Calculating of degree-based topological indices of nanostructures

Wei Gao\textsuperscript{a}, M. R. Rajesh Kanna\textsuperscript{b}, E. Suresh\textsuperscript{c} and Mohammad Reza Farahani\textsuperscript{d}

\textsuperscript{a}School of Information Science and Technology, Yunnan Normal University, Kunming, China; \textsuperscript{b}Department of Mathematics, Maharani’s Science College for Women, Mysore, India; \textsuperscript{c}Department of Mathematics, Velammal Engineering College, Chennai, India; \textsuperscript{d}Department of Applied Mathematics, Iran University of Science and Technology, Tehran, Iran

**ABSTRACT**

A larger amount of studies reveal that there is strong inherent connection between the chemical characteristics of nanostructures and their molecular structures. Degree-based topological indices introduced on these chemical molecular structures can help material scientists better understand its chemical and biological features, thus they can make up for the lack of chemical experiments. In this paper, by means of edge dividing trick, we present several degree-based indices of special widely employed nanostructures: SC\textsubscript{C}\textsubscript{[p,q]} nanotubes, polyphenylene dendrimers, H-Naphtalenic nanotubes \textit{NPX}\textsubscript{[m,n]}, \textit{TUC}\textsubscript{[m,n]} nanotubes and PAMAM dendrimers.

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1. Introduction

As the development of nanotechnology, more and more of nanomaterials are emerging every year. Thus, identification of the chemical properties of these nanomaterials has become more and more cumbersome. Fortunately, previous studies have shown that chemical characteristics of nanomaterials and their molecular structures are closely related. By defining the chemical topological indices to study indicators of these nanostructures can help researchers to determine their chemical properties, which make up for the chemical experiments defects.

Specifically, the nanostructure is modelled as a graph, where each vertex represents an atom and each edge denotes a chemical bond between two atoms. Let \( G \) be a (molecular) graph with vertex set \( V(G) \) and edge set \( E(G) \). A topological index can be regarded as a real-valued function \( f: G \rightarrow \mathbb{R}^+ \) which maps each nanostructure to a real number. As numerical descriptors of the molecular structure yielded from the corresponding nanostructures, topological indices have been proofed several applications in nanoengineering, for example, QSPR/QSAR study. In the past years, harmonic index, Wiener index, sum connectivity index were introduced to measure certain structural features of nanomolecules. There were several papers contributing to determine these topological indices of special molecular graph in chemical engineering (See Hosamani (2016), (Gao & Farahani, 2016; Gao & Wang, 2014, 2015, 2016, 2017), Gao and Farahani (2016), and (Gao, Farahani, & Jamil, 2016; Gao, Farahani, & Shi, 2016; Gao, Siddiqui, Imran, Jamil, & Farahani, 2016; Gao, Wang, & Farahani, 2016) for more detail). The notations and terminologies used but not clearly defined in our article can be referred in book (Bondy & Mutry, 2008) written by Bondy and Mutry.

Bollobas and Erdos (1998) defined the general Randic index which was stated as follows:

\[
R_k(G) = \sum_{u \in V(G)} (d(u)d(v))^k,
\]

where \( k \) is a real number and \( d(u) \) denotes the degree of vertex \( u \) in molecular graph \( G \). Liu and Gutman (2007) determined the estimating for general Randic index and its special cases. Throughout, we always assume that \( k \) is a real number.

By taking \( k = 1 \) and \( k = -1 \), formula (1) then becomes the second Zagreb index \((M_2(G))\) and the modified second Zagreb index \((M_2^*(G))\), respectively:

\[
M_2(G) = \sum_{u \in V(G)} d(u)d(v), \quad M_2^*(G) = \sum_{u \in V(G)} \frac{1}{d(u)d(v)}.
\]

Zhou and Trinajstic (2010) introduced the general sum connectivity index as follows:

\[
\chi_k(G) = \sum_{u \in V(G)} (d(u) + d(v))^k.
\]

By taking \( k = \frac{1}{2} \), formula (2) becomes the sum connectivity index \((\chi(G))\) which is formulated by:

\[
\chi(G) = \sum_{u \in V(G)} (d(u) + d(v))^{\frac{1}{2}}.
\]
Gao and Wang (2016) introduced the general harmonic index as:

$$H_k(G) = \sum_{uv \in E(G)} \left( \frac{2}{d(u) + d(v)} \right)^k. \quad (3)$$

If we take $k = 1$ in formula (3), then it becomes a normal harmonic index which was described by:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}.$$

Eliasi and Iranmanesh (2011) reported the ordinary geometric–arithmetic index (or, called general geometric–arithmetic index) as the extension of geometric–arithmetic index which was stated as follows:

$$OGA_k(G) = \sum_{uv \in E(G)} \left( \frac{2 \sqrt{d(u) d(v)}}{d(u) + d(v)} \right)^k. \quad$$

Clearly, GA (geometric–arithmetic) index is a special case of ordinary geometric–arithmetic index when $k = 1$.

Azari and Iranmanesh (2011) proposed the generalized Zagreb index of molecular graph $G$ expressed by:

$$M_{t_1, t_2}(G) = \sum_{uv \in E(G)} (d(u)^{t_1} d(v)^{t_2} + d(u)^{t_2} d(v)^{t_1}),$$

where $t_1$ and $t_2$ are arbitrary non-negative integers.

Several polynomials related to degree-based indices are also introduced. For instance, the first and the second Zagreb polynomials are expressed by:

$$M_1(G, x) = \sum_{uv \in E(G)} x^{d(u) + d(v)}$$

and

$$M_2(G, x) = \sum_{uv \in E(G)} x^{d(u)d(v)},$$

respectively.

Moreover, the third Zagreb index and third Zagreb polynomial are denoted as:

$$M_3(G) = \sum_{uv \in E(G)} |d(u) - d(v)|$$

and

$$M_3(G, x) = \sum_{uv \in E(G)} x^{d(u) - d(v)}.$$

The multiplicative version of first and second Zagreb indices were introduced by Gutman (2011) and Ghorbani and Azimi (2012) as follows:

$$PM_1(G) = \prod_{e=uv \in E(G)} (d(u) + d(v)),$$

and

$$PM_2(G) = \prod_{e=uv \in E(G)} (d(u)d(v)).$$

Several conclusions on $PM_1(G)$ and $PM_2(G)$ can be referred to Eliasi, Iranmanesh, and Gutma (2012) and Xu and Das (2012).

Furthermore, Ranjini, Lokesha, and Usha (2013) re-defined the Zagreb indices, i.e., the redefined first, second and third Zagreb indices of a (molecular) graph $G$ were manifested as follows:

$$\text{ReZG}_1(G) = \sum_{e=uv \in E(G)} \frac{d(u) + d(v)}{d(u)d(v)},$$

$$\text{ReZG}_2(G) = \sum_{e=uv \in E(G)} \frac{d(u)d(v)}{d(u) + d(v)}$$

and

$$\text{ReZG}_3(G) = \sum_{e=uv \in E(G)} d(u)d(v)(d(u) + d(v)),$$

respectively.

Although there have been several advances in distance-based indices of molecular graphs, the study of degree-based indices for special nanomolecular structures are still largely limited. In addition, as widespread and critical nanostructures, $SC_5C_7[p, q]$ nanotubes, polyphenylene dendrimers, H-Naphthalenic nanotubes $NPHX[m, n]$, $TUC_4[m, n]$ nanotubes and PAMAM dendrimers are widely used in medical science and material field. For these reasons, we give the exact expressions of above-mentioned degree-based indices for these nanostructures.

The rest of the context is arranged as follows: first, we present the degree-based indices of $SC_5C_7[p, q]$ nanotubes; then, the nanostructure of polyphenylene dendrimers are considered; third, we focus on the H-Naphtalenic nanotubes $NPHX[m, n]$; the degree-based indices computation of $TUC_4[m, n]$ nanotubes are presented in Section 5; at last, we consider three kinds of PAMAM dendrimers: $PD[1][n], PD[2][n]$ and $DS[1][n].$

2. Degree-based indices of $SC_5C_7[p, q]$ nanotubes

The purpose of this section is to manifest several degree-based indices of $SC_5C_7[p, q]$ nanotubes. Actually, this nanotube is a kind of $C_5C_7$-net which is obtained by alternating $C_5$ and $C_7$. This classical tiling of $C_5$ and $C_7$ can either cover a cylinder or a torus. A period of $SC_5C_7[p, q]$ (here $p$ is the number of heptagons in each row and $q$ is the number of periods in whole lattice) is consisted of three rows (see Figure 1 for more details on $i$-th period). Clearly, there are $8p$ vertices in one period of the lattice, and thus $|V(SC_5C_7[p, q])| = 8pq$. Using the similar fashion, there are $12p$ edges in one period and exists $2p$ extra edges joined to the end of this nanostructure. Therefore, we have $|E(SC_5C_7[p, q])| = 12pq - 2p.$
The main technique in this paper to obtain the desired conclusion is edge dividing approach. Throughout this paper, we use the following notations for edge dividing.

Let \( \delta(G) \) and \( \Delta(G) \) be the minimum and maximum degree of \( G \). We divide edge set \( E(G) \) and vertex set \( V(G) \) into several partitions: for any \( i, \delta(G) \leq i \leq 2 \Delta(G), \) let \( E_i = \{ e = uv \in E(G) | d(v) + d(u) = i \} \); for any \( j, (\delta(G))^2 \leq j \leq (\Delta(G))^2, \) let \( E_j = \{ e = uv \in E(G) | d(v) = d(u) = j \} \) and for any \( k, \delta(G) \leq k \leq \Delta(G), \) let \( V_k = \{ v \in V(G) | \ d(v) = k \}. \)

Now, we state the main conclusion in this section.

**Theorem 1:**

\[
R_k(\text{SC}_5 \text{C}_7[p, q]) = (12pq - 9p) \cdot 9^k + 6p \cdot 6^k + p \cdot 4^k, \\
\chi_k(\text{SC}_5 \text{C}_7[p, q]) = (12pq - 9p) \cdot 6^k + 6p \cdot 5^k + p \cdot 4^k, \\
H_k(\text{SC}_5 \text{C}_7[p, q]) = (12pq - 9p) \cdot \left(\frac{1}{3}\right)^k + 6p \cdot \left(\frac{2}{5}\right)^k + p \cdot \left(\frac{1}{2}\right)^k, \\
O\text{GA}_k(\text{SC}_5 \text{C}_7[p, q]) = (12pq - 8p) + 6p \cdot \left(\frac{2}{\sqrt{5}}\right)^k, \\
M_{\{i, j\}}(\text{SC}_5 \text{C}_7[p, q]) = (24pq - 18p) \cdot 3^{i+j} + 6p \cdot (2^i 3^j + 2^j 3^i) + p \cdot 2^{i+j+1}, \\
M_1(\text{SC}_5 \text{C}_7[p, q], x) = (12pq - 9p)x^6 + 6px^5 + px^4, \\
M_2(\text{SC}_5 \text{C}_7[p, q], x) = (12pq - 9p)x^6 + 6px^5 + px^4, \\
M_3(\text{SC}_5 \text{C}_7[p, q], x) = 6px + (12pq - 8p), \\
PM_1(\text{SC}_5 \text{C}_7[p, q]) = 6^{12pq - 9p} 5^{6p} 4^p, \\
PM_2(\text{SC}_5 \text{C}_7[p, q]) = 9^{12pq - 9p} 6^{6p} 4^p, \\
\text{Re}\text{ZG}_1(\text{SC}_5 \text{C}_7[p, q]) = 8pq, \\
\text{Re}\text{ZG}_2(\text{SC}_5 \text{C}_7[p, q]) = 18pq - \frac{3}{10}p.
\]

**Proof:** By observation of nanostructure \( \text{SC}_5 \text{C}_7[p, q] \), we infer three partitions of edge set:

- \( E_1 \) or \( E_2^* \): \( d(u) = d(v) = 2 \);
- \( E_6 \) or \( E_3^* \): \( d(u) = d(v) = 3 \);
- \( E_5 \) or \( E_4^* \): \( d(u) = 2 \) and \( d(v) = 3 \).

Furthermore, we get \(|E_1^*| = |E_2| = |E_3^*| = 6p, |E_6| = |E_4^*| = 12pq - 9p). Then, the result follows from the definitions of these degree-based indices.

**Remark 1:** From what we have deduced in Theorem 1, we yield that

\[
M_1^*(\text{SC}_5 \text{C}_7[p, q]) = \frac{4}{3}pq + \frac{p}{4}, \\
H(\text{SC}_5 \text{C}_7[p, q]) = 4pq - \frac{1}{10}p, \\
M_1(\text{SC}_5 \text{C}_7[p, q]) = 6p.
\]

### 3. Degree-based indices of polyphenylene dendrimers

The aim of this section is to show the degree-based indices of polyphenylene dendrimers \( D_n[n] \) and \( D_n[n]\), where \( n \in \mathbb{N} \). These two molecular structures are widely appeared in the nanomaterials. The kernel structure of \( D_n[n] \) and \( D_n[n]\) can be referred to Figure 2.

Additionally, the following Figure 3 present the \( D_n[n] \) with three growth stages.

The main results in this section are manifested as follows:

**Theorem 2:**

\[
R_k(D_n[n]) = 4 \cdot 12^k + (36 \cdot 2^n - 36) \cdot 9^k + (48 \cdot 2^n - 40) \cdot 6^k + (56 \cdot 2^n - 40) \cdot 4^k, \\
\chi_k(D_n[n]) = 4 \cdot 2^k + (36 \cdot 2^n - 36) \cdot 6^k + (48 \cdot 2^n - 40) \cdot 5^k + (56 \cdot 2^n - 40) \cdot 4^k, \\
H_k(D_n[n]) = 4 \cdot \left(\frac{2}{5}\right)^k + (36 \cdot 2^n - 36) \cdot \left(\frac{1}{3}\right)^k \\
+ (48 \cdot 2^n - 40) \cdot \left(\frac{2}{5}\right)^k \\
+ (56 \cdot 2^n - 40) \cdot \left(\frac{1}{2}\right)^k.
\]
Figure 2. The kernel of $D_4[n]$ and $D_2[n]$, respectively.

Figure 3. Polyphenylene dendrimers $D_2[n]$ with three growth stages.

$OGA_k(D_4[n]) = 4 \cdot \left(\frac{4 \sqrt{3}}{7}\right)^k + (48 \cdot 2^n - 40) \cdot \left(\frac{2 \sqrt{6}}{5}\right)^k + (92 \cdot 2^n - 76),$

$M_{1,0}(D_4[n]) = 4 \cdot \left(3^i 4^i + 4^i 3^i\right)$
$+ (72 \cdot 2^n - 72) \cdot 3^{i+1},$
$+ (48 \cdot 2^n - 40) \cdot (2^{i+1} 3^i + 2^i 3^{i+1}),$
$+ (56 \cdot 2^n - 40) \cdot 2^{i+1} 3^{i+1},$

$M_1(D_4[n], x) = 4x^7 + (36 \cdot 2^n - 36)x^6$
$+ (48 \cdot 2^n - 40)x^5 + (56 \cdot 2^n - 40)x^4,$

$M_2(D_4[n], x) = 4x^{12} + (36 \cdot 2^n - 36)x^9$
$+ (48 \cdot 2^n - 40)x^6 + (56 \cdot 2^n - 40)x^4,$

$M_3(D_4[n], x) = (48 \cdot 2^n - 36)x + (92 \cdot 2^n - 76),$

$PM_1(D_4[n]) = 2401 \cdot 6^{36 \cdot 2^n - 36} 4^{36 \cdot 2^n - 40} 4^{36 \cdot 2^n - 40},$

$PM_2(D_4[n]) = 20736 \cdot 9^{36 \cdot 2^n - 36} 6^{48 \cdot 2^n - 40} 4^{36 \cdot 2^n - 40},$

$ReZG_1(D_4[n]) = 120 \cdot 2^n - 95,$
ReZG$_2(D_4[n]) = \frac{838}{5} \cdot 2^n - \frac{946}{7}$,

ReZG$_3(D_4[n]) = 4280 \cdot 2^n - 3448$.

**Proof:** By observation of polyphenylene dendrimers $D_4[n]$, we infer four partitions of edge set:

- $E_1$ (or $E'_1$): $d(u) = d(v) = 2$;
- $E_6$ (or $E'_6$), $d(u) = d(v) = 3$;
- $E_5$ (or $E'_5$), $d(u) = 2$ and $d(v) = 3$;
- $E_7$ (or $E'_7$), $d(u) = 3$ and $d(v) = 4$.

Furthermore, we get $|E_1| = |E'_1| = 56 \cdot 2^n - 40$, $|E_6| = |E'_6| = 48 \cdot 2^n - 40$, $|E_5| = |E'_5| = 36 \cdot 2^n - 36$, and $|E_7| = |E'_7| = 6$. Then, the result follows from the definitions of these degree-based indices.

**Remark 2:** From what we have obtained in Theorem 2, we yield that

$$M_1(D_4[n]) = 680 \cdot 2^n - 548,$$

$$M_2(D_4[n]) = 836 \cdot 2^n - 676,$$

$$M_3(D_4[n]) = 26 \cdot 2^n - \frac{61}{3},$$

$$\chi(D_4[n]) = \frac{4}{\sqrt{7}} + \frac{36 \cdot 2^n - 36}{\sqrt{6}} + \frac{48 \cdot 2^n - 40}{\sqrt{5}} + 28 \cdot 2^n - 20,$$

$$H(D_4[n]) = \frac{296}{5} \cdot 2^n - 47,$$

$$GA(D_4[n]) = \frac{16 \sqrt{3}}{7} + (96 \cdot 2^n - 80) \frac{\sqrt{5}}{5} + (92 \cdot 2^n - 76),$$

$$M_5(D_4[n]) = 48 \cdot 2^n - 36.$$

**Theorem 3:** $R_k(D_2[n]) = (36 \cdot 2^n - 35) \cdot 9^k + (48 \cdot 2^n - 44) \cdot 6^k + (56 \cdot 2^n - 48) \cdot 4^k$,

$$\chi_k(D_2[n]) = (36 \cdot 2^n - 35) \cdot 6^k + (48 \cdot 2^n - 44) \cdot 5^k + (56 \cdot 2^n - 48) \cdot 4^k,$$

$$H_k(D_2[n]) = (36 \cdot 2^n - 35) \cdot \left(\frac{2}{3}\right)^k + (48 \cdot 2^n - 44) \cdot \left(\frac{2}{5}\right)^k + (56 \cdot 2^n - 48) \cdot \left(\frac{1}{2}\right)^k,$$

$$OGA_k(D_2[n]) = (48 \cdot 2^n - 44) \cdot \left(\frac{2 \sqrt{5}}{5}\right)^k + (92 \cdot 2^n - 83),$$

$$M_{(t,t)}(D_2[n]) = (72 \cdot 2^n - 70) \cdot 3^t \cdot 5^t + (48 \cdot 2^n - 44) \cdot (2^t \cdot 3^t + 2^t \cdot 3^t) + (56 \cdot 2^n - 48) \cdot 2^t \cdot 3^t \cdot 5^t,$$

$$M_1(D_2[n], x) = (36 \cdot 2^n - 35)x^6 + (48 \cdot 2^n - 44)x^5 + (56 \cdot 2^n - 48)x^4,$$

$$M_2(D_2[n], x) = (36 \cdot 2^n - 35)x^6 + (48 \cdot 2^n - 44)x^5 + (56 \cdot 2^n - 48)x^4,$$

$$M_3(D_2[n], x) = (48 \cdot 2^n - 44)x + (92 \cdot 2^n - 83),$$

$$PM_1(D_2[n]) = 56 \cdot 2^n - 48,$$

$$PM_2(D_2[n]) = 48 \cdot 2^n - 44,$$

$$PM_3(D_2[n]) = 36 \cdot 2^n - 35.$$
\[ GA(D_2[n]) = (96 \cdot 2^n - 88) \frac{\sqrt{6}}{5} + (92 \cdot 2^n - 83), \]

\[ M_3(D_2[n]) = 48 \cdot 2^n - 44. \]

### 4. Degree-based indices of H-Naphtalenic nanotubes

In this part, we consider the degree-based indices of H-Naphtalenic nanotubes \(NPHX[m, n]\) (here \(m\) is denoted as the number of pairs of hexagons in first row and \(n\) is represented as the number of alternative hexagons in a column) which is a trivalent decoration with sequence of \(C_6, C_6, C_6, C_6, C_6, C_6, \ldots\) in the first row and a sequence of \(C_6, C_6, C_6, C_6, C_6, \ldots\) in the other rows. That is to say, this nanolattice can be regarded as a plane tiling of \(C_6, C_6\) and \(C_6\). Thus, such type of tiling can either cover a cylinder or a torus (see Figure 4 as an example). Moreover, we can verify that \(|V(NPHX[m, n])| = 10mn\) and \(|E(NPHX[m, n])| = 15mn - 2m\).

Now, we present the main results in this section.

**Theorem 4:** \(R_k(NPHX[m, n]) = (15mn - 10m) \cdot 9^k + 8m \cdot 6^k,\)

\[ \chi_k(NPHX[m, n]) = (15mn - 10m) \cdot 6^k + 8m \cdot 5^k, \]

\[ H_k(NPHX[m, n]) = (15mn - 10m) \cdot \left( \frac{1}{3} \right)^k + 8m \cdot \left( \frac{2}{5} \right)^k, \]

\[ OGA_k(NPHX[m, n]) = 15mn - 10m + 8m \cdot \left( \frac{2\sqrt{6}}{5} \right)^k, \]

\[ M_{\xi_{1,2}}(NPHX[m, n]) = (30mn - 20m) \cdot 3^{4t + t}, \]

\[ M_1(NPHX[m, n], x) = (15mn - 10m)x^6 + 8mx^5, \]

\[ M_2(NPHX[m, n], x) = (15mn - 10m)x^9 + 8mx^6, \]

\[ M_3(NPHX[m, n], x) = 8mx + (15mn - 10m), \]

\[ PM_1(NPHX[m, n]) = 6^{15mn-10m} 5^{8m}, \]

\[ PM_2(NPHX[m, n]) = 9^{15mn-10m} 6^{8m}, \]

\[ ReZG_1(NPHX[m, n]) = 10mn, \]

\[ ReZG_2(NPHX[m, n]) = \frac{45}{2} mn - \frac{27}{5} m, \]

\[ ReZG_3(NPHX[m, n]) = 810mn - 300m. \]

**Proof:**

By observation of H-Naphtalenic nanotubes \(NPHX[m, n]\), we know two partitions of edge set:

- \(E_6\) (or \(E_6^*\)), \(d(u) = d(v) = 3;\)
- \(E_5\) (or \(E_5^*\)), \(d(u) = 2\) and \(d(v) = 3.\)

**Figure 4.** The molecular structure of \(NPHX[n, n].\)
Moreover, it is not hard to check that $|E_6| = |E_5^*| = 8m$ and $|E_6| = |E_5^*| = 15mn - 10m$. Thus, we get the desired formulations in terms of the definitions of these degree-based indices. □

**Remark 4:** Using the conclusions obtained in Theorem 4, we yield that
\[
\begin{align*}
M_1(NPHX[m, n]) &= 90mn - 20m, \\
M_2(NPHX[m, n]) &= 135mn - 42m, \\
M_2^*(NPHX[m, n]) &= \frac{5}{3}mn + \frac{2}{9}m, \\
H(NPHX[m, n]) &= 5mn - \frac{2}{15}m, \\
M_3(NPHX[m, n]) &= 8m.
\end{align*}
\]

**5. Degree-based indices of TUC\(_4\) [m, n] nanotubes**

In this part, we discuss the degree-based indices of TUC\(_4\)[m, n] nanotubes (here \(m\) is denoted as the number of squares in a row and \(n\) is represented as the number of squares in a column) which is a plane tiling of \(C_4\). This tessellation of \(C_4\) can either cover a cylinder or a torus. We verify that \(|V(TUC_4[m, n])| = m(n + 1)\) and \(|E(TUC_4[m, n])| = 2mn + m\). Figure 5 describes the 3D representation of this kind of nanostructure.

Again, using the trick of edge dividing, we get the following statement.

**Theorem 5:**
\[
\begin{align*}
R_k(TUC_4[m, n]) &= 2m \cdot 9^k + 2m \cdot 12^k + m \times (2n - 3) \cdot 16^k, \\
\chi_k(TUC_4[m, n]) &= 2m \cdot 6^k + 2m \cdot 7^k + m(2n - 3) \cdot 8^k, \\
H_k(TUC_4[m, n]) &= 2m \cdot \left(\frac{1}{3}\right)^k + 2m \cdot \left(\frac{2}{7}\right)^k + m(2n - 3) \cdot \left(\frac{1}{4}\right)^k, \\
OGA_k(TUC_4[m, n]) &= 2mn - m + 2m \cdot \left(\frac{4 \sqrt{3}}{7}\right)^k, \\
M_1(t_i, t_j)(TUC_4[m, n]) &= 4m \cdot 3^{i + j} + 2m \cdot (3^i 4^j + 3^j 4^i) + m(2n - 3) \cdot 2^{2i + 2j + 1}, \\
M_1(TUC_4[m, n], x) &= 2mx^6 + 2mx^7 + m(2n - 3)x^8, \\
M_2(TUC_4[m, n], x) &= 2mx^9 + 2mx^{12} + m(2n - 3)x^{16}, \\
M_3(TUC_4[m, n], x) &= 2mx + (2mn - m), \\
PM_1(TUC_4[m, n]) &= 6^m 7^m 8^m (2m - 5)^m, \\
PM_2(TUC_4[m, n]) &= 9^m 12^m 16^m (2m - 3)^m, \\
ReZG_1(TUC_4[m, n]) &= mnn - m, \\
ReZG_2(TUC_4[m, n]) &= 4mn + \frac{3}{7}m, \\
ReZG_3(TUC_4[m, n]) &= 256mn - 108m.
\end{align*}
\]

**Proof:** By observation of TUC\(_4\)[m, n] nanotubes, we ensure that its edge set can be divided into three partitions:

- \(E_6\) (or \(E_5^*\)), \(d(u) = d(v) = 3\);
- \(E_7\) (or \(E_1^*\)), \(d(u) = 3\) and \(d(v) = 4\);
- \(E_8\) (or \(E_1^*\)), \(d(u) = d(v) = 4\).

Moreover, it is not hard to check that \(|E_6| = |E_5^*| = 2m\), \(|E_7| = |E_1^*| = 2m\) and \(|E_8| = |E_1^*| = 2m(2n - 3)\). Therefore, we obtain the desired formulations in terms of the definitions of these degree-based indices. □

**Remark 5:** According to results presented in Theorem 5, we have
\[
\begin{align*}
M_1(TUC_4[m, n]) &= 16mn + 2m, \\
M_2(TUC_4[m, n]) &= 32mn - 6m, \\
M_2^*(TUC_4[m, n]) &= \frac{1}{8}mn + \frac{13}{144}m, \\
H(TUC_4[m, n]) &= \frac{1}{2}mn + \frac{41}{84}m, \\
M_3(TUC_4[m, n]) &= 2m.
\end{align*}
\]

**Figure 5.** The 3D expression of TUC\(_4\)[6, n].
6. Degree-based indices of PAMAM dendrimers

In this section, we first discuss the degree-based indices of PAMAM dendrimers with trifunctional core unit constructed by dendrimer generations $G_n$ with $n$ growth stages. We use $PD_1$ to denote this nanostructures with $n$ growth stages.

**Theorem 6:** $R_1(PD_1) = 3 \cdot 2^n \cdot 2^k + (6 \cdot 2^n - 3) \cdot 3^k + (18 \cdot 2^n - 9) \cdot 4^k + (21 \cdot 2^n - 12) \cdot 6^k$,

$\chi_1(PD_1) = 3 \cdot 2^n \cdot 3^k + (24 \cdot 2^n - 12) \cdot 4^k + (21 \cdot 2^n - 12) \cdot 5^k$,

$H_1(PD_1) = (3 \cdot 2^n) \cdot \left(\frac{2}{3}\right)^k + (24 \cdot 2^n - 12) \cdot \left(\frac{1}{2}\right)^k + (21 \cdot 2^n - 12) \cdot \left(\frac{2}{3}\right)^k$,

$O_{GA_1}(PD_1) = 3 \cdot 2^n \cdot \left(\frac{2\sqrt{2}}{3}\right)^k + (6 \cdot 2^n - 3) \cdot \left(\frac{\sqrt{3}}{2}\right)^k + (18 \cdot 2^n - 9) \cdot (21 \cdot 2^n - 12) \cdot \left(\frac{2\sqrt{6}}{5}\right)^k$,

$M_{[v,d]}(PD_1) = 3 \cdot 2^n (2^v + 2^h) + (6 \cdot 2^n - 3) (3^v + 3^h) + (18 \cdot 2^n - 9) 21 \cdot 2^n$,

$M_1(PD_1,x) = 3 \cdot 2^n x^3 + (24 \cdot 2^n - 12)x^4 + (21 \cdot 2^n - 12)x^5$,

$M_3(PD_1,x) = 3 \cdot 2^n x^2 + (6 \cdot 2^n - 3)x^3 + (18 \cdot 2^n - 9)x^4 + (21 \cdot 2^n - 12)x^5$,

$PM_1(PD_1) = 3^{3 \cdot 2^n} \cdot 2^{24 \cdot 2^n - 12} \cdot 5^{21 \cdot 2^n - 12}$,

$PM_2(PD_1) = 2^{3 \cdot 2^n} \cdot 3^{6 \cdot 2^n - 3} \cdot 4^{18 \cdot 2^n - 9} \cdot 6^{21 \cdot 2^n - 12}$,

$ReZ_{G_1}(PD_1) = 48 \cdot 2^n - 23$,

$ReZ_{G_2}(PD_1) = 42 \cdot 2^n - \frac{85}{4}$,

$ReZ_{G_3}(PD_1) = 1008 \cdot 2^n - 540$.

**Proof:** By observation of PAMAM dendrimer $PD_1$, we ensure that its edge set can be divided into four partitions:

- $E_1$ (or $E_1^*$), $d(u) = 1$ and $d(v) = 2$;
- $E_2$, $d(u) = 1$ and $d(v) = 3$;
- $E_3$, $d(u) = d(v) = 2$;
- $E_4$ (or $E_4^*$), $d(u) = 2$ and $d(v) = 3$.

Moreover, it is not hard to check that $|E_1| = |E_2| = 3 \cdot 2^n$, $|E_3| = 6 \cdot 2^n - 3$, $|E_4| = 18 \cdot 2^n - 9$ and $|E_2| = |E_3| = 21 \cdot 2^n - 12$. At last, the results obtained by means of definitions of these degree-based indices.

**Remark 6:** By taking the special value of $k$ in results of Theorem 5, we get

$M_1(PD_1) = 210 \cdot 2^n - 108$,

$M_2(PD_1) = 222 \cdot 2^n - 117$,

$M_3(PD_1) = \frac{23}{2} \cdot 2^n - \frac{21}{4}$,

$\chi_1(PD_1) = \frac{3}{\sqrt{3}} \cdot 2^n + 12 \cdot 2^n - 6 + \frac{21 \cdot 2^n - 12}{\sqrt{5}}$,

$H_1(PD_1) = \frac{112}{5} \cdot 2^n - \frac{54}{5}$,

$GA_1(PD_1) = (6 \cdot 2^n - 3) \cdot \sqrt{\frac{3}{2}} + \left((18 \cdot 2 \sqrt{2}) \cdot 2^n - 9\right) + (42 \cdot 2^n - 24) \cdot \sqrt{\frac{6}{5}}$,

$M_1(PD_1) = 36 \cdot 2^n - 18$.

Next, we determine the degree-based indices of PAMAM dendrimer with different core constructed by dendrimer generations $G_n$ with $n$ growth stages. We use $PD_2$ to denote this nanostructures with $n$ growth stages.

**Theorem 7:** $R_1(PD_2) = 4 \cdot 2^n \cdot 2^k + (8 \cdot 2^n - 4) \cdot 3^k + (24 \cdot 2^n - 11) \cdot 4^k + (28 \cdot 2^n - 14) \cdot 6^k$,

$\chi_1(PD_2) = 4 \cdot 2^n \cdot 3^k + (32 \cdot 2^n - 15) \cdot 4^k + (28 \cdot 2^n - 14) \cdot 5^k$,

$H_1(PD_2) = (4 \cdot 2^n) \cdot \left(\frac{2}{3}\right)^k + (32 \cdot 2^n - 15) \cdot \left(\frac{1}{2}\right)^k + (28 \cdot 2^n - 14) \cdot \left(\frac{2}{5}\right)^k$,

$O_{GA_1}(PD_2) = 4 \cdot 2^n \cdot \left(\frac{2\sqrt{2}}{3}\right)^k + (8 \cdot 2^n - 4) \cdot \left(\frac{\sqrt{3}}{2}\right)^k + (24 \cdot 2^n - 11) + (28 \cdot 2^n - 14) \cdot \left(\frac{2\sqrt{6}}{5}\right)^k$,
\[ M_{1,2}(PD_2) = 4 \cdot 2^n (2^i + 2^j) + (8 \cdot 2^n - 4) (3^i + 3^j) \]
\[ + (24 \cdot 2^n - 11) 2^{i+1} \]
\[ + (28 \cdot 2^n - 14) (2^i 3^j + 2^j 3^i) , \]
\[ M_1(PD_2, x) = 4 \cdot 2^n x^2 + (32 \cdot 2^n - 15) x^4 \]
\[ + (28 \cdot 2^n - 14) x^6 , \]
\[ M_2(PD_2, x) = 4 \cdot 2^n x^2 + (8 \cdot 2^n - 4) x^4 \]
\[ + (24 \cdot 2^n - 11) x^6 \]
\[ + (28 \cdot 2^n - 14) x^8 , \]
\[ M_3(PD_2, x) = (8 \cdot 2^n - 4) x^2 + (32 \cdot 2^n - 14) x \]
\[ + (24 \cdot 2^n - 11) , \]
\[ PM_1(PD_2) = 3^{4 \cdot 2^n} 4^{32 \cdot 2^{n-15}} 5^{28 \cdot 2^{n-14}} , \]
\[ PM_2(PD_2) = 2^{4 \cdot 2^n} 3^{8 \cdot 2^{n-4}} 4^{24 \cdot 2^{n-11}} 6^{28 \cdot 2^{n-14}} , \]
\[ ReZG_1(PD_2) = 64 \cdot 2^n - 28 , \]
\[ ReZG_2(PD_2) = \frac{994}{15} \cdot 2^n - \frac{154}{5} , \]
\[ ReZG_3(PD_2) = 1344 \cdot 2^n - 644 . \]

**Proof:**  By analysis of PAMAM dendrimer PD_2 structures, we yield the four dividings of its edge set.

- \( E_1 \) (or \( E_2^{+} \)), \( d(u) = 1 \) and \( d(v) = 2 \);
- \( E_1^{-} \), \( d(u) = 1 \) and \( d(v) = 3 \);
- \( E_2^{+} \), \( d(u) = d(v) = 2 \);
- \( E_2^{-} \) (or \( E_2^{0} \)), \( d(u) = 2 \) and \( d(v) = 3 \).

Moreover, it is not hard to check that \( |E_1| = |E_2^+| = 4 \cdot 2^n, |E_1^-| = 8 \cdot 2^n - 4, |E_2^0| = 24 \cdot 2^n - 11 \) and \( |E_2^-| = |E_2^0| = 28 \cdot 2^n - 14 \). At last, the results obtained by means of the definitions of these degree-based indices.

**Remark 7:** By taking the special value of \( k \) in results of Theorem 7, we get

\[ M_1(PD_2) = 280 \cdot 2^n - 130 , \]
\[ M_2(PD_2) = 296 \cdot 2^n - 140 , \]
\[ M_3(PD_2) = \frac{46}{3} \cdot 2^n - \frac{77}{12} , \]
\[ \chi(PD_2) = \frac{4 \cdot 2^n - 9}{\sqrt{3}} + 16 \cdot 2^n - \frac{15}{2} + \frac{28 \cdot 2^n - 14}{\sqrt{5}} . \]

\[ H(PD_2) = \frac{688}{15} \cdot 2^n - \frac{131}{10} , \]
\[ GA(PD_2) = \frac{8 \sqrt{2}}{3} \cdot 2^n + (4 \cdot 2^n - 2) \sqrt{3} \]
\[ + (24 \cdot 2^n - 11) + (56 \cdot 2^n - 28) \cdot \frac{\sqrt{6}}{5} , \]
\[ M_2(PD_2) = 48 \cdot 2^n - 22 . \]

At last, we compute the degree-based indices of other kinds of PAMAM dendrimer \( DS_1 \) with \( n \) growth stages.

**Theorem 8:** \( R_1(DS_1) = (14 \cdot 3^n - 10) \cdot 4^k + (4 \cdot 3^n - 4) \cdot 8^k \),
\[ \chi_1(DS_1) = 4 \cdot 3^n \cdot 5^k + (10 \cdot 3^n - 10) \cdot 4^k \]
\[ + (4 \cdot 3^n - 4) \cdot 6^k , \]
\[ H_1(DS_1) = (4 \cdot 3^n) \cdot \left( \frac{2}{5} \right)^k + (10 \cdot 3^n - 10) \cdot \left( \frac{1}{2} \right)^k \]
\[ + (4 \cdot 3^n - 4) \cdot \left( \frac{1}{3} \right)^k , \]
\[ OGA_1(DS_1) = 4 \cdot 3^n \left( \frac{2}{5} \right)^k + (10 \cdot 3^n - 10) \]
\[ + (4 \cdot 3^n - 4) \cdot \left( \frac{2 \sqrt{2}}{3} \right)^k , \]
\[ M_{1,2}(DS_1) = 4 \cdot 3^n \cdot (4^n + 4^i) + (10 \cdot 3^n - 10) 2^{i+1} + (4 \cdot 3^n - 4) \cdot (2^{i+2} + 2^{2i+1}) , \]
\[ M_1(DS_1, x) = 4 \cdot 3^n x^5 + (10 \cdot 3^n - 10) x^4 + (4 \cdot 3^n - 4) x^6 , \]
\[ M_2(DS_1, x) = (14 \cdot 3^n - 10) x^4 + (4 \cdot 3^n - 4) x^8 , \]
\[ M_3(DS_1, x) = 4 \cdot 3^n x^5 + (4 \cdot 3^n - 4) x^2 + (10 \cdot 3^n - 10) , \]
\[ PM_1(DS_1) = 5^{4 \cdot 3^n} 4^{10 \cdot 3^n - 10} 6^{4 \cdot 3^n - 4} , \]
\[ PM_2(DS_1) = 2^{40 \cdot 3^n - 32} , \]
\[ ReZG_1(DS_1) = 18 \cdot 3^n - 13 , \]
\[ ReZG_2(DS_1) = \frac{278}{15} \cdot 3^n - \frac{46}{3} , \]
\[ ReZG_3(DS_1) = 432 \cdot 3^n - 352 . \]
**Proof:** By analysis of PAMAM dendrimer $DS_1$ structures, we found that the edge set of $DS_1$ can be divided into three parts.

- $E_1$, $d(u) = 1$ and $d(v) = 4$;
- $E_2$, $d(u) = d(v) = 2$;
- $E_3$ (or $E_5$), $d(u) = 2$ and $d(v) = 4$.

Additionally, it is not hard to check that $|E_1| = 4 \cdot 3^n$, $|E_2| = 10 \cdot 3^n - 10$, and $|E_3| = |E_5| = 4 \cdot 3^n - 4$. Finally, the results deduced according to the definitions of these degree-based indices.

**Remark 8:** Again, in view of taking the special value of $k$ in results of Theorem 8, we get

\[
M_1(DS_1) = 84 \cdot 3^n - 64, \quad M_2(DS_1) = 88 \cdot 3^n - 72, \quad M_3^*(DS_1) = 4 \cdot 3^n - 3, \quad \chi(DS_1) = \frac{4 \cdot 3^n}{\sqrt{5}} + 5 \cdot 3^n - 5 + \frac{4 \cdot 3^n - 4}{\sqrt{6}}, \quad H(DS_1) = \frac{119}{15} \cdot 3^n - \frac{19}{3}, \quad GA(DS_1) = \frac{16}{5} \cdot 3^n + (10 \cdot 3^n - 10) + (8 \cdot 3^n - 8) \cdot \frac{\sqrt{2}}{3}, \quad M_4(DS_1) = 20 \cdot 3^n - 8.
\]

**7. Conclusion**

In this paper, by means of nanomolecular graph structural analysis, edge dividing technology and mathematical derivation, we present the degree-based indices (including general Randic index, general sum connectivity index, general harmonic index, general geometric-arithmetic index, multiplicative Zagreb indices and redefined Zagreb indices) of certain important and widely used nanostructures such as $SC_nC_2[p,q]$ nanotubes, polyphenylene dendrimers, H-Naphthalic nanotubes $NPHX[m, n]$, $TUC_4[m, n]$ nanotubes and three classes of PAMAM dendrimers. The result achieved in our paper illustrates the promising prospects of the application for chemical engineering and nanomaterial manufacturing.

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