Three New/Old Vertex-Degree-Based Topological Indices of Some Dendrimers Structure

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Received: February 21, 2017; Accepted: March 23, 2017; Published: March 30, 2017

Review Article

Abstract

There is a natural linkage between the molecular structures and the bio-medical and pharmacology characteristics. A topological index can be considered as transformation of chemical structure into real number and has been used as a predictor parameter. There are certain vertex-degree-based topological indices which has been used extensively in the chemical graph theory but recently no further attention is given to these topological indices. These are the reciprocals Randić’ index (RR), the reduced reciprocal Randić’ index (RRR) and the reduced second Zagreb index RM_2. In this paper we determine reciprocal Randić’ index (RR), the reduced second Zagreb index RM_2, and the reduced reciprocal Randić’ index (RRR) of Poly (Propyl) Ether Imine, porphyrin and Zinc-Porphyrin dendrimers.

Keywords: Randić’ index; Zagreb index; Porphyrin dendrimers; Poly (propyl) ether imine dendrimer; Zinc porphyrin dendrimer

1. Introduction

Dendrimers are highly branched, star-shaped macromolecules with nanometer-scale dimensions. Dendrimers are defined by three components: a central core, an interior dendritic structure (the branches), and an exterior surface with functional surface groups. Dendrimers have a huge range of applications in all branches of chemistry, especially in host–guest reactions and self-assembly procedures. Dendrimers are used in the formation of nanotubes, nanolatex, chemical sensors, micro/macro capsules, coloured glass, modified electrodes, and photon funnels such as artificial antennas [1-13]. Because dendrimers are widely used in different applied fields, the study of nanostar dendrimers has received a great deal of attention in both chemical and mathematical literature [13-24].

Molecules and molecular compounds are often modeled by molecular graphs. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. A graph G (V, E) with vertex set V and edge set E is connected, if there exists a connection between any pair of vertices in G. For a graph G, the degree of a vertex v is the number of edges incident with v and denoted by deg (v).

A graph can be recognized by a numeric number, a polynomial, a drawing, a sequence of numbers, or a matrix. A topological index is a numeric quantity associated with a graph that characterizes the topology of the graph and is invariant under graph automorphism. Many topological indices are widely used for quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies. Among various topological indices, degree based topological indices are the most important and widely used. These have great application in chemical graph theory. Since the 1970s, two degree based graph invariants have been extensively studied. These are the first Zagreb index M_1 and the second Zagreb index M_2, defined as

\[ M_1(G) = \sum_{v \in V(G)} (d_v)^2 \]

\[ M_2(G) = \sum_{uv \in E(G)} (d_u d_v) \]

Details on the two Zagreb topological indices can be found in [2-6]. Randić’ index was proposed by the chemist Randić [20] in 1975 and is defined as

\[ R(G) = \frac{1}{\sum_{uv \in E(G)} d(u)d(v)} \]

The widely used connectivity topological index is atom-bond connectivity (ABC) index introduced by Estrada et al. [10]. The ABC index of graph G is defined as
Geometric-arithmetic (GA) index is another well known topological index. It was shown that its predictive power is better than the Randić index for many physicochemical properties like entropy, boiling point, vaporization, enthalpy of formation and acentric factor etc. This topological index is defined by Vukićević [21] as follows:

$$GA(G) = \sum_{uv \in E(G)} \frac{\sqrt{d(u)d(v)}}{d(u) + d(v)}$$

For recent results on vertex-degree based topological indices, we refer Hua and Ning [22], Nadeem et al. [23, 24]. Recently, Gutman et al. [10, 13] re-introduced the neglected topological indices and succeed to demonstrate that these indices also have very promising applicative potential. The new/old topological indices studied by Gutman et al. [10, 13] are the following: The reciprocal Randić index ($RR$) is defined as (Figure 1).

$$RR(G) = \sum_{uv \in E(G)} \sqrt{d(u)d(v)}.$$  

Obviously it is a special case of general Randić index $\sum_{uv \in E(G)} \frac{d(u)d(v)}{\alpha}$ where $\alpha$ is a real number. The reduced Randić index is defined as

$$RRR(G) = \sum_{uv \in E(G)} \sqrt{(d(u) - 1)(d(v) - 1)}.$$

The reduced second Zagreb index is defined as

$$RM_2(G) = \sum_{uv \in E(G)} (d(u) - 1)(d(v) - 1)$$

2. Three New/Old Index of Poly (Propyl) Ether Imine Dendrimer

In this section, we study the RR, RRR and RM indices of PETIM dendrimer of generation with $n$ growth stages. The molecular structure for the growth of PETIM dendrimer is shown in Figure 2. It is easy to see that the graph of PETIM dendrimer has $24 \times 2^n - 23$ vertices and $24 \times 2^n - 24$ edges. Now we compute RR, RRR and $RM_2$ indices of PETIM dendrimer.

**Theorem 1** Let $G$ be the molecular graph of Poly(Propyl) Ether Imine (PETIM) dendrimer. Then

$$RR(G) = 2^{n+1} \times \sqrt{5} + 32 \times 2^n - 36 + 6\sqrt{6}(2^n - 1)$$

$$RM_2(G) = 28 \times 2^n - 30$$

$$RRR(G) = 2^{n+4} + 6\sqrt{2}(2^n - 1) - 18$$

**Proof.** Let $G$ be the graph of PETIM dendrimer. We have $|V(PETIM)| = 24 \times 2^n - 23$ and

![Figure 1. Basic molecular structure of Poly Propyl Ether Imine (PETIM) dendrimer.](image-url)
There are three partitions of edge set correspond to their degrees of end vertices which are:

\[ E_1(G) = \{ e = uv \in E(G): d_u = 1 \text{ and } d_v = 2 \} \]

\[ E_2(G) = \{ e = uv \in E(G): d_u = d_v = 2 \} \]

\[ E_3(G) = \{ e = uv \in E(G): d_u = 2 \text{ and } d_v = 3 \} \]

and

\[ |E_1(G)| = 2^{n+1}, |E_2(G)| = 16 \times 2^n - 18, |E_3(G)| = 6 \times 2^n - 6 \]

With the help of this partition we can easily find the required results. We apply these to the formulas of RR, RRR and RM to compute these indices for G. Since,

\[
RR(G) = \sum_{e \in E(G)} \sqrt{(d_u')(d_v')}
\]

\[
= \sum_{u \in D_1(G)} \sqrt{(d_u')(d_v')} + \sum_{u \in D_2(G)} \sqrt{(d_u')(d_v')} + \sum_{u \in D_3(G)} \sqrt{(d_u')(d_v')}
\]

\[
= |E_1(G)| \sqrt{1 \times 2} + |E_2(G)| \sqrt{2 \times 2} + |E_3(G)| \sqrt{2 \times 3}
\]

\[
= (2^{n+1}) \sqrt{2} + (16 \times 2^n - 18) \sqrt{4} + (6 \times 2^n - 6) \sqrt{6}
\]

\[
= 2^{n+1} \sqrt{2} + 32 \times 2^n - 36 + 6 \sqrt{6}(2^n - 1)
\]

\[
RRR(G) = \sum_{e \in E(G)} (d_u' - 1)(d_v' - 1)
\]

\[
= \sum_{u \in D_1(G)} (d_u' - 1)(d_v' - 1) + \sum_{u \in D_2(G)} (d_u' - 1)(d_v' - 1) + \sum_{u \in D_3(G)} (d_u' - 1)(d_v' - 1)
\]

\[
= |E_1(G)|((1-1)(2-1)+|E_2(G)|(2-1)(2-1)+|E_3(G)|(2-1)(3-1))
\]

\[
= (2^{n+1}) \times 0 + (16.2^n - 18) \times 1 + (6.2^n - 6) \times 2
\]

\[
= (16.2^n - 18) + (12.2^n - 12)
\]

\[
= 28 \times 2^n - 30
\]

\[
RM_2(G) = \sum_{e \in E(G)} (d_u - 1)(d_v - 1)
\]

\[
= |E_1(G)|((1-1)(1-1)+|E_2(G)|(2-1)(2-1)+|E_3(G)|(2-1)(3-1))
\]

\[
= (2^{n+1}) \times 0 + (16.2^n - 18) \times 1 + (6.2^n - 6) \times \sqrt{2}
\]

\[
= (16.2^n - 18) + 6 \sqrt{2}(2^n - 1)
\]

\[
= 2^{n+1} + 6 \sqrt{2}(2^n - 1)
\]

3. Three New/Old Index of Porphyrin Dendrimers

We consider the class of Porphyrin dendrimers, denoted by \( D_{n,n} \), where n is steps of growth. Note that \( n=2^m \), where \( m \geq 2 \) (Figure 3). In the graph of \( D_{n,n} \),
there are total 96-10 vertices and 105
-11 edges. Figure 3 shows the graph of porphyrin dendrimer with growth stage n=3. Now we compute RR, RRR and RM
2 indices of Porphyrin \( D_n P_n \) dendrimer.

Theorem 2 Let \( D_n P_n \) be a Porphyrin dendrimer. Then

\[
RR(D_n P_n) = (18\sqrt{3} + 48\sqrt{6} + 107)n - (6\sqrt{6} + 10)
\]

\[
RM_2(D_n P_n) = 206n - 17
\]

\[
RRR(D_n P_n) = (36 + 48\sqrt{2} + 8\sqrt{6})n - (6\sqrt{2} + 5)
\]

Proof. Let G be the graph of \( D_n P_n \) dendrimer. We have \(|V(D_n P_n)| = 96n - 10\) and \(|E(D_n P_n)| = 105n - 11\). There are six partitions of edge set correspond to their degrees of end vertices which are

- \( E_1(G) = \{ (u,v) \in E(G) : d_u = 1 \text{ and } d_v = 3 \} \)
- \( E_2(G) = \{ (u,v) \in E(G) : d_u = 1 \text{ and } d_v = 4 \} \)
- \( E_3(G) = \{ (u,v) \in E(G) : d_u = d_v = 2 \} \)
- \( E_4(G) = \{ (u,v) \in E(G) : d_u = 2 \text{ and } d_v = 3 \} \)
- \( E_5(G) = \{ (u,v) \in E(G) : d_u = d_v = 3 \} \)
- \( E_6(G) = \{ (u,v) \in E(G) : d_u = 3 \text{ and } d_v = 4 \} \)

and

- \( |E_1(D_n P_n)| = 2n \)
- \( |E_2(D_n P_n)| = 24n \)
- \( |E_3(D_n P_n)| = 10n - 5 \)
- \( |E_4(D_n P_n)| = 48n - 6 \)
- \( |E_5(D_n P_n)| = 13n \)
- \( |E_6(D_n P_n)| = 8n \)

With the help of this partition we can easily find the required results. We apply these to the formulas of RR, RRR and RM
2 to compute these indices for G. Since,

\[
RR(D_n P_n) = \sum_{uv \in E(D_n P_n)} \sqrt{(d_u)(d_v)}
\]

\[
RM_2(D_n P_n) = \sum_{uv \in E(D_n P_n)} \sqrt{(d_u)(d_v)} + \sum_{uv \in E_1(D_n P_n)} \sqrt{(d_u)(d_v)} + \sum_{uv \in E_2(D_n P_n)} \sqrt{(d_u)(d_v)} + \sum_{uv \in E_3(D_n P_n)} \sqrt{(d_u)(d_v)} + \sum_{uv \in E_4(D_n P_n)} \sqrt{(d_u)(d_v)} + \sum_{uv \in E_5(D_n P_n)} \sqrt{(d_u)(d_v)}
\]

\[
= \sqrt{(1 \times 3)} |E_1(D_n P_n)| + \sqrt{(1 \times 4)} |E_2(D_n P_n)| + \sqrt{(2 \times 2)} |E_3(D_n P_n)| + \sqrt{(2 \times 3)} |E_4(D_n P_n)| + \sqrt{(3 \times 3)} |E_5(D_n P_n)| + \sqrt{(3 \times 4)} |E_6(D_n P_n)|
\]

\[
= \sqrt{3(2n)} + 2\sqrt{24n} + 2\sqrt{10n - 5} + \sqrt{48n - 6} + \sqrt{13n} + 2\sqrt{8n}
\]

\[
= (18\sqrt{3} + 48\sqrt{6} + 107)n - (6\sqrt{6} + 10)
\]
4. Three New/Old Index of Zinc-Porphyrin Dendrimer

We consider the class of dendrimer Zinc-Porphyrin DPZ\(_n\) (Figure 3), where \(n\) is the steps of growth and \(n \geq 1\). In the molecular graph of DPZ\(_n\) there are total \(56 \times 2^n - 7\) vertices and \(64 \times 2^n - 4\) edges. Figure 3 shows the graph of Zinc-Porphyrin dendrimer with growth stage \(n=3\). Now we compute RR, RRR and RM\(_2\) indices of Zinc-Porphyrin DPZ\(_n\) dendrimer.

**Theorem 3** Let DPZ\(_n\) be a Zinc-Porphyrin dendrimer. Then

\[
\begin{align*}
RR(DPZ_n) &= 2^{n+3}(7 + 5\sqrt{6}) - 2^{3}(7 + 2\sqrt{6} - 3) \\
RM_2(DPZ_n) &= 128 \times 2^n - 76 \\
RRR(DPZ_n) &= (32 + 40\sqrt{2}) 	imes 2^n - (36 + 16\sqrt{2} - 4\sqrt{6})
\end{align*}
\]

**Proof.** Let G be the graph of Zinc-Porphyrin DPZ\(_n\) dendrimer. We have \(|V(G)| = 56 \times 2^n - 7\) and \(|E(G)| = 64 \times 2^n - 4\). There are three partitions of edge set correspond to their degrees of end vertices which are

\[
\begin{align*}
E_1(G) &= \{e = uv \in E(G) : d_u = d_v = 2\} \\
E_2(G) &= \{e = uv \in E(G) : d_u = 2 \text{ and } d_v = 3\} \\
E_3(G) &= \{e = uv \in E(G) : d_u = d_v = 3\}
\end{align*}
\]

and

\[
|E_1(G)| = 16 \times 2^n - 4, |E_2(G)| = 40 \times 2^n - 16, |E_3(G)| = 8 \times 2^n - 16
\]

With the help of this partition we can easily find the required results. We apply these to the formulas of RR, RRR and RM\(_2\) to compute these indices for G. Since,

\[
RR(DPZ_n) = \sum_{uv \in \hat{E}(DPZ_n)} \sqrt{(d_u - 1)(d_v - 1)}
\]

\[
= \sum_{uv \in E_1(DPZ_n)} \sqrt{(d_u - 1)(d_v - 1)} + \sum_{uv \in E_2(DPZ_n)} \sqrt{(d_u - 1)(d_v - 1)} + \sum_{uv \in E_3(DPZ_n)} \sqrt{(d_u - 1)(d_v - 1)}
\]

\[
= \sqrt{(1-1)(3-1)|E_1(DPZ_n)|} + \sqrt{(1-1)(4-1)|E_2(DPZ_n)|} + \sqrt{(3-1)(3-1)|E_3(DPZ_n)|} + \sqrt{(3-1)(4-1)|E_3(DPZ_n)|}
\]

\[
= (10n - 5) + \sqrt{2}(48n - 6) + 2(13n) + \sqrt{6}(8n)
\]

\[
= (36 + 48\sqrt{2} + 8\sqrt{6})n - (6\sqrt{2} + 5)
\]

\[
= 206n - 17
\]

\[
RRR(DPZ_n) = \sum_{uv \in \hat{E}(DPZ_n)} \sqrt{(d_u - 1)(d_v - 1)}
\]

\[
= \sum_{uv \in E_1(DPZ_n)} \sqrt{(d_u - 1)(d_v - 1)} + \sum_{uv \in E_2(DPZ_n)} \sqrt{(d_u - 1)(d_v - 1)} + \sum_{uv \in E_3(DPZ_n)} \sqrt{(d_u - 1)(d_v - 1)}
\]

\[
= \sqrt{(2-1)(2-1)|E_1(DPZ_n)|} + \sqrt{(2-1)(3-1)|E_1(DPZ_n)|} + \sqrt{(3-1)(3-1)|E_3(DPZ_n)|} + \sqrt{(3-1)(4-1)|E_3(DPZ_n)|}
\]

\[
= (16n - 2) + \sqrt{2}(40n - 4) + \sqrt{6}(40n - 2) + \sqrt{3}(4n)
\]

\[
= n^3(7 + 5\sqrt{6}) - 2^n(7 + 2\sqrt{6} - \sqrt{3})
\]

\[
RM_2(DPZ_n) = \sum_{uv \in \hat{E}(DPZ_n)} (d_u - 1)(d_v - 1)
\]

\[
= \sum_{uv \in E_1(DPZ_n)} (d_u - 1)(d_v - 1) + \sum_{uv \in E_2(DPZ_n)} (d_u - 1)(d_v - 1) + \sum_{uv \in E_3(DPZ_n)} (d_u - 1)(d_v - 1)
\]

\[
= (2-1)(2-1)|E_1(DPZ_n)| + (2-1)(3-1)|E_2(DPZ_n)| + (3-1)(3-1)|E_3(DPZ_n)| + (3-1)(4-1)|E_3(DPZ_n)|
\]

\[
= 128n - 76
\]

\[
RM_2(DPZ_n) = \sum_{uv \in \hat{E}(DPZ_n)} (d_u - 1)(d_v - 1)
\]

\[
= \sum_{uv \in E_1(DPZ_n)} (d_u - 1)(d_v - 1) + \sum_{uv \in E_2(DPZ_n)} (d_u - 1)(d_v - 1) + \sum_{uv \in E_3(DPZ_n)} (d_u - 1)(d_v - 1)
\]

\[
= (2-1)(2-1)|E_1(DPZ_n)| + (2-1)(3-1)|E_2(DPZ_n)| + (3-1)(3-1)|E_3(DPZ_n)| + (3-1)(4-1)|E_3(DPZ_n)|
\]

\[
= 128n - 76
\]
\[
= \sqrt{(2-1)(2-1)} |E_1(DPZ_n)| + \sqrt{(2-1)(3-1)} |E_2(DPZ_n)| \\
+ \sqrt{(3-1)(3-1)} |E_1(DPZ_n)| + \sqrt{(3-1)(4-1)} |E_4(DPZ_n)| \\
= \sqrt{(2-1)(2-1)} |E_1(DPZ_n)| + \sqrt{(2-1)(3-1)} |E_2(DPZ_n)| \\
= (32 + 40\sqrt{2}) \times 2^n - (36 + 16\sqrt{2} - 4\sqrt{6})
\]

5. Conclusion

In this paper we deal with three dendrimers families and studied their topological indices. We determined Randić' index (RR), the reduced second Zagreb index RM_2, and the reduced reciprocal Randić index (RRR) for these dendrimers families. Randić' index (RR) has proven its worth in so many drugs design and have been used at various occasions.

References