Distance indices calculating for two classes of dendrimer

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ABSTRACT
In ecological studies, topological indices are defined to test the ecological and chemical characteristics, such as oxidation, melting point, boiling point, toxicity, and other biological activity. As a basic molecular structure, dendrimers widely appeared in chemical, biology, pharmacy, medicine, and material engineering. In this paper, we study the chemical properties of two kinds of dendrimers from the mathematical point of view. Several vertex distance-based indices are determined. Furthermore, the edge distance-based indices of one class of nanocore structure are also considered.

1. Introduction
It has been over 35 years since the studies of topological indices for molecular structures were conducted. Distance-based and degree-based topological indices are numerical parameters of molecular structure, which are of great importance in physics, chemistry, and pharmacology science.

Specifically, let \( G = (V(G), E(G)) \) be a molecular graph with vertex set \( V(G) \) and edge set \( E(G) \), then a topological index can be regarded as a positive real function \( f: G \to \mathbb{R}^+ \). Being numerical descriptors of the molecular structure deduced from the corresponding molecular graph, topological indices can be applied in theoretical chemistry, like QSAR/QSPR study. For example, harmonic index, Wiener index, PI index, Randic index, and sum connectivity index can be used to reflect certain structural features and chemical characteristics of organic molecules. In recent years, several articles made contribution to covering certain distance-based and degree-based indices of special molecular graph (Gao, Farahani, & Shi, 2016; Gao & Siddiqui, 2017; Gao, Siddiqui, Imran, Jamil, & Farahani, 2016; Gao & Wang, 2015, 2016, 2017; Gao, Wang, & Farahani, 2016; Gao, Yan, & Shi, 2017; Gao et al., 2017; Sardar, Zafar, & Zhao, 2017). The notations and terminologies are used but undefined in this paper (Bondy & Murty, 2008).

For any \( e = uv \in E(G) \), let

\[
m_u(e) = |\{x|x \in V(G), d(u, x) < d(v, x)\}|,
\]

\[
m_v(e) = |\{x|x \in V(G), d(u, x) > d(v, x)\}|,
\]

\[
m_v(e) = |\{x|x \in V(G), d(u, x) < d(v, x)\}|,
\]

\[
m_u(e) = |\{x|x \in V(G), d(u, x) > d(v, x)\}|.
\]

Some researchers have introduced a distance-based version of the atom-bond connectivity index, and it was called the second atom-bond connectivity index being denoted as

\[
ABC_2(G) = \sum_{e=uv \in E(G)} \sqrt{n_u(e) + n_v(e) - 2},
\]

The edge version of atom-bond connectivity index (the third atom-bond connectivity index) was defined as

\[
ABC_3(G) = \sum_{e=uv \in E(G)} \frac{\sqrt{m_u(e) + m_v(e) - 2}}{m_u(e)m_v(e)}.
\]

raised a distance-based version of the geometric–arithmetic index, and was called the second geometric–arithmetic index which can be stated as

\[
GA_2(G) = \sum_{e=uv \in E(G)} \frac{2\sqrt{n_u(e)n_v(e)}}{n_u(e) + n_v(e)}.
\]

The third geometric–arithmetic index was introduced as

\[
GA_3(G) = \sum_{e=uv \in E(G)} \frac{2\sqrt{m_u(e)m_v(e)}}{m_u(e) + m_v(e)}.
\]

As a traditional topological index, the vertex PI index and PI index of molecular graph \( G \) were defined as
The vertex PI polynomial, as the extension of vertex PI index, was introduced being stated as

$$\text{PI}_v(G) = \sum_{e=uv} (n_u(e) + n_v(e)),$$

$$\text{PI}(G) = \sum_{e=uv} (m_u(e) + m_v(e)).$$

The corresponding PI polynomial was stated as

$$\text{PI}_v(G, x) = \sum_{uv \in E(G)} x^{n_u(e)+n_v(e)}.$$

The corresponding distance-based polynomial, the Szeged polynomial, and edge Szeged polynomial are defined as

$$\text{Sz}(G) = \sum_{e=uv} n_u(e)n_v(e),$$

$$\text{Sz}_e(G) = \sum_{e=uv} m_u(e)m_v(e).$$

Other distance-based index, the Szeged index, and edge Szeged index are defined as

$$\text{Sz}(G, x) = \sum_{e=uv} x^{n_u(e) + n_v(e)},$$

$$\text{Sz}_e(G, x) = \sum_{e=uv} x^{m_u(e)+m_v(e)}.$$

For any edge $e = uv$, let

$$n(e) = |\{x|x \in V(G), d(u, x) = d(v, x)\}|,$$

$$m(e) = |\{x|x \in E(G), d(u, x) = d(v, x)\}|.$$

Then, the modified version of Szeged index for a molecular graph $G$ was defined as

$$\text{Sz}^*_v(G) = \sum_{uv \in E(G)} \left( \left( n_u(e) + \frac{n(e)}{2} \right) \left( n_v(e) + \frac{n(e)}{2} \right) \right),$$

$$\text{Sz}_e^*(G) = \sum_{e=uv} \left( m_u(e) + \frac{m(e)}{2} \right) \left( m_v(e) + \frac{m(e)}{2} \right).$$

In past decades, the computation of distance-based indices for certain special chemical molecular structure raised much attention among chemists. Although there have been many results in distance-based indices of molecular graphs, the research of indices for special chemical structures are still largely limited. In addition, as widespread and critical chemical structures, tetrathiafulvalene (TTF) and 4,4'-bipyridinium dendrimers are widely applied in medical science and pharmaceutical engineering. For all these reasons, we

![Figure 1. Molecular graph of dendrimers using TTF units as branching centers. D (Gao, Wang, Jamil, & Farahani, 2016d).](image-url)
give a deep discussion on the computation of the two dendrimers mentioned above (Ashrafi, Manoochehrian, & Yousefi-Azari, 2006; Graovac & Ghorbani, 2010; Gutman & Ashrafi, 2008; Tabar, Purtula, & Gutman, 2010).

The main contribution of our work is twofold. On the one hand, we will manifest certain vertex distance-based indices of TTF. On the other hand, some important vertex distance-based indices of 4,4′-bipyridinimu dendrimers will be discussed. At last, as supplement contribution, the edge distance-based indices of \( \text{CNC}_7[n] \) are presented.

### 2. Main results and proofs

In this part, we present our main results on vertex distance-based indices of two finite families of dendrimer: TTF and 4,4′-bipyridinimiu dendrimers. Then, as supplemental results, the edge distance-based indices of one-heptagonal carbon nanocones are discussed.

#### 2.1. Vertex distance-based indices of TTF

The dendrimers built from a starting atom, such as nitrogen, to which carbon are part of a new group of macromolecules. 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

![Figure 2](image2.png) Branched monomer was obtained by CsOH-HaO-promoted Thioben-zylation.

![Figure 3](image3.png) Methyl-terminated monomer.

![Table 1](image4.png)

| Class of edge | \( n_1(e) \) | \( n_2(e) \) | Number of edges |
|---------------|---------------|---------------|-----------------|
| \( e_1 \)     | 62 - 2\(^2\) - 37 | 62 - 2\(^2\) - 37 | 1               |
| \( e_2 \)     | 62 - 2\(^2\) - 35 | 31 - 2\(^2\) - 19 | 4               |
| \( e_3 \)     | 62 - 2\(^2\) - 35 | 62 - 2\(^2\) - 40 | 4               |
| \( e_4 \)     | 31 - 2\(^2\) - 29 | 31 - 2\(^2\) - 29 | 2               |
| \( e_5 \)     | 93 - 2\(^2\) - 53 | 31 - 2\(^2\) - 21 | 4               |
| \( e_6 \)     | 93 - 2\(^2\) - 52 | 31 - 2\(^2\) - 22 | 4               |
| \( e_7 \)     | 93 - 2\(^2\) - 51 | 31 - 2\(^2\) - 23 | 4               |
| \( e_8 \)     | 93 - 2\(^2\) - 51 | 31 - 2\(^2\) - 26 | 8               |
| \( e_9 \)     | 93 - 2\(^2\) - 48 | 31 - 2\(^2\) - 26 | 8               |
| \( e_{10} \)  | 93 - 2\(^2\) - 48 | 31 - 2\(^2\) - 26 | 8               |
| \( e_{11} \)  | 93 - 2\(^2\) - 45 | 31 - 2\(^2\) - 29 | 4               |
| \( e_{12} \)  | 93 - 2\(^2\) - 44 | 31 - 2\(^2\) - 30 | 4               |
atom or group of atoms) and grows out to the periphery. In each repeated step, a number of monomers will be added to the actual structure. In a radial manner, resulting quasi concentric shells are called generations. The periphery in a convergent synthesis is first set up and then the branches which are called Dendron's are connected to the core.

We first discuss a kind of dendrimers named TTF, and see Figure 1 as an example of this molecular structure where TTF units were used as branching centers. Several contributions on TTF and other dendrimers. In this subsection, we aim to determine the distance-based indices of TTF by means of distance computation.

We use \( D[k] \) to denote the molecular graph TTF with \( k \) generation. By simply calculating, we have \(|V(D[k])| = 124 \cdot 2^k - 74\). In order to determine the vertex distance-based index of \( D[k] \), we divide \( E(D[k]) \) into two parts \( A \) and \( B \) (see Figures 2 and 3, respectively) where \( A \) includes the edges of the core and \( B \) is the subset containing all remaining edges of \( D[k] \). In view of the symmetry of core, we yield the value of \( n_i(e), n_k(e) \), and the number of such kind of edges (as we indicate in Figures 2 and 3, there are 12 kinds of edges in part \( A \) and 19 kinds of edges in part \( B \) which are manifested in Tables 1 and 2 for part \( A \) and part \( B \), respectively.

\[
ABC_2(D[k]) = \sqrt{124 \cdot 2^k - 76} + \frac{4 \sqrt{93 \cdot 2^k - 56}}{62 \cdot 2^k - 37} + \frac{4 \sqrt{124 \cdot 2^k - 77}}{(62 \cdot 2^k - 35)(31 \cdot 2^k - 19)} + \frac{2 \sqrt{62 \cdot 2^k - 60}}{31 \cdot 2^k - 29} + \frac{124 \cdot 2^k - 76}{93 \cdot 2^k - 53(31 \cdot 2^k - 21)} + \frac{124 \cdot 2^k - 76}{93 \cdot 2^k - 51(31 \cdot 2^k - 26)} + \frac{124 \cdot 2^k - 76}{93 \cdot 2^k - 44(31 \cdot 2^k - 30)} + \frac{124 \cdot 2^k - 76}{124 \cdot 2^k - 31 \cdot 2^{k+1} - 43(31 \cdot 2^{k+1} - 31)} + \frac{124 \cdot 2^k - 76}{124 \cdot 2^k - 31 \cdot 2^{k+1} - 41} + \frac{124 \cdot 2^k - 76}{124 \cdot 2^k - 31 \cdot 2^{k+1} - 35}.
\]
Using the definition of distance-based indices, we get

\[
GA_2(D[k]) = 4 \cdot 2^k - 1 + \frac{8 \sqrt{(62 \cdot 2^k - 35)(31 \cdot 2^k - 19)}}{93 \cdot 2^k - 54} + \frac{8 \sqrt{(62 \cdot 2^k - 35)(62 \cdot 2^k - 40)}}{124 \cdot 2^k - 75} \\
+ \frac{8 \sqrt{(93 \cdot 2^k - 53)(31 \cdot 2^k - 21)}}{124 \cdot 2^k - 74} + \frac{8 \sqrt{(93 \cdot 2^k - 52)(31 \cdot 2^k - 22)}}{124 \cdot 2^k - 74} + \frac{8 \sqrt{(93 \cdot 2^k - 51)(31 \cdot 2^k - 23)}}{124 \cdot 2^k - 74} \\
+ \frac{16 \sqrt{(93 \cdot 2^k - 51)(31 \cdot 2^k - 26)}}{124 \cdot 2^k - 77} + \frac{32 \sqrt{(93 \cdot 2^k - 48)(31 \cdot 2^k - 26)}}{124 \cdot 2^k - 74} + \frac{8 \sqrt{(93 \cdot 2^k - 45)(31 \cdot 2^k - 29)}}{124 \cdot 2^k - 74} \\
+ \frac{8 \sqrt{(93 \cdot 2^k - 44)(31 \cdot 2^k - 30)}}{124 \cdot 2^k - 74} + \sum_{i=1}^{k} \frac{2^{i+2} \sqrt{(124 \cdot 2^k - 31 \cdot 2^{k-i+1} - 43)(31 \cdot 2^{k-i+1} - 31) - 40)(31 \cdot 2^{k-i+1} - 35)}}{124 \cdot 2^k - 74} \\
+ \sum_{i=1}^{k} \frac{2^{i+3} \sqrt{(31 \cdot 2^{k-i+1} - 35)(31 \cdot 2^{k-i+1} - 32)}}{124 \cdot 2^k - 76} + \sum_{i=1}^{k} \frac{2^{i+3} \sqrt{(124 \cdot 2^k - 31 \cdot 2^{k-i+1} - 37)(31 \cdot 2^{k-i+1} - 37)}}{124 \cdot 2^k - 74} \\
+ \sum_{i=1}^{k} \frac{2^{i+3} \sqrt{(124 \cdot 2^k - 31 \cdot 2^{k-i+1} - 35)(31 \cdot 2^{k-i} - 19)}}{124 \cdot 2^k - 74} + \sum_{i=1}^{k} \frac{2^{i+3} \sqrt{(124 \cdot 2^k - 31 \cdot 2^{k-i+1} - 35)(31 \cdot 2^{k-i+1} - 40)}}{124 \cdot 2^k - 75} \\
+ \sum_{i=1}^{k} \frac{2^{i+3} \sqrt{(124 \cdot 2^k - 31 \cdot 2^{k-i} - 53)(31 \cdot 2^{k-i} - 21)}}{124 \cdot 2^k - 74} + \sum_{i=1}^{k} \frac{2^{i+3} \sqrt{(124 \cdot 2^k - 31 \cdot 2^{k-i} - 52)(31 \cdot 2^{k-i} - 22)}}{124 \cdot 2^k - 74} \\
+ \sum_{i=1}^{k} \frac{2^{i+3} \sqrt{(124 \cdot 2^k - 31 \cdot 2^{k-i} - 51)(31 \cdot 2^{k-i} - 23)}}{124 \cdot 2^k - 74} + \sum_{i=1}^{k} \frac{2^{i+4} \sqrt{(31 \cdot 2^{k-i} - 23)(31 \cdot 2^{k-i} - 26)}}{62 \cdot 2^{k-i} - 49} \\
+ \sum_{i=1}^{k} \frac{2^{i+3} \sqrt{(124 \cdot 2^k - 31 \cdot 2^{k-i} - 48)(31 \cdot 2^{k-i} - 26)}}{124 \cdot 2^k - 74} + \sum_{i=1}^{k} \frac{2^{i+3} \sqrt{(124 \cdot 2^k - 31 \cdot 2^{k-i} - 45)(31 \cdot 2^{k-i} - 29)}}{124 \cdot 2^k - 74} \\
+ \sum_{i=1}^{k} \frac{2^{i+3} \sqrt{(124 \cdot 2^k - 31 \cdot 2^{k-i} - 44)(31 \cdot 2^{k-i} - 30)}}{124 \cdot 2^k - 74},
\]

\[
PI_1(D[k], x) = (84 \cdot 2^k - 45)x^{124 \cdot 2^k - 74} + 4x^{93 \cdot 2^k - 54} + (16 \cdot 2^k - 12) x^{124 \cdot 2^k - 75} \\
+ 2x^{62 \cdot 2^k - 58} + 8x^{124 \cdot 2^k - 77} + \sum_{i=1}^{k} 2^{i+1} x^{124 \cdot 2^k - 31 \cdot 2^{k-i+1} - 38} \\
+ (4 \cdot 2^k - 4)x^{124 \cdot 2^k - 76} + (4 \cdot 2^k - 4)x^{31 \cdot 2^{k-i+1} - 32} \\
+ \sum_{i=1}^{k} 2^{i+2} x^{124 \cdot 2^k - 31 \cdot 2^{k-i} - 54} + (4 \cdot 2^k - 4)x^{62 \cdot 2^k - 38} + \sum_{i=1}^{k} 2^{i+3} x^{62 \cdot 2^k - 49},
\]
\[ Sz(D[k]) = 391250 \cdot 2^k - 300328 \cdot 2^{2k} - 42160k \cdot 2^k + 261392k \cdot 2^{2k} - 76337, \]

\[ \begin{align*}
& Sz(D[k], x) = x^{(62 \cdot 2^{2i-37})} + 4x^{(62 \cdot 2^{2i-35}(31 \cdot 2^{2i-19})} + 4x^{(62 \cdot 2^{2i-35}(62 \cdot 2^{2i-40})} + 2x^{(31 \cdot 2^{2i-29})} \\
& + 4x^{(93 \cdot 2^{3i-53}(31 \cdot 2^{2i-21})} + 4x^{(93 \cdot 2^{3i-52}(31 \cdot 2^{2i-22})} + 4x^{(93 \cdot 2^{3i-51}(31 \cdot 2^{2i-23})} \\
& + 8x^{(93 \cdot 2^{3i-50}(31 \cdot 2^{2i-26})} + 16x^{(93 \cdot 2^{3i-48}(31 \cdot 2^{2i-26})} + 4x^{(93 \cdot 2^{3i-45}(31 \cdot 2^{2i-29})} \\
& + 4x^{(93 \cdot 2^{3i-44}(31 \cdot 2^{2i-30})} + \sum_{i=1}^{k} 2^{+1} x^{(124 \cdot 2^{3i-31} \cdot 2^{2i-31} - 43(31 \cdot 2^{2i-31} - 31)} \\
& + \sum_{i=1}^{k} 2^{+1} x^{(124 \cdot 2^{3i-31} - 31 \cdot 2^{2i-31} - 41)} + \sum_{i=1}^{k} 2^{+1} x^{(124 \cdot 2^{3i-31} - 31 \cdot 2^{2i-31} - 35)} \\
& + \sum_{i=1}^{k} 2^{+1} x^{(31 \cdot 2^{2i-31} - 35)} + \sum_{i=1}^{k} 2^{+1} x^{(124 \cdot 2^{3i-31} - 31 \cdot 2^{2i-31} - 37)} (31 \cdot 2^{2i-31} - 37) \\
& + \sum_{i=1}^{k} 2^{+1} x^{(124 \cdot 2^{3i-31} - 31 \cdot 2^{2i-31} - 35)} (31 \cdot 2^{2i-31} - 19) + \sum_{i=1}^{k} 2^{+2} x^{(124 \cdot 2^{3i-31} - 31 \cdot 2^{2i-31} - 35)(31 \cdot 2^{2i-31} - 40)} \\
& + \sum_{i=1}^{k} 2^{+1} x^{(31 \cdot 2^{2i-31} - 19)} + \sum_{i=1}^{k} 2^{+2} x^{(124 \cdot 2^{3i-31} - 31 \cdot 2^{2i-31} - 21)} \\
& + \sum_{i=1}^{k} 2^{+2} x^{(124 \cdot 2^{3i-31} - 31 \cdot 2^{2i-31} - 52)(31 \cdot 2^{2i-31} - 22)} + \sum_{i=1}^{k} 2^{+2} x^{(124 \cdot 2^{3i-31} - 31 \cdot 2^{2i-31} - 23)} \\
& + \sum_{i=1}^{k} 2^{+3} x^{(124 \cdot 2^{3i-31} - 23)(31 \cdot 2^{2i-31} - 26)} + \sum_{i=1}^{k} 2^{+4} x^{(124 \cdot 2^{3i-31} - 48)(31 \cdot 2^{2i-31} - 26)} \\
& + \sum_{i=1}^{k} 2^{+2} x^{(124 \cdot 2^{3i-31} - 45)(31 \cdot 2^{2i-31} - 29)} + \sum_{i=1}^{k} 2^{+2} x^{(124 \cdot 2^{3i-31} - 31 \cdot 2^{2i-31} - 30)} \\
\end{align*} \]

\[ Sz^*_e(D[k]) = 92256 \cdot 2^k - 522474 \cdot 2^{2k} + 100905 \cdot 2^k - 31372k \cdot 2^k + 449916 \cdot 2^k + 276768k \cdot 2^{2k} - 103116. \]

### 2.2. Vertex distance-based indices of 4,4'-bipyridinium dendrimers

In this subsection, we present the above-mentioned distance-based indices of 4,4'-bipyridinium dendrimers. The structure of 4,4'-bipyridinium dendrimers with \( n \) stages (which is denoted by \( G_n \)) can be referred to Figure 4. Some contributions on these structures in the field of chemical science can be referred to (Balzani et al., 2006; Bongard, Moller, Rao, Corr, & Walder, 2005; Ewais, Nagdy, & Hameed, 2006; Giananta et al., 2009; Kathiresan & Walder, 2011; Kim et al., 2007; Oh et al., 2004; Ong et al., 2005; Marchioni et al., 2004; Rajakumar & Srinivasan, 2014). By computation, we yield \( |V(G_n)| = 16 \cdot 2^n - 6 \).

Let \( h_i \) be a hexagon in the \( i \)-stage and \( e_{i-1,j} \) be the edge connected \( h_i \) and \( h_{i+1} \). Suppose that \( e \in E(h_i) \) for all six edges, we have \( n_e(e) = 3 \) and there are \( 2^n \) such hexagons. If

| Table 2. Distance computation for part \( B \) (1 ≤ \( i \) ≤ \( k \)). |
|---|---|---|
| Class of edge \( e \) | \( n_e(e) \) | Number of edges |
| \( e_1 \) | 124 \cdot 2^i - 31 \cdot 2^{2i-13} - 43 | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_2 \) | 124 \cdot 2^i - 31 \cdot 2^{2i-14} - 41 | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_3 \) | 124 \cdot 2^i - 75 | 1 | 2^{i+1} |
| \( e_4 \) | 124 \cdot 2^i - 31 \cdot 2^{2i-13} - 40 | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_5 \) | 124 \cdot 2^i - 31 \cdot 2^{2i-14} - 40 | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_6 \) | 124 \cdot 2^i - 31 \cdot 2^{2i-13} - 41 | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_7 \) | 124 \cdot 2^i - 31 \cdot 2^{2i-14} - 35 | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_8 \) | 124 \cdot 2^i - 31 \cdot 2^{2i-13} - 37 | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_9 \) | 124 \cdot 2^i - 31 \cdot 2^{2i-14} - 37 | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_{10} \) | 124 \cdot 2^i - 31 \cdot 2^{2i-13} - 35 | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_{11} \) | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_{12} \) | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_{13} \) | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_{14} \) | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_{15} \) | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_{16} \) | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_{17} \) | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_{18} \) | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
| \( e_{19} \) | 31 \cdot 2^{2i-1} - 31 | 2^{i+1} |
\[ e \in E(h_{n-1}), \text{ we get } n_n(e) = 11 \text{ for four of edges, } n_n(e) = 19 \text{ for other two edges, and there are } 2^{n-1} \text{ such hexagons.} \]

Continue such computation until we reach the first stage. If \( e \in E(h_1) \), we obtain \( n_n(e) = 4 \cdot 2^n - 5 \) for four of edges, \( n_n(e) = 8 \cdot 2^n - 13 \) for other two edges, and there are two such hexagons. Suppose that \( e \in E(h_2) \) for all six edges, we have \( n_n(e) = 8 \cdot 2^n - 6 \) and there are two such hexagons.

Next, we determine the value of \( n_n(e) \) for \( e_{i-1} \) (the presentation of edges can be referred to Figure 4). Obviously, we infer \( n_n(e_{n-1}) = 6, n_n(e_{n-2}) = 7, n_n(e_{n-1}) = 8 \) and there are \( 2^n \) such edges. Moreover, we deduce \( n_n(e_{n-1}) = 22, n_n(e_{n-2}) = 23, n_n(e_{n-1}) = 24 \) and there are \( 2^{n-1} \) such edges. Continue such computation until we reach the first stage. We check that \( n_n(e_{1}) = 8 \cdot 2^n - 10, n_n(e_{0}) = 8 \cdot 2^n - 9 \) and there are two such edges. Assume that \( e \) is the edge between two central hexagons, we verify \( n_n(e) = 8 \cdot 2^n - 3 \).

In terms of the definition of distance-based indices, we get

\[
\begin{align*}
ABC_2(G_n) &= \sum_{i=1}^{n} 2^i \left( 2 \sqrt{\frac{16 \cdot 2^n - 8}{(16 \cdot 2^n - 13)(16 \cdot 2^n - 16 \cdot 2^{n-1} + 7)} + 4 \sqrt{\frac{16 \cdot 2^n - 8}{(8 \cdot 2^{n-5} - 5)(16 \cdot 2^n - 8 \cdot 2^{n-1} - 1)}} \right) \\
+ 6 \sqrt{\frac{16 \cdot 2^n - 8}{8 \cdot 2^n(8 \cdot 2^n - 6)}} + \sum_{i=2}^{n} 2^i \left( \sqrt{\frac{16 \cdot 2^n - 8}{(16 \cdot 2^n - 10)(16 \cdot 2^n - 16 \cdot 2^{n-1} + 4)}} \right) \\
+ \sqrt{\frac{16 \cdot 2^n - 8}{(16 \cdot 2^n - 9)(8 \cdot 2^n - 9)(8 \cdot 2^n - 3)}},
\end{align*}
\]

\[
\begin{align*}
GA_2(G_n) &= \sum_{i=1}^{n} 2^i \left( 2 \sqrt{\frac{16 \cdot 2^n - 8}{(16 \cdot 2^n - 13)(16 \cdot 2^n - 16 \cdot 2^{n-1} + 7)} + 4 \sqrt{\frac{8 \cdot 2^n - 5}{(16 \cdot 2^n - 8 \cdot 2^{n-1} - 1)}} \right) \\
+ 6 \sqrt{\frac{8 \cdot 2^n(8 \cdot 2^n - 3)}{8 \cdot 2^n - 3}} + \sum_{i=2}^{n} 2^i \left( \sqrt{\frac{16 \cdot 2^n - 8}{(16 \cdot 2^n - 10)(16 \cdot 2^n - 16 \cdot 2^{n-1} + 4)}} \right) \\
+ \sqrt{\frac{16 \cdot 2^n - 8}{(16 \cdot 2^n - 9)(8 \cdot 2^n - 9)(8 \cdot 2^n - 3)}},
\end{align*}
\]

\[
\begin{align*}
\pi_1(G_n) &= 320 \cdot 2^{2n} - 264 \cdot 2^n + 54, \\
\pi_1(G_n, x) &= (20 \cdot 2^n - 9)x^{16 \cdot 2^{n-6}},
\end{align*}
\]

\[
\begin{align*}
Sz(G_n, x) &= \sum_{i=1}^{n} 2^i \left( 2x^{(16 \cdot 2^n - 13)(16 \cdot 2^n - 16 \cdot 2^{n-1} + 7)} + 4x^{(8 \cdot 2^{n-5} - 5)(16 \cdot 2^n - 8 \cdot 2^{n-1} - 1)}) \\
+ 6x^{8 \cdot 2^n(8 \cdot 2^n - 6)} + \sum_{i=2}^{n} 2^i \left( x^{(16 \cdot 2^n - 10)(16 \cdot 2^n - 16 \cdot 2^{n-1} + 4)} \\
+ x^{(16 \cdot 2^n - 9)(16 \cdot 2^n - 16 \cdot 2^{n-1} + 3)} + x^{(16 \cdot 2^n - 8)(16 \cdot 2^n - 16 \cdot 2^{n-1} + 2)} \\
+ 2 \left( x^{(8 \cdot 2^n - 10)(8 \cdot 2^n + 4)} + x^{(8 \cdot 2^n - 9)(8 \cdot 2^n + 3)} + x^{(8 \cdot 2^n - 3)} \right),
\end{align*}
\]

\[
\begin{align*}
Sz^*_p(G_n) &= 1792n \cdot 2^n + 1344n \cdot 2^n - 3553 \cdot 2^n + 3142 \cdot 2^n + 561.
\end{align*}
\]
2.3. Edge distance-based indices of one-heptagonal carbon nanocones

As a supplement, we present the edge distance-based indices of one-heptagonal carbon nanocones $\text{CNC}_7[n]$ which is widely used in chemical engineering. The detail molecular structure and some important results can be found (Adil, Assal, Khan, Al-Warthan, & Siddiqui, 2013; Alipour & Ashrafi, 2009; Ashrafi & Gholami-Nezhaad, 2009; Doynov, Bozadjiev, Dimitrov, & Bozadjiev, 2011; Siddiqui, Warad, Adil, Mahfouz, & Al-Arifi, 2012). In view of molecular structure analysis, we get $|E(\text{CNC}_7[n])| = \frac{7}{2}(3n^2 + 5n + 2)$. The whole molecular graph $\text{CNC}_7[n]$ can be divided into seven parts since its symmetry structure and the center is $C_7$. Hence, by means of its symmetry, the edge distance-based indices can be calculated and stated as follows.
\[
\begin{align*}
ABC_s(CNC_3[n]) &= \frac{7(n+1)}{2} \sqrt{9n^2 + 15n + 4} + 7 \sum_{j=1}^{n} (n+j+1) \sqrt{\frac{21n^2 + 33n + 4 - j}{2}} \\
& \quad - \left( \frac{3}{2} j^2 + (3n + \frac{3}{2})j - (n+1) \right) \left( \frac{7}{2} (3n^2 + 5n + 2) - \frac{3}{2} j^2 - (3n + \frac{5}{2})j \right),
\end{align*}
\]

\[
\begin{align*}
GA_s(CNC_3[n]) &= 7(n+1) + 7 \sum_{j=1}^{n} (n+j+1) \sqrt{\frac{21n^2 + 33n + 4 - j}{2}} \\
& \quad - \left( \frac{3}{2} j^2 + (3n + \frac{3}{2})j - (n+1) \right) \left( \frac{7}{2} (3n^2 + 5n + 2) - \frac{3}{2} j^2 - (3n + \frac{5}{2})j \right),
\end{align*}
\]

\[
\begin{align*}
PI(CNC_3[n], x) &= 7(n+1)x^{9n^2 + 15n + 6} + 7 \sum_{j=1}^{n} (n+j+1)x^{\frac{21n^2 + 33n + 4 - j}{2}},
\end{align*}
\]

\[
\begin{align*}
Sz_s(CNC_3[n], x) &= 7(n+1)x^{\frac{1}{3}(3n^3 + 5n + 2)j} + 7 \sum_{j=1}^{n} (n+j+1)x^{\frac{1}{3}(3n^3 + 5n + 2)j - (n+1)j} \left( \frac{7}{2} (3n^2 + 5n + 2) - \frac{3}{2} j^2 - (3n + \frac{5}{2})j \right),
\end{align*}
\]

\[
\begin{align*}
Sz_s^*(CNC_3[n]) &= \frac{2835}{16} n^6 + \frac{37023}{40} n^5 + \frac{32319}{16} n^4 + \frac{9443}{4} n^3 + \frac{3129}{2} n^2 + \frac{11221}{20} n + \frac{343}{4},
\end{align*}
\]

3. Conclusion

In our paper, according to the analysis of molecular graph, structural, distance calculating, and mathematical derivation, we mainly determine the distance-based indices of two classes of dendrimers: TTF and 4,4′-bipyridinium dendrimer. As supplement conclusion, we report the edge distance-based indices of CNC_3[n]. The theoretical formulations obtained in our work illustrate the promising prospects of their application for the pharmacy and chemical engineering.

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