n-1},\\
&d^{(n)}_{22232}=d^{(n-1)}_{22232}+12\times 2^{n-1},\ d^{(n)}_{22322}=d^{(n-1)}_{22322}+15\times 2^{n-1},\\
&d^{(n)}_{23223}=d^{(n-1)}_{23223}+12\times 2^{n-1},\ d^{(n)}_{13223}=d^{(n-1)}_{13223}+6\times 2^{n-1},\\
&d^{(n)}_{32223}=d^{(n-1)}_{32223}+3\times 2^{n-1}
\end{aligned}
$$

and for any $(i_1 i_2 i_3 i_4 i_5)\neq(12223),(22231),(22232),(22322),(23223)$,(13223), (32223), we have $d^{(n)}_{i_1 i_2 i_3 i_4 i_5}=0$.

Thus,

$$
\begin{aligned}
&{}^4\chi(PD_1[n]) = {}^4\chi(PD_1[n-1])+\\
&(\frac{3}{\sqrt{1\times 2\times 2\times 2\times 3}}+\frac{6}{\sqrt{2\times 2\times 2\times 3\times 1}}\\
&+\frac{12}{\sqrt{2\times 2\times 2\times 3\times 2}}+\frac{15}{\sqrt{2\times 2\times 3\times 2\times 2}}\\
&+\frac{12}{\sqrt{2\times 3\times 2\times 2\times 3}}+\frac{6}{\sqrt{1\times 3\times 2\times 2\times 3}}
\end{aligned}
$$

$$+\frac{3}{\sqrt{3\times2\times2\times2\times3}})\times 2^{n-1}$$

$$= {}^4\chi(PD_1[n-1]) + \frac{1}{8}(5\sqrt{2}+9\sqrt{3}+3\sqrt{6}+4)\times 2^n$$

$$= {}^4\chi(PD_1[n-2]) + \frac{1}{8}(5\sqrt{2}+9\sqrt{3}+3\sqrt{6}+4)(2^n+2^{n-1})$$

$$\vdots$$

$$= {}^4\chi(PD_1[0]) + \frac{1}{8}(5\sqrt{2}+9\sqrt{3}+3\sqrt{6}+4)(2^n+2^{n-1}+\ldots+2^2+2)$$

Hence,

$${}^4\chi(PD_1[n]) = \frac{1}{4}[(3\sqrt{2}+3\sqrt{3}+2\sqrt{6}+2) + (5\sqrt{2}+9\sqrt{3}+3\sqrt{6}+4)(2^n-1)]$$

The proof is now complete.

CONCLUSION

In this paper, we have discussed the 2-order, 3-order and 4-order connectivity indices of the PAMAM dendrimers. We believe that the results in this paper can be extended to the study of *m*-order connectivity index of PAMAM dendrimers where *m* ≥ 5. Another direction is to investigate the *m*-order connectivity index of PAMAM dendrimers and other families of dendrimers, in general.

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