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Third Order and Third Sum Connectivity Indices of Tetrathiafulvalene Dendrimers

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Abstract: The *m*-order connectivity index ${}^m\chi(G)$ of a graph G is ${}^m\chi(G) = \sum_{v_{i_1}v_{i_2}\dots v_{i_{m+1}}} \frac{1}{\sqrt{d_{i_1}d_{i_2}\dots d_{i_{m+1}}}}$, where $d_{i_1}d_{i_2}\dots d_{i_{m+1}}$ runs over all paths of length *m* in G and d_i denotes the degree of vertex v_i. Also ${}^{ms}X(G) = \sum_{v_{i_1}v_{i_2}\dots v_{i_{m+1}}} \frac{1}{\sqrt{d_{i_1}+d_{i_2}+\dots+d_{i_{m+1}}}}$ its m -sum connectivity index. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this paper, we will study 3-order connectivity and 3-sum connectivity indices of an infinite family of tetrathiafulvalene dendrimer .

Key words:

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.

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. Randic (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 (Trinajastic, 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

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

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. In particular, 3-order connectivity index is defined as follows:

$$ {}^3\chi(G) = \sum_{i_1i_2i_3i_4} \frac{1}{\sqrt{d_{i_1}d_{i_2}d_{i_3}d_{i4}}} $$

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Recently, a closely related variant of the Randić connectivity index called the sum-connectivity index was introduced by Zhou and Trinajstic [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

$$^{s}X(G) = \sum_{u,v} \frac{1}{\sqrt{d_u + d_v}},$$

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 [4,8].
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 $i_1 ... i_{m+1}$ runs over all paths of length m in G. In particular, 3-sum connectivity index are defined as

$$^{3s}X(G) = \sum_{i_1 i_2 i_3 i_4} \frac{1}{\sqrt{d_{i_1} + d_{i_2} + d_{i_3} + d_{i_4}}}$$

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 and sum connectivity index of some dendrimer nanostars, where *m* = 2 and 3 (see [1,2,3,5,7,9]).

In Sections 2 and 3, we study the 3-order and the 3-sum connectivity indices of an infinite family of tetrathiafulvalene dendrimers, respectively.

2. *Third-Order Connectivity Index of Dendrimer* $TD_2[n]$:

In this section, we will study the 3-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.

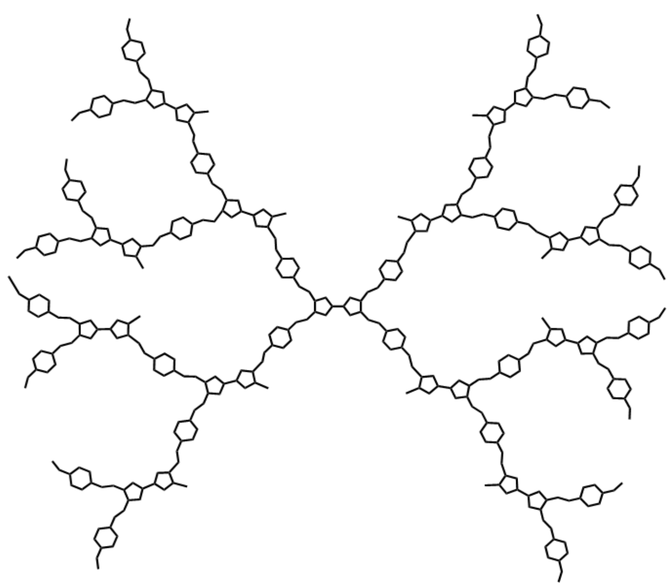

Fig. 1: Tetrathiafulvalene dendrimer of generations G_n has grown 2 stages, $TD_2[2]$

Now we give our main results.

Theorem 1. Let $n \in N_0$. The third-order connectivity index of $TD_2[n]$ is computed as follows

$$^3\chi(TD_2[n]) = \begin{cases} \frac{1}{18}(24\sqrt{3}+74\sqrt{6}+108), & if\ n=0; \\ \frac{1}{18}[(24\sqrt{3}+74\sqrt{6}+108)+(18\sqrt{2}+12\sqrt{3}+91\sqrt{6}+162)(2^{n+1}-2)], & if\ n \geq 1. \end{cases}$$

Proof. Note that the core of the structure that means the number of stage equal to zero. Firstly, we compute $^3\chi(TD_2[0])$. Let $d_{i_1i_2i_3i_4}$ denote the number of 3-paths whose three consecutive vertices are of degree i_1, i_2, i_3, i_4 respectively . By the same way, we use $d^{(n)}_{i_1i_2i_3i_4}$ to mean $d_{i_1i_2i_3i_4}$ in $n-th$ stages. Particularly, $d^{(n)}_{i_1i_2i_3i_4} = d^{(n)}_{i_4i_3i_2i_1}$.

It is easy to see that

$$d^{(0)}_{1232} = 8,\ d^{(0)}_{2232} = 44,\ d^{(0)}_{2233} = 4,\ d^{(0)}_{2323} = 8,\ d^{(0)}_{2332} = 12,\ d^{(0)}_{3223} = 12,\ d^{(0)}_{3233} = 8.$$

Therefore,

$$\begin{aligned} ^3\chi(TD_2[0]) &= \frac{8}{\sqrt{1\times2\times3\times2}} + \frac{44}{\sqrt{2\times2\times3\times2}} + \frac{4}{\sqrt{2\times2\times3\times3}} + \frac{8}{\sqrt{2\times3\times2\times3}} + \frac{12}{\sqrt{2\times3\times3\times2}} \\ &+ \frac{12}{\sqrt{3\times2\times2\times3}} + \frac{8}{\sqrt{3\times2\times3\times3}} \\ &= \frac{1}{18}(24\sqrt{3}+74\sqrt{6}+108). \end{aligned}$$

Secondly, we construct the relation between $^3\chi(TD_2[n])$ and $^3\chi(TD_2[n-1])$ for $n \geq 1$.
By simple reduction, we obtain

$$d^{(n)}_{1232} = d^{(n-1)}_{1232} + 4\times2^n,\ d^{(n)}_{1323} = d^{(n-1)}_{1323} + 2\times2^n,\ d^{(n)}_{1332} = d^{(n-1)}_{1332} + 4\times2^n,\ d^{(n)}_{2232} = d^{(n-1)}_{2232} + 50\times2^n,$$
$$d^{(n)}_{2233} = d^{(n-1)}_{2233} + 6\times2^n,\ d^{(n)}_{2323} = d^{(n-1)}_{2323} + 14\times2^n,\ d^{(n)}_{2332} = d^{(n-1)}_{2332} + 20\times2^n,\ d^{(n)}_{3223} = d^{(n-1)}_{3223} + 14\times2^n,$$
$$d^{(n)}_{3233} = d^{(n-1)}_{3233} + 16\times2^n,$$

and for any $(i_1i_2i_3i_4) \neq (1232), (1323), (1332), (2232), (2233), (2323), (2332), (3223), (3233)$, we have $d^{(n)}_{i_1i_2i_3i_4} = 0$.

Therefore

$$\begin{aligned} ^3\chi(TD_2[n]) &= {}^3\chi(TD_2[n-1]) + \Big(\frac{4}{\sqrt{1\times2\times3\times2}} + \frac{2}{\sqrt{1\times3\times2\times3}} + \frac{4}{\sqrt{1\times3\times3\times2}} \\ &+ \frac{50}{\sqrt{2\times2\times3\times2}} + \frac{6}{\sqrt{2\times2\times3\times3}} + \frac{14}{\sqrt{2\times3\times2\times3}} + \frac{20}{\sqrt{2\times3\times3\times2}} \\ &+ \frac{14}{\sqrt{3\times2\times2\times3}} + \frac{16}{\sqrt{3\times2\times3\times3}}\Big)\times2^n \\ &= {}^3\chi(TD_2[n-1]) + \frac{1}{18}(18\sqrt{2}+12\sqrt{3}+91\sqrt{6}+162)\times2^n. \end{aligned}$$

From the above recursion formula, we have

$$^3\chi(TD_2[n]) = {}^3\chi(TD_2[n-1]) + \frac{1}{18}(18\sqrt{2}+12\sqrt{3}+91\sqrt{6}+162)\times2^n$$

$$= {}^{3}\chi(TD_2[n-2]) + \frac{1}{18}(18\sqrt{2} + 12\sqrt{3} + 91\sqrt{6} + 162)(2^n + 2^{n-1})$$
$$\vdots$$
$$= {}^{3}\chi(TD_2[0]) + \frac{1}{18}(18\sqrt{2} + 12\sqrt{3} + 91\sqrt{6} + 162)(2^n + 2^{n-1} + ... + 2^2 + 2).$$

Therefore,

$${}^{3}\chi(TD_2[n]) = \frac{1}{18}[(24\sqrt{3} + 74\sqrt{6} + 108) + (18\sqrt{2} + 12\sqrt{3} + 91\sqrt{6} + 162)(2^{n+1} - 2)].$$

The proof is now complete.

3. *Third-Sum Connectivity Index of Dendrimer* $TD_2[n]$:

In this section, we will study the 3-sum connectivity index of the same family of dendrimers as shown in Figure 1.

Theorem 2. Let $n \in \mathrm{N}_0$. The third-sum connectivity index of $TD_2[n]$ is

$${}^{3s}\chi(TD_2[n]) = \begin{cases} \frac{1}{165}(165\sqrt{8}+594\sqrt{10}+120\sqrt{11}+2420), \ if \ n = 0; \\ \frac{1}{165}[(165\sqrt{8}+594\sqrt{10}+120\sqrt{11}+2420)+(165\sqrt{8}+1782\sqrt{10}+480\sqrt{11}+6160)(2^n-1)], \ if \ n \geq 1. \end{cases}$$

Proof. We first compute ${}^{3s}\chi(TD_2[0])$. Let $d_{i_1i_2i_3i_4}$ denote the number of 3-paths whose three consecutive vertices are of degree i_1, i_2, i_3, i_4 respectively . Similarly we use $d^{(n)}_{i_1i_2i_3i_4}$ to mean $d_{i_1i_2i_3i_4}$ in $n-th$ stages. Particularly, $d^{(n)}_{i_1i_2i_3i_4} = d^{(n)}_{i_4i_3i_2i_1}$.
It is easy to see that

$$d^{(0)}_{1232} = 8,\ d^{(0)}_{2232} = 44,\ d^{(0)}_{2233} = 4,\ d^{(0)}_{2323} = 8,\ d^{(0)}_{2332} = 12,\ d^{(0)}_{3223} = 12,\ d^{(0)}_{3233} = 8.$$

Therefore,

$$\begin{aligned} {}^{3s}\chi(TD_2[0]) = & \frac{8}{\sqrt{1+2+3+2}} + \frac{44}{\sqrt{2+2+3+2}} + \frac{4}{\sqrt{2+2+3+3}} + \frac{8}{\sqrt{2+3+2+3}} + \frac{12}{\sqrt{2+3+3+2}} \\ & + \frac{12}{\sqrt{3+2+2+3}} + \frac{8}{\sqrt{3+2+3+3}} \\ & = \frac{1}{165}(165\sqrt{8} + 594\sqrt{10} + 120\sqrt{11} + 2420). \end{aligned}$$

By using the same way in Theorem 1, we can find the relation between ${}^{3s}X(TD_2[n])$ and ${}^{3s}X(TD_2[n-1])$ for $n \geq 1$.

Now we have

$d^{(n)}_{1232} = d^{(n-1)}_{1232} + 4\times 2^n$, $d^{(n)}_{1323} = d^{(n-1)}_{1323} + 2\times 2^n$, $d^{(n)}_{1332} = d^{(n-1)}_{1332} + 4\times 2^n$, $d^{(n)}_{2232} = d^{(n-1)}_{2232} + 50\times 2^n$,
$d^{(n)}_{2233} = d^{(n-1)}_{2233} + 6\times 2^n$, $d^{(n)}_{2323} = d^{(n-1)}_{2323} + 14\times 2^n$, $d^{(n)}_{2332} = d^{(n-1)}_{2332} + 20\times 2^n$, $d^{(n)}_{3223} = d^{(n-1)}_{3223} + 14\times 2^n$,
$d^{(n)}_{3233} = d^{(n-1)}_{3233} + 16\times 2^n$,
and for any $(i_1i_2i_3i_4) \neq (1232),(1323),(1332),(2232),(2233),(2323),(2332),(3223),(3233)$, we have $d^{(n)}_{i_1i_2i_3i_4} = 0$.

Therefore,

$$
\begin{aligned}
{}^{3s}\chi(TD_2[n]) = {}^{3s}\chi(TD_2[n-1]) + (&\frac{4}{\sqrt{1+2+3+2}} + \frac{2}{\sqrt{1+3+2+3}} + \frac{4}{\sqrt{1+3+3+2}} \\
&+ \frac{50}{\sqrt{2+2+3+2}} + \frac{6}{\sqrt{2+2+3+3}} + \frac{14}{\sqrt{2+3+2+3}} + \frac{20}{\sqrt{2+3+3+2}} \\
&+ \frac{14}{\sqrt{3+2+2+3}} + \frac{16}{\sqrt{3+2+3+3}}) \times 2^n \\
= {}^{3s}\chi(TD_2[n-1]) + &\frac{1}{330}(165\sqrt{8} + 1782\sqrt{10} + 480\sqrt{11} + 6160) \times 2^n.
\end{aligned}
$$

From the above recursion formula, we have

$$
\begin{aligned}
{}^{3s}\chi(TD_2[n]) &= {}^{3s}\chi(TD_2[n-1]) + \frac{1}{330}(165\sqrt{8} + 1782\sqrt{10} + 480\sqrt{11} + 6160) \times 2^n \\
&= {}^{3s}\chi(TD_2[n-2]) + \frac{1}{330}(165\sqrt{8} + 1782\sqrt{10} + 480\sqrt{11} + 6160)(2^n + 2^{n-1}) \\
&\vdots \\
&= {}^{3s}\chi(TD_2[0]) + \frac{1}{330}(165\sqrt{8} + 1782\sqrt{10} + 480\sqrt{11} + 6160)(2^n + 2^{n-1} + \ldots + 2^2 + 2) \\
&= \frac{1}{165}[(165\sqrt{8} + 594\sqrt{10} + 120\sqrt{11} + 2420) + \\
&\quad \frac{1}{2}(165\sqrt{8} + 1782\sqrt{10} + 480\sqrt{11} + 6160)(2^{n+1} - 2)].
\end{aligned}
$$

Hence, we obtain

$$
\begin{aligned}
{}^{3s}\chi(TD_2[n]) = &\frac{1}{165}[(165\sqrt{8} + 594\sqrt{10} + 120\sqrt{11} + 2420) + \\
&(165\sqrt{8} + 1782\sqrt{10} + 480\sqrt{11} + 6160)(2^n - 1)].
\end{aligned}
$$

The proof is now complete.

4. Conclusion:

In this paper, we have discussed the 3-order and 3-sum connectivity indices of tetrathiafulvalene dendrimers. We believe the technique used in this paper can be extended to study the connectivity indices of other families of dendrimers as well. In our next paper, we will determine the 4-order and 4-sum connectivity indices of tetrathiafulvalene dendrimers.

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