Fourth order and fourth sum connectivity indices of tetrathiafulvalene dendrimers

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ABSTRACT

The *m*-order connectivity index ${}^m\chi(G)$ of a graph G is

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

where $d_{i_1} d_{i_2} \ldots d_{i_{m+1}}$ runs over all paths of length *m* in G and d_i denotes the degree of vertex v_i. Also,

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

is its *m*-sum connectivity index. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this paper, the 4-order connectivity and 4-sum connectivity indices of tetrathiafulvalene dendrimers are computed.

Keywords: 4-order connectivity index; 4-sum connectivity index; Dendrimer; Graph.

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.

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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. Randić (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 (Trinajastić, 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

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

where $i_1 \ldots i_{m+1}$ (for simplicity) runs over all paths of length m in G and d_i denote the degree of vertex v_i. In particular, 4-order connectivity index is defined as follows:

$$^{4}\chi(G) = \sum_{i_1 \ldots i_5} \frac{1}{\sqrt{d_{i_1} d_{i_2} d_{i_3} d_{i_4} d_{i_5}}}.$$

Recently, a closely related variant of the Randić connectivity index called the sum-connectivity index was introduced by Zhou and Trinajstić [10,11]. For a simple connected graph G, its sum-connectivity index $X(G)$ is defined as the sum over all edges of the graph of the terms $(d_u + d_v)^{-1/2}$, that is

$$^{s}X(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}$$

where d_u and d_v are the degrees of the vertices *u* and *v*, respectively. It is a graph-based molecular structure descriptor. It has been found that the sum-connectivity index correlates well with π-electronic energy of benzenoid hydrocarbons, and it is frequently applied in quantitative structure property and structure-activity studies [4,7].

The *m*-sum connectivity index of *G* is defined as

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

where $i_1 i_2 \ldots i_{m+1}$ runs over all paths of length m in G. In particular, 4-sum connectivity index are defined as

$$^{4s}X(G) = \sum_{i_1 \ldots i_5} \frac{1}{\sqrt{d_{i_1} + d_{i_2} + d_{i_3} + d_{i_4} + d_{i5}}}.$$

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 index of some dendrimer nanostars, where *m* = 2 and 3, see [1,2,3,5,8,9].

In Section 2, the 4-connectivity index of an infinite family of tetrathiafulvalene dendrimers is computed. The 4-sum connectivity index of this family of dendrimers is studied in Section 3.

2. FOURTH-ORDER CONNECTIVITY INDEX OF DENDRIMER

In recent research in mathematical chemistry, particular attention is paid to distance-based graph invariants. In this section, we will study the 4-order connectivity index of some infinite family of dendrimers. We consider tetrathiafulvalene dendrimer by construction of dendrimer generations G_n has grown *n* stages. We denote this graph by $TD_2[n]$. Figure 1 shows the generations G_2 has grown 2 stages.

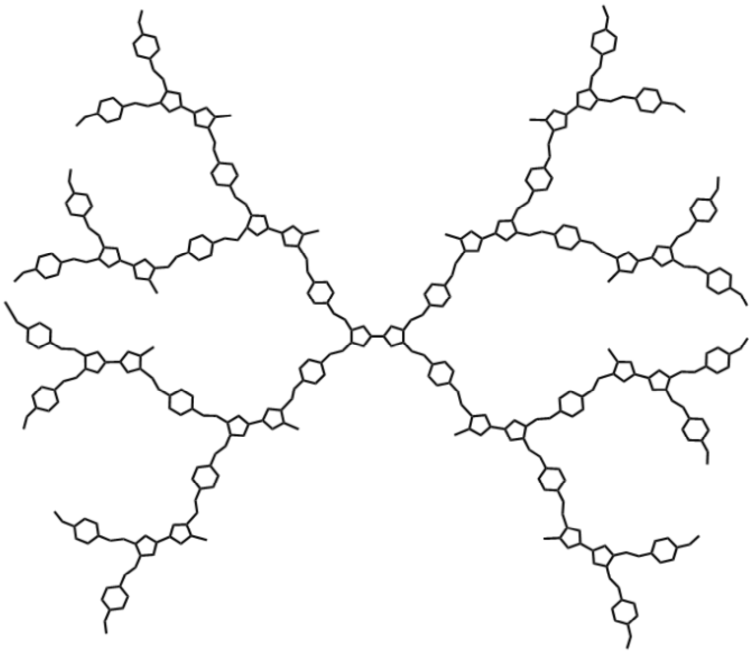

Figure 1. Tetrathiafulvalene Dendrimer of Generations G_n has Grown 2 Stages, $TD_2[2]$.

Now we give our main results.

Theorem 1. Let $n \in N_0$. The fourth-order connectivity index of $TD_2[n]$ is

$$^4\chi(TD_2[n]) = \begin{cases} \frac{1}{9}\left(47\sqrt{2}+27\sqrt{3}+6\sqrt{6}\right) & if\ n=0 \\ \frac{1}{9}\left[\left(47\sqrt{2}+27\sqrt{3}+6\sqrt{6}\right)+\left(58\sqrt{2}+42\sqrt{3}+5\sqrt{6}+6\right)\left(2^{n+1}-2\right)\right] & if\ n \geq 1 \end{cases}.$$

Proof. Note that the core of this structure means that the number of stage equal to zero. First, we compute $^4\chi(TD_2[0])$. 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 $d^{(n)}_{i_1i_2i_3i_4i_5}$ to mean $d_{i_1i_2i_3i_4i_5}$ in $n-th$ stages. Particularly, $d^{(n)}_{i_1i_2i_3i_4i_5} = d^{(n)}_{i_5i_4i_3i_2i_1}$.

When n = 0, we have

$$d^{(0)}_{12322}=8,\ d^{(0)}_{23223}=44,\ d^{(0)}_{22322}=16,\ d^{(0)}_{32233}=4,\ d^{(0)}_{22323}=4,\ d^{(0)}_{22332}=8,\ d^{(0)}_{23233}=8,\ d^{(0)}_{23232}=4,$$

$$d^{(0)}_{32332}=16,\ d^{(0)}_{32323}=2,\ d^{(0)}_{33233}=4.$$

Therefore, we have

$$^{4}\chi(TD_2[0]) = \frac{8}{\sqrt{1\times2\times3\times2\times2}} + \frac{44}{\sqrt{2\times3\times2\times2\times3}} + \frac{16}{\sqrt{2\times2\times3\times2\times2}} +$$

$$\frac{4}{\sqrt{3\times2\times2\times3\times3}} + \frac{4}{\sqrt{2\times2\times3\times2\times3}} + \frac{8}{\sqrt{2\times2\times3\times3\times2}}$$

$$\frac{8}{\sqrt{2\times3\times2\times3\times3}} + \frac{4}{\sqrt{2\times3\times2\times3\times2}} + \frac{16}{\sqrt{3\times2\times3\times3\times2}} \ \frac{2}{\sqrt{3\times2\times3\times2\times3}} +$$

$$\frac{4}{\sqrt{3\times3\times2\times3\times3}}$$

$$= \frac{1}{9}(47\sqrt{2} + 27\sqrt{3} + 6\sqrt{6})$$

Now, we construct the relation between $^{4}\chi(TD_2[n])$ and $^{4}\chi(TD_2[n-1])$ for $n \geq 1$.

By simple reduction, we have

$d_{12322}^{(n)} = d_{12322}^{(n-1)} + 4\times2^{n}$, $d_{23223}^{(n)} = d_{23223}^{(n-1)} + 50\times2^{n}$, $d_{22322}^{(n)} = d_{22322}^{(n-1)} + 20\times2^{n}$, $d_{32233}^{(n)} = d_{32233}^{(n-1)} + 6\times2^{n}$, $d_{22323}^{(n)} = d_{22323}^{(n-1)} + 6\times2^{n}$, $d_{22332}^{(n)} = d_{22332}^{(n-1)} + 10\times2^{n}$, $d_{23233}^{(n)} = d_{23233}^{(n-1)} + 14\times2^{n}$, $d_{23232}^{(n)} = d_{23232}^{(n-1)} + 6\times2^{n}$, $d_{32332}^{(n)} = d_{32332}^{(n-1)} + 30\times2^{n}$, $d_{32323}^{(n)} = d_{32323}^{(n-1)} + 4\times2^{n}$, $d_{33233}^{(n)} = d_{33233}^{(n-1)} + 8\times2^{n}$, $d_{13233}^{(n)} = d_{13233}^{(n-1)} + 2\times2^{n}$, $d_{13232}^{(n)} = d_{13232}^{(n-1)} + 2\times2^{n}$, $d_{13323}^{(n)} = d_{13323}^{(n-1)} + 2\times2^{n}$, $d_{13322}^{(n)} = d_{13322}^{(n-1)} + 2\times2^{n}$,

and for any

$(i_1 i_2 i_3 i_4 i_5) \neq (12322), (23223), (22322), (32233), (22323), (22332), (23233), (23232), (32332), (32323), (33233), (13233), (13232), (13323), (13322)$, we have $d_{i_1 i_2 i_3 i_4 i_5}^{(n)} = 0$.

Therefore,

$$^{4}\chi(TD_4[n]) = {}^{4}\chi(TD_2[n-1]) + \frac{4\times2^{n}}{\sqrt{1\times2\times3\times2\times2}} + \frac{50\times2^{n}}{\sqrt{2\times3\times2\times2\times3}} +$$

$$\frac{20\times2^{n}}{\sqrt{2\times2\times3\times2\times2}} + \frac{6\times2^{n}}{\sqrt{3\times2\times2\times3\times3}} +$$

$$\frac{6\times2^{n}}{\sqrt{2\times2\times3\times2\times3}} + \frac{10\times2^{n}}{\sqrt{2\times2\times3\times3\times2}} + \frac{14\times2^{n}}{\sqrt{2\times3\times2\times3\times3}} +$$

$$\frac{6\times 2^n}{\sqrt{2\times 3\times 2\times 3\times 2}}+\frac{30\times 2^n}{\sqrt{3\times 2\times 3\times 3\times 2}}+\frac{4\times 2^n}{\sqrt{3\times 2\times 3\times 2\times 3}}+\frac{8\times 2^n}{\sqrt{3\times 3\times 2\times 3\times 3}}+$$

$$\frac{2\times 2^n}{\sqrt{1\times 3\times 2\times 3\times 3}}+\frac{2\times 2^n}{\sqrt{1\times 3\times 2\times 3\times 2}}+\frac{2\times 2^n}{\sqrt{1\times 3\times 3\times 2\times 3}}+\frac{2\times 2^n}{\sqrt{1\times 3\times 3\times 2\times 2}}$$

$$= {}^4\chi(TD_2[n-1])+\frac{1}{9}(58\sqrt{2}+42\sqrt{3}+5\sqrt{6}+6)\times 2^n.$$

From the above recursion formula, we have

$$\begin{aligned}{}^4\chi(TD_2[n]) &= {}^4\chi(TD_2[n-1])+\frac{1}{9}(58\sqrt{2}+42\sqrt{3}+5\sqrt{6}+6)\times 2^n\\ &= {}^4\chi(TD_2[n-2])+\frac{1}{9}(58\sqrt{2}+42\sqrt{3}+5\sqrt{6}+6)(2^n+2^{n-1})\\ &\ \vdots\\ &= {}^4\chi(TD_2[0])+\frac{1}{9}(58\sqrt{2}+42\sqrt{3}+5\sqrt{6}+6)(2^n+2^{n-1}+\ldots+2^2+2)\\ &=\frac{1}{9}[(47\sqrt{2}+27\sqrt{3}+6\sqrt{6})+(58\sqrt{2}+42\sqrt{3}+5\sqrt{6}+6)(2^n+2^{n-1}+\ldots+2^2+2)]\end{aligned}$$

Therefore,

$${}^4\chi(TD_2[n])=\frac{1}{9}[(47\sqrt{2}+27\sqrt{3}+6\sqrt{6})+(58\sqrt{2}+42\sqrt{3}+5\sqrt{6}+6)(2^{n+1}-2)].$$

The proof is now complete. □

3. FOURTH-SUM CONNECTIVITY INDEX OF DENDRIMER

In this section, we shall compute the 4-sum connectivity index of the same family of dendrimer as shown in Figure 1.

Theorem 2. Let $n \in N_0$. The fourth-sum connectivity index of $TD_2[n]$ is

$$ {}^{4s}\chi(TD_2[n]) = \begin{cases} \frac{4}{5}\sqrt{10}+\frac{16}{11}\sqrt{11}+5\sqrt{12}+\frac{30}{13}\sqrt{13}+\frac{2}{7}\sqrt{14} & if\ n=0; \\ (\frac{4}{5}\sqrt{10}+\frac{16}{11}\sqrt{11}+5\sqrt{12}+\frac{30}{13}\sqrt{13}+\frac{2}{7}\sqrt{14}\ ) & if\ \ n\geq 1. \\ +(\frac{2}{5}\sqrt{10}+\frac{24}{11}\sqrt{11}+\frac{19}{3}\sqrt{12}+\frac{54}{13}\sqrt{13}+\frac{4}{7}\sqrt{14}\ )(2^n-2) & \end{cases} $$

Proof. Firstly we compute ${}^{4s}\chi(TD_2[0])$. 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. In the same way, we use $d^{(n)}_{i_1i_2i_3i_4i_5}$ to mean $d_{i_1i_2i_3i_4i_5}$ in $n-th$ stages. Particularly, $d^{(n)}_{i_1i_2i_3i_4i_5} = d^{(n)}_{i_5i_4i_3i_2i_1}$. When $n = 0$, we obtain

$d^{(0)}_{12322} = 8$, $d^{(0)}_{23223} = 44$, $d^{(0)}_{22322} = 16$, $d^{(0)}_{32233} = 4$, $d^{(0)}_{22323} = 4$, $d^{(0)}_{22332} = 8$, $d^{(0)}_{23233} = 8$, $d^{(0)}_{23232} = 4$, $d^{(0)}_{32332} = 16$, $d^{(0)}_{32323} = 2$, $d^{(0)}_{33233} = 4$. Therefore, we have

$$ {}^{4s}\chi(TD_2[0]) = \frac{8}{\sqrt{1+2+3+2+2}} + \frac{44}{\sqrt{2+3+2+2+3}} + \frac{16}{\sqrt{2+2+3+2+2}} + $$

$$ \frac{4}{\sqrt{3+2+2+3+3}} + \frac{4}{\sqrt{2+2+3+2+3}} + \frac{8}{\sqrt{2+2+3+3+2}} $$

$$ \frac{8}{\sqrt{2+3+2+3+3}} + \frac{4}{\sqrt{2+3+2+3+2}} + \frac{16}{\sqrt{3+2+3+3+2}} \ \frac{2}{\sqrt{3+2+3+2+3}} + $$

$$ \frac{4}{\sqrt{3+3+2+3+3}} = \frac{4}{5}\sqrt{10}+\frac{16}{11}\sqrt{11}+5\sqrt{12}+\frac{30}{13}\sqrt{13}+\frac{2}{7}\sqrt{14}. $$

Then, similar to that of Theorem 1, we compute ${}^{4s}\chi(TD_2[n])$. The relation between $d^{(n)}_{i_1i_2i_3i_4i_5}$ and $d^{(n-1)}_{i_1i_2i_3i_4i_5}$ for $n \geq 1$ is

$d^{(n)}_{12322} = d^{(n-1)}_{12322} + 4\times 2^n$, $d^{(n)}_{23223} = d^{(n-1)}_{23223} + 50\times 2^n$, $d^{(n)}_{22322} = d^{(n-1)}_{22322} + 20\times 2^n$, $d^{(n)}_{32233} = d^{(n-1)}_{32233} + 6\times 2^n$, $d^{(n)}_{22323} = d^{(n-1)}_{22323} + 6\times 2^n$, $d^{(n)}_{22332} = d^{(n-1)}_{22332} + 10\times 2^n$, $d^{(n)}_{23233} = d^{(n-1)}_{23233} + 14\times 2^n$, $d^{(n)}_{23232} = d^{(n-1)}_{23232} + 6\times 2^n$, $d^{(n)}_{32332} = d^{(n-1)}_{32332} + 30\times 2^n$, $d^{(n)}_{32323} = d^{(n-1)}_{32323} + 4\times 2^n$, $d^{(n)}_{33233} = d^{(n-1)}_{33233} + 8\times 2^n$, $d^{(n)}_{13233} = d^{(n-1)}_{13233} + 2\times 2^n$, $d^{(n)}_{13232} = d^{(n-1)}_{13232} + 2\times 2^n$, $d^{(n)}_{13323} = d^{(n-1)}_{13323} + 2\times 2^n$, $d^{(n)}_{13322} = d^{(n-1)}_{13322} + 2\times 2^n$

and for any

$(i_1i_2i_3i_4i_5) \neq (12322), (23223), (22322), (32233), (22323), (22332), (23233), (23232), (32332), (32323), (33233), (13233), (13232), (13323), (13322)$, we have $d^{(n)}_{i_1i_2i_3i_4i_5} = 0$.

Therefore,

$$
\begin{aligned}
{}^{4s}\chi(TD_4[n]) &= {}^{4s}\chi(TD_2[n-1]) + \frac{4\times 2^n}{\sqrt{1+2+3+2+2}} + \frac{50\times 2^n}{\sqrt{2+3+2+2+3}} + \\
&\frac{20\times 2^n}{\sqrt{2+2+3+2+2}} + \frac{6\times 2^n}{\sqrt{3+2+2+3+3}} + \\
&\frac{6\times 2^n}{\sqrt{2+2+3+2+3}} + \frac{10\times 2^n}{\sqrt{2+2+3+3+2}} + \frac{14\times 2^n}{\sqrt{2+3+2+3+3}} + \\
&\frac{6\times 2^n}{\sqrt{2+3+2+3+2}} + \frac{30\times 2^n}{\sqrt{3+2+3+3+2}} + \frac{4\times 2^n}{\sqrt{3+2+3+2+3}} + \frac{8\times 2^n}{\sqrt{3+3+2+3+3}} + \\
&\frac{2\times 2^n}{\sqrt{1+3+2+3+3}} + \frac{2\times 2^n}{\sqrt{1+3+2+3+2}} + \frac{2\times 2^n}{\sqrt{1+3+3+2+3}} + \frac{2\times 2^n}{\sqrt{1+3+3+2+2}} \\
&= {}^{4s}\chi(TD_2[n-1]) + (\frac{2}{5}\sqrt{10} + \frac{24}{11}\sqrt{11} + \frac{19}{3}\sqrt{12} + \frac{54}{13}\sqrt{13} + \frac{4}{7}\sqrt{14})\times 2^n.
\end{aligned}
$$

From the above recursion formula, we obtain

$$
\begin{aligned}
{}^{4s}\chi(TD_2[n]) &= {}^{4s}\chi(TD_2[n-1]) + (\frac{2}{5}\sqrt{10} + \frac{24}{11}\sqrt{11} + \frac{19}{3}\sqrt{12} + \frac{54}{13}\sqrt{13} + \frac{4}{7}\sqrt{14})\times 2^n. \\
&= {}^{4s}\chi(TD_2[n-2]) + (\frac{2}{5}\sqrt{10} + \frac{24}{11}\sqrt{11} + \frac{19}{3}\sqrt{12} + \frac{54}{13}\sqrt{13} + \frac{4}{7}\sqrt{14})(2^n + 2^{n-1}) \\
&\vdots \\
&= {}^{4s}\chi(TD_2[0]) + (\frac{2}{5}\sqrt{10} + \frac{24}{11}\sqrt{11} + \frac{19}{3}\sqrt{12} + \frac{54}{13}\sqrt{13} + \frac{4}{7}\sqrt{14})\ (2^n + 2^{n-1} + \ldots + 2^2 + 2)
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
{}^{4s}\chi(TD_2[n]) &= (\frac{4}{5}\sqrt{10} + \frac{16}{11}\sqrt{11} + 5\sqrt{12} + \frac{30}{13}\sqrt{13} + \frac{2}{7}\sqrt{14}) + \\
&(\frac{2}{5}\sqrt{10} + \frac{24}{11}\sqrt{11} + \frac{19}{3}\sqrt{12} + \frac{54}{13}\sqrt{13} + \frac{4}{7}\sqrt{14})(2^n - 2)
\end{aligned}
$$

The proof is now complete. □

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