

**SOME NEW/OLD DEGREE-BASED TOPOLOGICAL
INDICES OF NANOSTAR DENDRIMERS**

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Abstract: Gutman, Furtula and Elphick reintroduced some degree based topological indices, some of these topological indices failed to get the attention of mathematical chemist in past.

Received: 2017-09-08

Revised: 2017-10-27

Published: January 22, 2017

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url: www.acadpubl.eu

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These are the reciprocal Randić index (RR), the reduced reciprocal Randić index (RRR), the reduced second Zagreb index (RM_2) and the forgotten index (F). In this paper, we computed these indices for *Nanostar Dendrimers*.

AMS Subject Classification: 05C90, 05C35, 05C12

Key Words: the reduced second Zagreb index, the forgotten index, reciprocal Randić index, the reduced reciprocal Randić index, Nanostar dendrimers

1. Introduction

Graph theory applied in the study of molecular structure represents an interdisciplinary science, called chemical graph theory or molecular topology. By using tools taken from graph theory, set theory and statistics it attempt to identify structural features involved in structure-property activity relationship. Topological indices is a subsection of chemical graph theory, which correlates certain physico-chemical properties of the underlying chemical compound. Hundreds of papers have been published on topological indices so far.

Let Σ is the set of all finite simple graphs. A topological index is a function $Top : \Sigma \rightarrow R$ with the property that $Top(G_1) = Top(G_2)$, if G_1 and G_2 are isomorphic. Due to their chemical significance a lot of research has been done on topological indices of different graph families.

Nano-biotechnology is a rapidly advancing area of scientific and technological opportunity that applies the tools and processes of nano-fabrication to build devices for studying bio-systems. One of the main object of this area is Dendrimers. Dendrimers are highly ordered branched macromolecules which have attracted much theoretical and experimental attention.

In this paper, G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The number of elements in $V(G)$ and $E(G)$ is represented as $|V(G)|$ and $|E(G)|$, respectively. For a vertex $u \in V(G)$, the number of vertices adjacent to the vertex u is called the *degree* of u , denoted as $d(u)$. In 1975 Milan Randić introduced the very first vertex-degree based topological index [35], defined as

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

In 1998, Bollobàs et. al. introduced the *general Randić index* by replacing $-\frac{1}{2}$ by any real number α as follows,

$$R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^\alpha$$

The *first* and *second Zagreb indices* are among the oldest and most famous topological indices, introduced by Gutman and Trinajstić [34] defined as follows

$$M_1(G) = \sum_{v \in V(G)} d(v)^2 = \sum_{uv \in E(G)} (d(u) + d(v))$$

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

Recently, Todeschini et. al. [37, 38] proposed the *multiplicative* variants of ordinary Zagreb indices, defined as

$$\prod_1(G) = \prod_{v \in V(G)} d(v)^2$$

$$\prod_2(G) = \prod_{uv \in E(G)} d(u)d(v)$$

Zhou et. al. [40] replaced the term $d(u)d(v)$ by $d(u) + d(v)$ and introduced the *sum connectivity index* as

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u) + d(v)}}$$

and the *general sum connectivity index* is defined as

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v))^\alpha$$

where α is any real number. For recent progress on these vertex-degree based topological indices see [8, 9, 10, 21, 23, 30, 33, 36, 39]

I. Gutman et. al. [22, 24] presented the neglected topological indices that earlier have been considered in the chemical and/or mathematical literature, but, that evaded the attention of most mathematical chemists. Recently, they succeed to demonstrate that these indices also have very promising applicative potential. The new/old topological indices studied by I. Gutman et. al. are the following: The *reciprocal Randić index* is defined as

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

It is, of course, a special case of *general Randić index* $\sum_{uv \in E(G)} (d(u)d(v))^\alpha$, where α is any real number. The *reduced reciprocal 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

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

In a study on the structure-dependency of the total π -electron energy, beside the first Zagreb index, it was indicated that another term on which this energy depends is of the form

$$F(G) = \sum_{v \in V(G)} d(v)^3 = \sum_{uv \in E(G)} (d(u)^2 + d(v)^2)$$

Recently, this sum was named *forgotten index*, or shortly the *F - index*.

2. Nanostar Dendrimers

Dendrimer is a synthetic 3-dimensional macromolecule that is prepared in a stepwise fashion from simple branched monomer units. The nanostar dendrimer is a part of a new group of macromolecules that appear to photon funnels just like artificial antennas. From polymer chemistry point of view, dendrimers are nearly perfect mono-disperse macromolecules with a regular and highly branched three dimensional architecture. Some topological indices of polyomino chains are discussed in [1]-[7], [29, 32], [11]-[20]. In this section, we will compute the reciprocal Randić index, reduced reciprocal Randić index, reduced second Zagreb index and forgotten index of nanostar dendrimers.

2.1. Nanostar Dendrimer $NS_1[n]$, $n > 1$

$NS_1[n]$ is the first class of these macromolecules, where $n > 1$ is the defining parameter, Fig 1. There are $140 \cdot 2^n - 127$ edges. The technique to find the certain topological indices we partitions the edge set of graph $NS_1[n]$ based on degrees of end vertices of each edge.

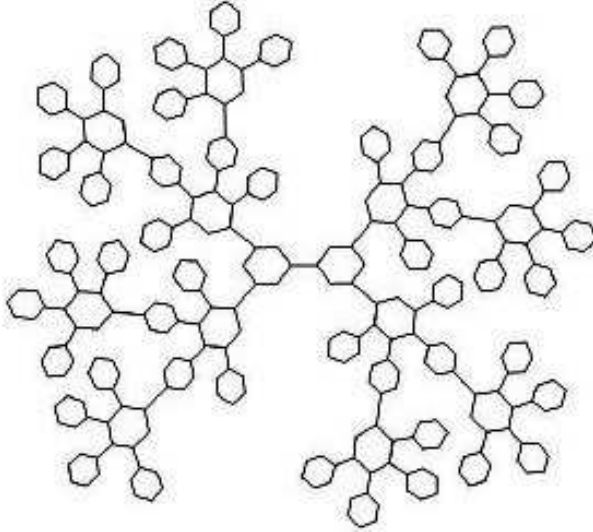
Theorem 1. Consider G be the graph of $NS_1[n]$, then

$$RR(G) = (21 + 12\sqrt{6})2^{n+1} - 3(4\sqrt{6} + 3) \quad (1)$$

$$RRR(G) = 3(1 + \sqrt{2})2^{n+3} - 6(2\sqrt{2} + 1) \quad (2)$$

$$RM_2(G) = 21 \cdot 2^{n+2} - 36 \quad (3)$$

$$F(G) = 129 \cdot 2^{n+2} - 208 \quad (4)$$

Figure 1: $NS_1[n]$ with $n = 2$.

Proof. Consider the graph of $NS_1[n]$. There are three type of edges in graph of this nanostar dendrimer based on degrees of end vertices of each edge, which are

$$E_1 = \{uv \in E(G) | d(u) = 2 \text{ and } d(v) = 2\}$$

$$E_2 = \{uv \in E(G) | d(u) = 2 \text{ and } d(v) = 3\}$$

$$E_3 = \{uv \in E(G) | d(u) = 3 \text{ and } d(v) = 3\}$$

The number of edges in E_1, E_2 and E_3 are $12 \cdot 2^n, 24 \cdot 2^n - 12$ and $6 \cdot 2^n - 3$. By using these we compute RR, RRR, RM_2 and F indices of $NS_1[n]$. Since,

$$\begin{aligned} RR(G) &= \sum_{uv \in E(G)} \sqrt{d(u)d(v)} \\ &= \sum_{uv \in E_1(G)} \sqrt{d(u)d(v)} + \sum_{uv \in E_2(G)} \sqrt{d(u)d(v)} + \sum_{uv \in E_3(G)} \sqrt{d(u)d(v)} \\ &= 12 \cdot 2^n \sqrt{2 \cdot 2} + (24 \cdot 2^n - 12) \sqrt{2 \cdot 3} + (6 \cdot 2^n - 3) \sqrt{3 \cdot 3} \\ &= (21 + 12\sqrt{6})2^{n+1} - 3(4\sqrt{6} + 3) \end{aligned}$$

which is the required (1) result.

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

$$\begin{aligned}
&= \sum_{uv \in E_1(G)} \sqrt{(d(u)-1)(d(v)-1)} + \sum_{uv \in E_2(G)} \sqrt{(d(u)-1)(d(v)-1)} \\
&+ \sum_{uv \in E_3(G)} \sqrt{(d(u)-1)(d(v)-1)} \\
&= 12 \cdot 2^n \sqrt{(2-1)(2-1)} + (24 \cdot 2^n - 12) \sqrt{(2-1)(3-1)} \\
&+ (6 \cdot 2^n - 3) \sqrt{(3-1)(3-1)} \\
&= 3(1 + \sqrt{2})2^{n+3} - 6(2\sqrt{2} + 1)
\end{aligned}$$

which is the required (2) result.

$$\begin{aligned}
RM_2(G) &= \sum_{uv \in E(G)} (d(u)-1)(d(v)-1) \\
&= \sum_{uv \in E_1(G)} (d(u)-1)(d(v)-1) + \sum_{uv \in E_2(G)} (d(u)-1)(d(v)-1) \\
&+ \sum_{uv \in E_3(G)} (d(u)-1)(d(v)-1) \\
&= 12 \cdot 2^n (2-1)(2-1) + (24 \cdot 2^n - 12)(2-1)(3-1) \\
&+ (6 \cdot 2^n - 3)(3-1)(3-1) \\
&= 21 \cdot 2^{n+2} - 36
\end{aligned}$$

which is the required (3) result.

$$\begin{aligned}
F(G) &= \sum_{uv \in E(G)} (d(u)^2 + d(v)^2) \\
&= \sum_{uv \in E_1(G)} (d(u)^2 + d(v)^2) + \sum_{uv \in E_2(G)} (d(u)^2 + d(v)^2) \\
&+ \sum_{uv \in E_3(G)} (d(u)^2 + d(v)^2) \\
&= 12 \cdot 2^n (2^2 + 2^2) + (24 \cdot 2^n - 12)(2^2 + 3^2) + (6 \cdot 2^n - 3)(3^2 + 3^2) \\
&= 129 \cdot 2^{n+2} - 208
\end{aligned}$$

which is the required (4) result, and the proof is complete. \square

2.2. Nanostar Dendrimer $NS_2[n]$, $n > 1$

$NS_2[n]$ is the second class of these macromolecules, where $n > 1$ is the defining parameter, Fig 2. There are $140 \cdot 2^n - 127$ edges. The technique to find the

certain topological indices we partitions the edge set of graph $NS_2[n]$ based on degrees of end vertices of each edge.

Theorem 2. Consider G be the graph of $NS_2[n]$, then

$$RR(G) = (55 + 12\sqrt{6})2^{n+2} - (201 + 44\sqrt{6}) \tag{5}$$

$$RRR(G) = (8 + 3\sqrt{2})2^{n+4} - 2(22\sqrt{2} + 59) \tag{6}$$

$$RM_2(G) = 37 \cdot 2^{n+3} - 276 \tag{7}$$

$$F(G) = 215 \cdot 2^{n+3} - 1586 \tag{8}$$

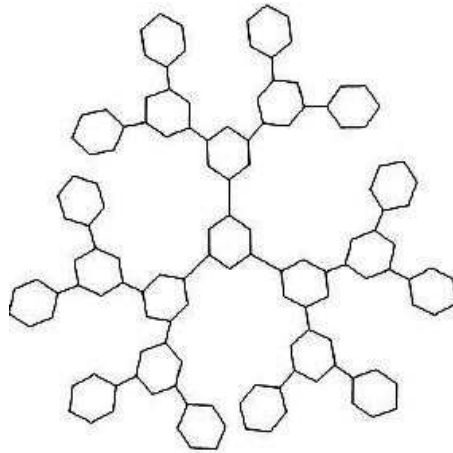


Figure 2: $NS_2[n]$ with $n = 2$.

Proof. Consider the graph of $NS_2[n]$. There are three types of edges in this nanostar dendrimer’s graph based on degrees of end vertices of each edge, which are

$$E_1 = \{uv \in E(G) | d(u) = 2 \text{ and } d(v) = 2\}$$

$$E_2 = \{uv \in E(G) | d(u) = 2 \text{ and } d(v) = 3\}$$

$$E_3 = \{uv \in E(G) | d(u) = 3 \text{ and } d(v) = 3\}$$

The number of edges in E_1, E_2 and E_3 are $56 \cdot 2^n - 48, 48 \cdot 2^n - 44$ and $36 \cdot 2^n - 35$. By using these we compute RR, RRR, RM_2 and F indices of $NS_2[n]$. Since,

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

$$\begin{aligned}
&= \sum_{uv \in E_1(G)} \sqrt{d(u)d(v)} + \sum_{uv \in E_2(G)} \sqrt{d(u)d(v)} + \sum_{uv \in E_3(G)} \sqrt{d(u)d(v)} \\
&= (56 \cdot 2^n - 48)\sqrt{2 \cdot 2} + (48 \cdot 2^n - 44)\sqrt{2 \cdot 3} + (36 \cdot 2^n - 35)\sqrt{3 \cdot 3} \\
&= (55 + 12\sqrt{6})2^{n+2} - (201 + 44\sqrt{6})
\end{aligned}$$

which is the required (5) result.

$$\begin{aligned}
RRR(G) &= \sum_{uv \in E(G)} \sqrt{(d(u) - 1)(d(v) - 1)} \\
&= \sum_{uv \in E_1(G)} \sqrt{(d(u) - 1)(d(v) - 1)} + \sum_{uv \in E_2(G)} \sqrt{(d(u) - 1)(d(v) - 1)} \\
&\quad + \sum_{uv \in E_3(G)} \sqrt{(d(u) - 1)(d(v) - 1)} \\
&= (56 \cdot 2^n - 48)\sqrt{(2 - 1)(2 - 1)} + (48 \cdot 2^n - 44)\sqrt{(2 - 1)(3 - 1)} + \\
&\quad (36 \cdot 2^n - 35)\sqrt{(3 - 1)(3 - 1)} \\
&= (8 + 3\sqrt{2})2^{n+4} - 2(22\sqrt{2} + 59)
\end{aligned}$$

which is the required (6) result.

$$\begin{aligned}
RM_2(G) &= \sum_{uv \in E(G)} (d(u) - 1)(d(v) - 1) \\
&= \sum_{uv \in E_1(G)} (d(u) - 1)(d(v) - 1) + \sum_{uv \in E_2(G)} (d(u) - 1)(d(v) - 1) \\
&\quad + \sum_{uv \in E_3(G)} (d(u) - 1)(d(v) - 1) \\
&= (56 \cdot 2^n - 48)(2 - 1)(2 - 1) + (48 \cdot 2^n - 44)(2 - 1)(3 - 1) + \\
&\quad (36 \cdot 2^n - 35)(3 - 1)(3 - 1) \\
&= 37 \cdot 2^{n+3} - 276
\end{aligned}$$

which is the required (7) result.

$$\begin{aligned}
F(G) &= \sum_{uv \in E(G)} (d(u)^2 + d(v)^2) \\
&= \sum_{uv \in E_1(G)} (d(u)^2 + d(v)^2) + \sum_{uv \in E_2(G)} (d(u)^2 + d(v)^2) \\
&\quad + \sum_{uv \in E_3(G)} (d(u)^2 + d(v)^2)
\end{aligned}$$

$$\begin{aligned} &= (56 \cdot 2^n - 48)(2^2 + 2^2) + (48 \cdot 2^n - 44)(2^2 + 3^2) + (36 \cdot 2^n - 35)(3^2 + 3^2) \\ &= 215 \cdot 2^{n+3} - 1586 \end{aligned}$$

which is the required (8) result, and the proof is complete. \square

3. Concluding Remarks and Open Problems

Recently, Gutman, Furtula and Elphick introduced reciprocal Rindić index, reduced reciprocal Randić index, reduced second Zagreb index and forgotten index with great significant applications in chemical graph theory. In this article, we computed these topological indices for Nanostar Dendrimers. Some future work that can be done is to find these topological indices for Polyomino chains, benzenoid systems or some other chemical structures.

Acknowledgments

The authors are very grateful to the referees for their constructive suggestions and useful comments, which improved this work very much. This research was supported by Key Project of Sichuan Provincial Department of Education under grant 17ZA0079.

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