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SECOND ORDER AND SECOND SUM CONNECTIVITY INDICES OF TETRATHIAFULVALENE DENDRIMERS

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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 in G. The m* -sum connectivity index changes the multiplication with addition, in the above index. A dendrimer is a hyperbranched molecule built up from branched units called monomers. In this paper, the 2-order connectivity and 2-sum connectivity indices of an infinite family of tetrathiafulvalene dendrimer are computed.

Key words: *Randic connectivity index, Sum-connectivity index, Dendrimers.*

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 molecule 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 worthy in practical application, the connectivity index (Randic, 1975) being one of them [1]. This index has been used in predicting physico-chemical properties such as boiling point and solubility partition. The molecular connectivity index χ is related to the branching of molecules. Next, Kier and Hall (1986) extended this to higher orders and introduced modifications to account for heteroatoms [2].

Molecular connectivity indices are the most popular topological indices (Trinajastic, 1992), used in predicting physicochemical properties such as boiling point, solubility partition, coefficient etc, (Murray et al., 1975; Kier and Hall, 1976) or biological activities (Kier et al., 1975; Kier and Murray, 1975) [2].

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Let *G* be a simple connected graph of order *n*. For an integer *m* ≥ 1, the *m*-order connectivity index of the graph *G* associated to a covalently bonded molecule 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 $i_1 \ldots i_{m+1}$ runs over all paths of length m in *G* and d_i denotes the degree of vertex v_i. In particular, the 2-order connectivity index is defined as follows:

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

Recently, a variant of the Randić connectivity index, called the sum-connectivity index was introduced by Zhou and Trinajstic [3,4]. 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 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 QSPR and structure-activity QSAR studies [2,5].

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, the 2-sum connectivity index is defined as

$$^{2s}X(G)=\sum_{i_1 i_2 i_3}\frac{1}{\sqrt{d_{i_1}+d_{i_2}+d_{i_3}}}.$$

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 the *m*-order connectivity index and *m*-sum connectivity index in some dendrimer nanostars, where *m* = 2 and 3 (see [6,7,8,9,10]).

In this paper, we shall study the 2-connectivity and 2-sum connectivity indices of an infinite family of tetrathiafulvalene dendrimers.

RESULTS AND DISCUSSIONS

In this section, we first study the 2-order connectivity index of some infinite family of dendrimers. We consider the tetrathiafulvalene dendrimer of generation G_n (i.e. grown in *n* stages). We denote this graph by $TD_2[n]$. Figure 1 shows the generation G_2 dendrimer.

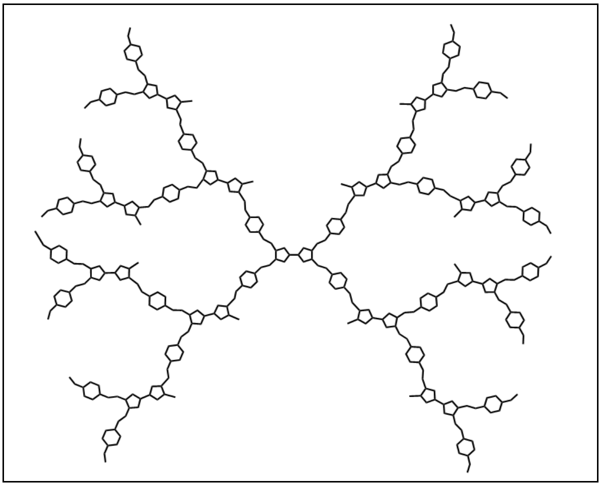

Figure 1. Tetrathiafulvalene dendrimer of generation G_n: n=2, symbolized $TD_2[2]$

We can now give our main results.

Theorem 1. Let $n \in \mathrm{N}_0$. The second-order connectivity index of $TD_2[n]$ is computed as follows

$$^{2}\chi(TD_2[n]) = \begin{cases} \frac{1}{3}(8\sqrt{2}+27\sqrt{3}+2\sqrt{6}), & if\ n = 0; \\ \frac{1}{3}(8\sqrt{2}+27\sqrt{3}+2\sqrt{6})+\frac{1}{3}(15\sqrt{2}+31\sqrt{3}+2\sqrt{6}+2)(2^{n+1}-2), & if\ n \geq 1. \end{cases}$$

Proof. The core of the structure means the stage zero. Firstly, we compute $^{2}\chi(TD_2[0])$. Let $d_{i_1i_2i_3}$ denote the number of 2-paths whose three consecutive vertices are of degree i_1, i_2, i_3, respectively. In the same way, we use $d^{(n)}_{i_1i_2i_3}$ to mean $d_{i_1i_2i_3}$ in $n-th$ stages. Particularly, $d^{(n)}_{i_1i_2i_3} = d^{(n)}_{i_3i_2i_1}$. It is easy to see that

$$d^{(0)}_{123} = 4,\ d^{(0)}_{223} = 24,\ d^{(0)}_{232} = 30,\ d^{(0)}_{233} = 12,\ d^{(0)}_{323} = 4.$$

Therefore, we have

$$^{2}\chi(TD_2[0]) = \frac{4}{\sqrt{1\times2\times3}} + \frac{24}{\sqrt{2\times2\times3}} + \frac{30}{\sqrt{2\times3\times2}} + \frac{12}{\sqrt{2\times3\times3}} + \frac{4}{\sqrt{3\times2\times3}}$$

$$= \frac{1}{3}(8\sqrt{2} + 27\sqrt{3} + 2\sqrt{6}).$$

Secondly, we construct the relation between $^{2}\chi(TD_2[n])$ and $^{2}\chi(TD_2[n-1])$ for $n \geq 1$.

By simple reduction, we have

$$d_{123}^{(n)} = d_{123}^{(n-1)} + 2\times2^n,\ d_{132}^{(n)} = d_{132}^{(n-1)} + 2\times2^n,\ d_{133}^{(n)} = d_{133}^{(n-1)} + 2\times2^n,$$

$$d_{223}^{(n)} = d_{223}^{(n-1)} + 28\times2^n,$$

$$d_{232}^{(n)} = d_{232}^{(n-1)} + 34\times2^n,\ d_{233}^{(n)} = d_{233}^{(n-1)} + 22\times2^n,\ d_{323}^{(n)} = d_{323}^{(n-1)} + 8\times2^n,$$

and for any $(i_1i_2i_3) \neq (123),(132),(133),(223),(232),(233),(323),$ we have $d_{i_1i_2i_3}^{(n)} = 0.$

Therefore,

$$^{2}\chi(TD_2[n]) = {}^{2}\chi(TD_2[n-1]) + \frac{2\times2^n}{\sqrt{1\times2\times3}} + \frac{2\times2^n}{\sqrt{1\times3\times2}} + \frac{2\times2^n}{\sqrt{1\times3\times3}} + \frac{28\times2^n}{\sqrt{2\times2\times3}}$$

$$+ \frac{34\times2^n}{\sqrt{2\times3\times2}} + \frac{22\times2^n}{\sqrt{2\times3\times3}} + \frac{8\times2^n}{\sqrt{3\times2\times3}}$$

$$= {}^{2}\chi(TD_2[n-1]) + \frac{1}{3}(15\sqrt{2} + 31\sqrt{3} + 2\sqrt{6} + 2)\times2^n.$$

From the above recursion formula, we have

$$^{2}\chi(TD_2[n]) = {}^{2}\chi(TD_2[n-1]) + \frac{1}{3}(15\sqrt{2} + 31\sqrt{3} + 2\sqrt{6} + 2)\times2^n$$

$$= {}^{2}\chi(TD_2[n-2]) + \frac{1}{3}(15\sqrt{2} + 31\sqrt{3} + 2\sqrt{6} + 2)(2^n + 2^{n-1})$$

$$\vdots$$

$$= {}^{2}\chi(TD_2[0]) + \frac{1}{3}(15\sqrt{2} + 31\sqrt{3} + 2\sqrt{6} + 2)(2^n + 2^{n-1} + \ldots + 2^2 + 2).$$

Thus,

$$^{2}\chi(TD_2[n]) = \frac{1}{3}(8\sqrt{2} + 27\sqrt{3} + 2\sqrt{6}) + \frac{1}{3}(15\sqrt{2} + 31\sqrt{3} + 2\sqrt{6} + 2)(2^{n+1} - 2).$$

The proof is now complete.

Now, we shall study the 2-sum connectivity index of the same family of dendrimer as shown in Figure 1.

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

$$^{2s}\chi(TD_2[n]) = \begin{cases} \frac{1}{21}(14\sqrt{6}+162\sqrt{7}+42\sqrt{8}), & if\ n=0; \\ \frac{1}{21}(14\sqrt{6}+162\sqrt{7}+42\sqrt{8})+\frac{1}{84}(56\sqrt{6}+768\sqrt{7}+315\sqrt{8})(2^{n+1}-2), & if\ n \geq 1. \end{cases}$$

Proof. We first compute $^{2s}\chi(TD_2[0])$. Let $d_{i_1i_2i_3}$ denote the number of 2-paths whose three consecutive vertices are of degree i_1, i_2, i_3, respectively. Similarly we use $d^{(n)}_{i_1i_2i_3}$ to mean $d_{i_1i_2i_3}$ in $n-th$ stages. Particularly, $d^{(n)}_{i_1i_2i_3} = d^{(n)}_{i_3i_2i_1}$.

It is easy to see that

$$d^{(0)}_{123} = 4,\ d^{(0)}_{223} = 24,\ d^{(0)}_{232} = 30,\ d^{(0)}_{233} = 12,\ d^{(0)}_{323} = 4.$$

Therefore, we have

$$^{2s}\chi(TD_2[0]) = \frac{4}{\sqrt{1+2+3}} + \frac{24}{\sqrt{2+2+3}} + \frac{30}{\sqrt{2+3+2}} + \frac{12}{\sqrt{2+3+3}} + \frac{4}{\sqrt{3+2+3}}$$
$$= \frac{1}{21}(14\sqrt{6}+162\sqrt{7}+42\sqrt{8}).$$

By using the same way in Theorem 1, we can find the relation between $^{2s}X(TD_2[n])$ and $^{2s}X(TD_2[n-1])$ for $n \geq 1$.

We have

$$d^{(n)}_{123} = d^{(n-1)}_{123} + 2\times 2^n,\ d^{(n)}_{132} = d^{(n-1)}_{132} + 2\times 2^n,\ d^{(n)}_{133} = d^{(n-1)}_{133} + 2\times 2^n,$$
$$d^{(n)}_{223} = d^{(n-1)}_{223} + 28\times 2^n,$$

$d^{(n)}_{232} = d^{(n-1)}_{232} + 34\times 2^n$, $d^{(n)}_{233} = d^{(n-1)}_{233} + 22\times 2^n$, $d^{(n)}_{323} = d^{(n-1)}_{323} + 8\times 2^n$, and for any $(i_1i_2i_3) \neq (123),(132),(133),(223),(232),(233),(323)$, we have $d^{(n)}_{i_1i_2i_3} = 0$.

Therefore,

$$^{2s}\chi(TD_2[n]) = {}^{2s}\chi(TD_2[n-1]) + \frac{2\times 2^n}{\sqrt{1+2+3}} + \frac{2\times 2^n}{\sqrt{1+3+2}} + \frac{2\times 2^n}{\sqrt{1+3+3}} + \frac{28\times 2^n}{\sqrt{2+2+3}}$$
$$+\frac{34\times 2^n}{\sqrt{2+3+2}} + \frac{22\times 2^n}{\sqrt{2+3+3}} + \frac{8\times 2^n}{\sqrt{3+2+3}}$$
$$= {}^{2s}\chi(TD_2[n-1]) + \frac{1}{84}(56\sqrt{6}+768\sqrt{7}+315\sqrt{8})\times 2^n.$$

From the above recursion formula, we have

$$^{2s}\chi(TD_2[n]) = {}^{2s}\chi(TD_2[n-1]) + \frac{1}{84}(56\sqrt{6}+768\sqrt{7}+315\sqrt{8})\times 2^n$$

$$= {}^{2s}\chi(TD_2[n-2]) + \frac{1}{84}(56\sqrt{6} + 768\sqrt{7} + 315\sqrt{8})(2^n + 2^{n-1})$$

$$\vdots$$

$$= {}^{2s}\chi(TD_2[0]) + \frac{1}{84}(56\sqrt{6} + 768\sqrt{7} + 315\sqrt{8})(2^n + 2^{n-1} + \ldots + 2^2 + 2).$$

Hence,

$${}^{2s}\chi(TD_2[n]) = \frac{1}{21}(14\sqrt{6} + 162\sqrt{7} + 42\sqrt{8}) + \frac{1}{84}(56\sqrt{6} + 768\sqrt{7} + 315\sqrt{8})(2^{n+1} - 2).$$

The proof is now complete.

CONCLUSION

In this paper, we have discussed the 2-order- and 2-sum connectivity indices of tetrathiafulvalene dendrimers. We believe the technique used in this paper can be extended to study the connectivity indices of some other families of dendrimers as well. In our next papers, we will determine the *m*-order and *m*-sum connectivity indices of tetrathiafulvalene dendrimers, where *m* = 3 and 4.

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