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Computing Vertex PI Index of Tetrathiafulvalene Dendrimers

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ABSTRACT

General formulas are obtained for the vertex Padmakar-Ivan index (PI_v) of tetrathiafulvalene (TTF) dendrimer, whereby TTF units we are employed as branching centers. The PI_v index is a Wiener-Szeged-like index developed very recently. This topological index is defined as the summation of all sums of $n_u(e)$ and $n_v(e)$, over all edges of connected graph G.

Keywords: Dendrimer nanostar, PI_v index.

1 INTRODUCTION

A simple graph G consist of a pair of the vertex and edge-sets of which are represented by $V(G)$ and $E(G)$, respectively. If e is an edge of G, connecting the vertices u and v then we write $e = uv$. If x and y are arbitrary vertices of a connected graph G then $d(x,y)$ denotes the distance between x and y. In mathematical chemistry, a new interdisciplinary branch of mathematics, a topological index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. Molecular graph is a mathematically model molecules (simple graph) in order to gain insight into the physical properties of these chemical compounds such as chemical reactivity or biological activity. Atom of this molecule can be represented as a vertex of graph by replacing the atoms with vertices. Chemical bonds are then represented as an edge in the graph. There are too many examples of such descriptors, which are applicable in chemistry.

Khadikar and Co–authors defined a topological index and called it Padmakar–Ivan index (PI). It is defined as $PI(G) = \sum_{e=uv}[m_u(e|G) + m_v(e|G)]$, where $m_u(e|G)$ is the number

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of edges of G lying closer to u than to v and $m_v(e|G)$ is the number of edges of G lying closer to v than to u. This is the edge version of PI index and in [1–3], the edge–PI index has been computed for some graphs.

The vertex version of PI index was introduced in [4] by Khalifeh *et al.* as $PI_v(G) = \sum_{e=uv}[n_u(e|G) + n_v(e|G)]$, such that $n_u(e|G)$ is the number of vertices of G lying closer to u than to v and $n_v(e|G)$ is defined analogously. Notice that vertices equidistant from both ends of the edge $e = uv$ are not counted. If G is a bipartite graph then $PI_v = |V(G)||E(G)|$, because G is without odd cycles. This index can be characterized bipartite graphs.

In this paper, the PI_v index of a class of dendrimers, Figure 1, named tetrathiafulvalene (TTF), is computed, whereby TTF units were employed as branching centers [5].

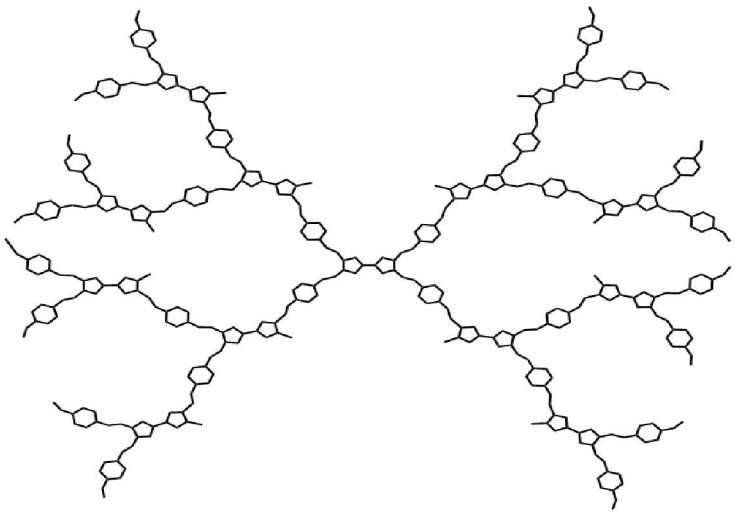

Figure 1. Molecular graph of dendrimers using TTF units as branching centers. *D*[2]

The dendrimers are part of a new group of macromolecules which is built from a starting atom, such as nitrogen, to which carbon and other elements are added by a repeating series of chemical reactions that produce a spherical branching structure. In a divergent synthesis of a dendrimer, one starts from the core (a multi connected atom or group of atoms) and growths out to the periphery. In each repeated step, a number of monomers are added to the actual structure, in a radial manner, in resulting quasi concentric shells, called generations. In a convergent synthesis, the periphery is first built up and next the branches (called dendrons) are connected to the core. The dendrimer promises to have great applications but first the structure and the energy transfer mechanism must be understood [5–7]. The PI index of dendrimer of Figure 1 was computed in [8]. Some

researchers computed the PI_v index of classes of fullerenes, nanotubes, nanocones, dendrimers and nanostars [9-19]. We encourage the reader to consult these papers for computational techniques, mathematical properties and chemical meaning of this topological index into account.

3 RESULTS AND DISCUSSION

Throughout this section $D[k]$ denotes the molecular graph of a nanostar dendrimer with exactly k generation, Figure 1. The graph $\mathbf{T} = D[k]$ has exactly $124 \times 2^k - 74$ vertices. Also, we assume that V and E denote the set of all edges and vertices of $D[k]$. To compute the PI_v index of $\mathbf{T}$, we first consider a partition of E into two subsets A and B such that A contains the edges of the core, Figure 2, and B is the set of all remaining edges of $\mathbf{T}$, Figure 3. Thus $PI_v(\mathbf{T}) = \Sigma_{f\in A}[n_u(f) + n_v(f)] + \Sigma_{e\in B}[n_u(e) + n_v(e)]$. Denote the number of vertices of one branch of B by $g(k)$. The we have $g(k) = 31 \times (2^k - 1)$. By the symmetry of core, it is enough to compute $n_u(f_i)$, $n_v(f_i)$, where $1 \le i \le 12$. In Table 1, $n_u(f_i)$, $n_v(f_i)$ and L_i are given, where L_i is the number of similar edges as f_i.

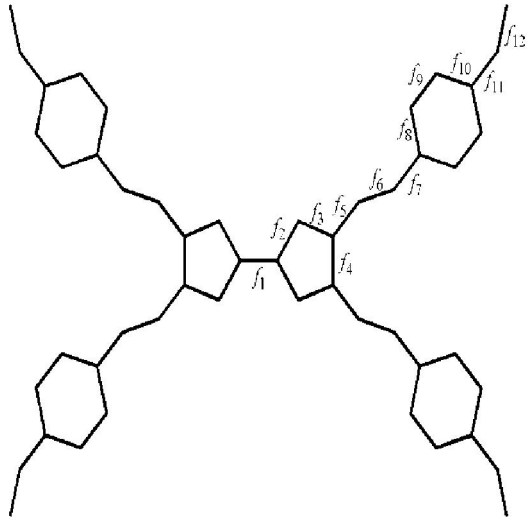

Figure 2. Branched monomer was obtained by CsOH–HaO–promoted thioben–zylation.

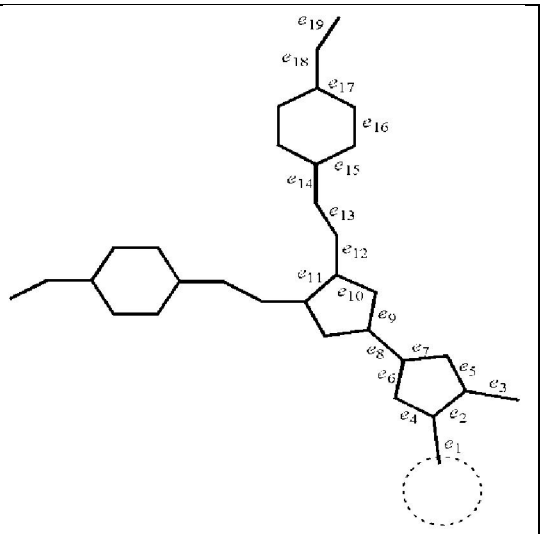

Figure 3. Methyl-terminated monomer.

By Table 1, $\Sigma_{f\in A}[n_u(f) + n_v(f)] = 65722 \times 2^k - 3962$.

1	$n_u(f_i\|\boldsymbol{D}[\boldsymbol{k}])$	$n_v(f_i\|\boldsymbol{D}[\boldsymbol{k}])$	L_i
f_1	$n/2$	$n/2$	1
f_2	$2 + n/2$	$12 + g(k)$	4
f_3	$2 + n/2$	$22 + 2g(k)$	4
f_4	$2 + g(k)$	$2 + g(k)$	2
f_5	$15 + n/2 + g(k)$	$10 + g(k)$	4
f_6	$16 + n/2 + g(k)$	$9 + g(k)$	4
f_7	$17 + n/2 + g(k)$	$8 + g(k)$	4
f_8	$17 + n/2 + g(k)$	$5 + g(k)$	8
f_9	$20 + n/2 + g(k)$	$5 + g(k)$	8
f_{10}	$20 + n/2 + g(k)$	$5 + g(k)$	8
f_{11}	$23 + n/2 + g(k)$	$2 + g(k)$	4
f_{12}	$24 + n/2 + g(k)$	$1 + g(k)$	4

In Table 2, $n_u(e_i)$, $n_v(e_i)$ and L_i, the number of similar edges as e_i, for a representative set of edges in B are given. By Table 2, $\Sigma_{e\in B}[n_u(e) + n_v(e)] = 16368 \times 2^{2k} - 26136 \times 2^k + 9768$.

1	$n_u(e_i\|\boldsymbol{D}[\boldsymbol{k}])$	$n_v(e_i\|\boldsymbol{D}[\boldsymbol{k}])$	L_i
e_1	$n - g(k - i + 1)$	$g(k - i + 1)$	$4(2^{i-1})$
e_2	$2 + n - g(k - i + 1)$	3	$4(2^{i-1})$
e_3	$n - 1$	1	$4(2^{i-1})$
e_4	$3 + n - g(k - i + 1)$	$-4 + g(k - i + 1)$	$4(2^{i-1})$
e_5	$3 + n - g(k - i + 1)$	$-4 + g(k - i + 1)$	$4(2^{i-1})$
e_6	$2 + n - g(k - i + 1)$	$-4 + g(k - i + 1)$	$4(2^{i-1})$
e_7	$-4 + g(k - i + 1)$	3	$4(2^{i-1})$
e_8	$6 + n - g(k - i + 1)$	$-6 + g(k - i + 1)$	$4(2^{i-1})$
e_9	$8 + n - g(k - i + 1)$	$12 + g(k - i)$	$8(2^{i-1})$
e_{10}	$8 + n - g(k - i + 1)$	$-9 + g(k - i + 1)$	$8(2^{i-1})$
e_{11}	$12 + g(k - i)$	$12 + g(k - i)$	$4(2^{i-1})$
e_{12}	$-10 + n - g(k - i)$	$10 + g(k - i)$	$8(2^{i-1})$
e_{13}	$-9 + n - g(k - i)$	$9 + g(k - i)$	$8(2^{i-1})$
e_{14}	$-8 + n - g(k - i)$	$8 + g(k - i)$	$8(2^{i-1})$
e_{15}	$8 + g(k - i)$	$5 + g(k - i)$	$16(2^{i-1})$
e_{16}	$-5 + n - g(k - i)$	$5 + g(k - i)$	$16(2^{i-1})$
e_{17}	$-5 + n - g(k - i)$	$5 + g(k - i)$	$16(2^{i-1})$
e_{18}	$-2 + n - g(k - i)$	$2 + g(k - i)$	$8(2^{i-1})$
e_{19}	$-1 + n - g(k - i)$	$1 + g(k - i)$	$8(2^{i-1})$

From these calculations we have:

Theorem. The PI_v index of $\mathbf{T} = D[k]$ is computed as follows:

$$PI_v(\mathbf{T}) = 16368 \times 4^k - 19564 \times 2^k + 5806.$$

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