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# Some Degree-Based Topological Indices of Base-3 Sierpiński Graphs

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**Abstract:** In this paper, a recursive relation between base-3 Sierpiński graphs rank n and n-1 of some topostructural indices is studied. Based on this relation, The formulae of the First Zagreb index, Second Zagreb index, Randić connectivity index, sum-connectivity index, Geometric-Arithmetic index and Atom-Bond Connectivity index of base-3 Sierpiński graphs are derived.

**Keywords:** Topological Index, Base-3 Sierpiński Graphs, Zagreb Index, Sum-Connectivity Index, Geometric-Arithmetic Index, Atom-Bond Connectivity Index, Sankruti Index

## 1. Introduction

In this paper, we only consider undirected graph without loops and multiple edges. Let $G$ be a graph, we denote $V(G)$ and $E(G)$ the vertex set and edge set of $G$, respectively. We denote by $d_v$ the degree of a vertex $v$ of a graph $G$. We denote by $E_{a,b}$ the set of edges $uv$ with $\{d_u, d_v\} = \{a, b\}$, i.e. $E_{a,b} = \{uv \mid \{a, b\} = \{d_u, d_v\}\}$. Let $s_G(v) = \sum_{u \in N(v)} d_u$, and the summation of the degrees of all the neighbors of a vertex $u$ be $s_G(u)$, i.e. $s_G(u) = \sum_{v \in N(u)} d(v)$ and $E'_{a,b} = \{uv \mid \{a, b\} = \{s_G(u), s_G(v)\}\}$. In chemical graph theory, the vertices of the graph correspond to the atoms of molecules and the edges correspond to chemical bonds.

Klavžar et al. [9] defined the Sierpiński graphs $S(n,k)$ in 1997. The Sierpiński graphs $S(n,k)$ were related to the Tower of Hanoi problems and the universal topological spaces problems. The authors defined $S(n,k)$ as follows.

$V(S(n,k)) = \{1, 2, 3, \cdots, k\}^n, k \geq 1, n \geq 1$ and two different vertices $I = (i_1, i_2, \cdots, i_n)$, and $J = (j_1, j_2, \cdots, j_3)$ are adjacent if $I \sim J$, where $I \sim J \Leftrightarrow \exists h \in \{1, 2, \cdots, n\}$ such that

i)  $\forall t, t < h \Rightarrow i_t = j_t$,
ii) $i_h \neq j_h$,
iii) $\forall t, t > h \Rightarrow i_t = j_h \& j_t = i_h$ [9]

Hinz et al. [5] discussed the definition and properties of Sierpiński graph, Sierpiński-type graphs, Sierpiński triangle graphs and Sierpiński-like graphs. Because we only focus on Base-3 Sierpiński Graphs $S(n,3)$, we simplify the notation from $S(n,3)$ to $S^n$. In Figure 1 the Base-3 Sierpiński Graphs are illustrated with $n \in \{1, 2, 3, 4\}$.
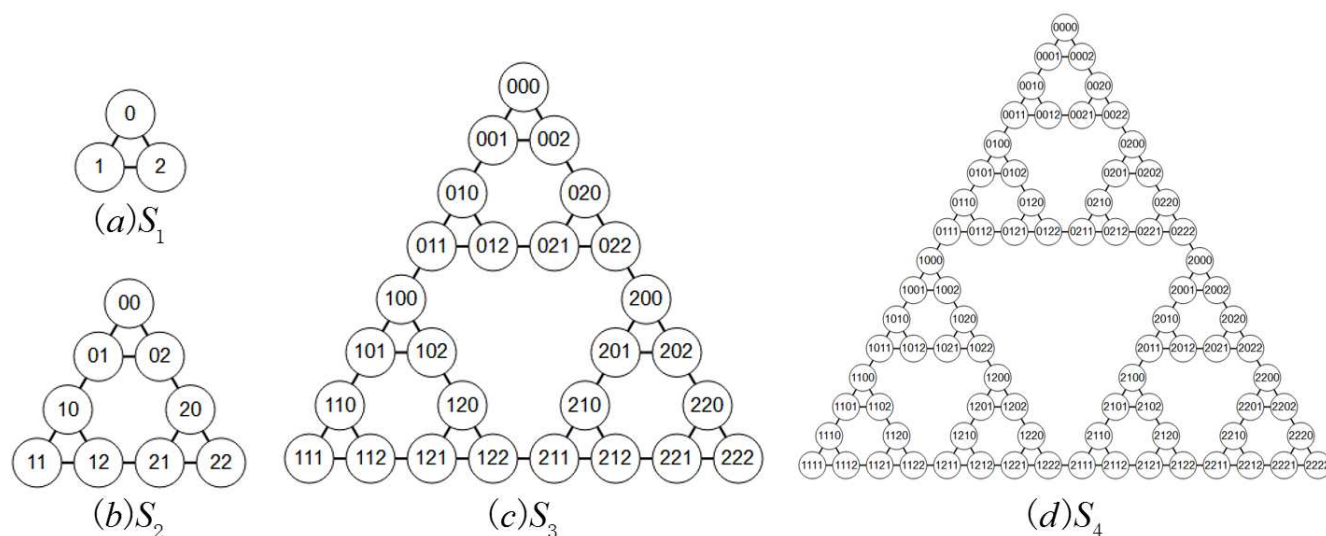
**Figure 1.** *The Sierpiński Triangles with n=1,2,3,4.*

$S^1$ is $K_3$ and three vertices are labeled with 0, 1, and 2. $S^2$ consists of three copies of $S^1$, if we consider a $S^1$ as a vertex, $S^2$ can be considered as another type of $K_3$. The vertices labels of $S^2$ can be considered by adding $S^1$ vertex labels before to three copies of $S^1$ vertex labels. So $S^{n+1}$ is composed with three copies of $S^n$, $S^{n+1}$ is another type of $K_3$ that all three vertices are replaced by $S^n$, and $S^n$ vertex labels are composed by adding $S^1$ vertex labels before to three copies of $S^n$ vertex labels. The relationship of $S^{n+1}$ and $S^n$ is illustrated in Figure 2.
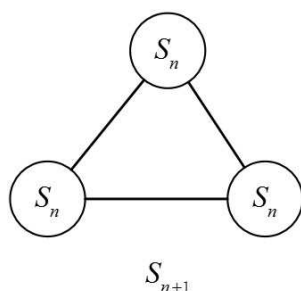


**Figure 2.** *The Base-3 Sierpiński Graphs $S^{n+1}$.*

By the definition of the Base-3 Sierpiński Graphs $S^i$, we have

*Observation 1.* If G is an $S^n$ graph with n ≥ 2, then $E(S^n) = E_{2,3} \cup E_{3,3}$ with $|E_{2,3}| = 6$ and $|E_{3,3}| = \dfrac{3^{n+1}-15}{2}$; If n=2, then $E(S^n) = E'_{6,8} \cup E'_{8,8}$ with $|E'_{6,8}| = |E'_{8,8}| = 6$; If $n \geq 3$, then $E(S^n) = E'_{6,8} \cup E'_{8,8} \cup E'_{8,9} \cup E'_{9,9}$ with $|E'_{8,8}| = 3$, $|E'_{6,8}| = |E'_{8,9}| = 6$, $|E'_{9,9}| = \dfrac{3^{n+1}-33}{2}$.

In chemical graph theory, the atoms of molecules can be considered as the vertices of graph and chemical bonds be considered as the edges of graph [12, 14]. The mathematical quantities derived from a graph representation of the molecule are called graph invariants. Single indices derived from a molecular graph are called topological indices.

Topological indices are sensitive to one or more structural features of the molecule such as size, shape, symmetry, branching, and topological indices are divided into two categories: *topostructural* and *topochemical indices* [11]. In this paper, we only focus on some of the *topostructural indices*, including First Zagreb index $Zg_1(G)$, Second Zagreb index $Zg_2(G)$, Randić connectivity index $R(G)$, sum-connectivity index $X(G)$, Geometric-Arithmetic index $GA(G)$ and Atom-Bond Connectivity index $ABC(G)$.

The First Zagreb index were introduced by Gutman and Trinajstić [6]. When they studied the molecular structure's π electron energy, they found the approximate expressions of M1 and M2. The First Zagreb index and the Second Zagreb index are very important topostructural indices in chemical graph theory [7].

The First Zagreb index $Zg_1(G)$ is defined as the sum of squares of the vertex degrees $d_u$ and $d_v$ of vertices $u$ and $v$ in G (see [6, 7, 13])

$$Zg_1(G) = \sum_{e=uv \in E(G)} (d_u + d_v) \qquad (1)$$

The Second Zagreb index $Zg_2(G)$ is defined as the sum of squares of the vertex degrees $d_u$ and $d_v$ of vertices $u$ and $v$ in G (see [6, 7, 13]) and deduced as formula (2).

$$Zg_2(G) = \sum_{e=uv \in E(G)} (d_u d_v) \qquad (2)$$

According to the above Zagreb indices, the First Zagreb polynomial $Zg_1(G,x)$ and the Second Zagreb polynomial $Zg_1(G,x)$ have been defined. They are defined as

$$Zg_1(G,x) = \sum_{e=uv \in E(G)} x^{d_u + d_v} \qquad (3)$$

and

$$Zg_2(G,x) = \sum_{e=uv\in E(G)} x^{d_u d_v} \qquad (4)$$

Kinkar and Gutman studied the properties of $Zg_1(G,x)$, $Zg_2(G,x)$ for some chemical structures in 2004 [1].

The Randić index $R(G)$, proposed by Randić [10, 12] in 1975, is well correlated with a variety of physico-chemical properties of alkanes. And this index has become one of the most popular molecular descriptors. The Randić index $R(G)$ is defined on the ground of vertex degrees

$$R(G) = \sum_{e=uv\in E(G)} \frac{1}{\sqrt{d_u d_v}} \qquad (5)$$

If more information about the Randić index of polymeric networks modelled by generalized Sierpiński graphs is wanted, please refer to Estradamoreno et al. [18].

The sum-connectivity index was introduced by Zhou and Trinajstić [15] which is very similar to the Randić connectivity index. The sum-connectivity index is defined (see [15]) as

$$X(G) = \sum_{e=uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}} \qquad (6)$$

As molecular structure descriptor based on graph theory, $X(G)$ and R(G) are both well related with each other and with the π-electronic energy of benzenoid hydrocarbons [16].

Fath-Tabar et al. were introduced the Geometric-Arithmetic index in 2010 (see [17]) is defined as

$$GA(G) = \sum_{e=uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \qquad (7)$$

The GA index is well correlated with a variety of physico-chemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation and acentric factor [3, 8].

By Estrada et al. [4], the Atom-Bond Connectivity index is defined as

$$ABC(G) = \sum_{e=uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \qquad (8)$$

The ABC index correlates well with the experimental heats of formation of alkanes [4]. The mathematical properties of this index have been studied extensively.

The Forgotten index $F(G)$ is defined as the sum of cubic of the vertex degrees in G (see [13])

$$F(G) = \sum_{v\in V(G)} (d(v)^3) = \sum_{uv\in E(G)} \left( d_u^2 + d_v^2 \right) \qquad (9)$$

The Harmonic index H(G) (see [19]) is defined as

$$H(G) = \sum_{ev\in E(G)} \frac{2}{d_u + d_v} \qquad (10)$$

More recently, motivated by the previous research on topological descriptors and their applications, Hosamani [20] proposed the Sanskruti index which can be utilized to guess the bioactivity of chemical compounds and shows good correlation with entropy of an octane isomers.

The Sankruti index of a graph G is defined as

$$\mathcal{S}(G) = \sum_{uv\in E(G)} \left( \frac{s_G(u)s_G(v)}{s_G(u) + s_G(v) - 2} \right)^3 \qquad (11)$$

Darafsheh [2] have discussed Wiener index formulae, Szeged index formulae and PI-index formulae of intersection graph and Hypercube (n-Cube) graph by using automorphism group method, and asserted recursion process method be good at to the graph with the same shape repeated several times, so he gave Wiener index formulae of Linear Chain, Polyphenylene and Linear Phenylene graph by using recursion formulae method. The recursion formulae method will be used to derived the formulae of the First Zagreb index $Zg_1(G)$, Second Zagreb index $Zg_2(G)$, the first Zagreb polynomial, the second Zagreb polynomial, sum-connectivity index $X(G)$, Geometric-Arithmetic index $GA(G)$, Atom-Bond Connectivity index ABC(G), forgotten index F(G), harmonic index H(G) and Sankruti index $\mathcal{S}(G)$ of base-3 Sierpiński graphs.

## 2. Main Results

Let $\phi(x,y)$ be a function on $\mathbb{Z}\times\mathbb{Z} \to R$ and a degree-based topological index $f(G)$ is defined as

$$f(G) = \sum_{uv\in E(G)} \phi(d_u, d_v).$$

By observing the structure of the base-3 Sierpiński graphs, we have the following recursive formulation of $f(S^n)$:
If $n \geq 3$, then

$$\begin{cases} f(S^n) &= 3f(S^{n-1}) - 12\phi(2,3) + 15\phi(3,3), \\ f(S^1) &= 3\phi(2,2) \\ f(S^2) &= 6(\phi(2,3) + \phi(3,3)) \end{cases} \qquad (12)$$

*Theorem 1.* $Zg_1(S^n) = 3^{n+2} - 15$.
*Proof.* It can be verified that $Zg_2(S^1) = 12$ and $Zg_2(S^2) = 66$ thus the theorem holds for $n = 1, 2$. Let $\phi(x,y) = x + y$. Then the degree-based topological index $f(G)$ in formula (1) is the first Zagreb index $Zg_1(G)$. By formula (1), we have If $n \geq 3$, then

$$\begin{cases} f(S^n) &= 3f(S^{n-1}) + 30, \\ f(S^2) &= 66 \end{cases}$$

By solving this recursive formulation, we have $Zg_1(S^n) = f(S^n) = 3^{n+2} - 15$.

*Theorem 2.* $Zg_2(S^1) = 12$; if $n \geq 2$, we have

$$Zg_2(S^n) = \frac{9(3^{n+1} - 7)}{2}.$$

*Proof.* It can be verified that $Zg_2(S^1) = 12$ and $Zg_2(S^2) = 90$ thus the theorem holds for $n = 1, 2$. Now we consider the case $n \geq 3$. Let $\phi(x,y) = xy$. Then the degree-based topological index $f(G)$ in formula (2) is the second Zagreb index $Zg_2(G)$. By formula (2), we have if $n \geq 3$, then

$$\begin{cases} f(S^n) &= 3f(S^{n-1}) + 63, \\ f(S^2) &= 90 \end{cases}$$

By solving this recursive formulation, we have

$$Zg_2(S^n) = \frac{9(3^{n+1} - 7)}{2} \text{ for } n \geq 2.$$

*Theorem 3.* $X(S^1) = \frac{3}{2}$ if $n \geq 2$, we have

$$X(S^n) = \frac{5\sqrt{6} \times 3^n + 24\sqrt{5} - 25\sqrt{6}}{20}.$$

*Proof.* It can be verified that $X(S^1) = \frac{3}{2}$ and

$X(S^2) = 6(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}})$ thus the theorem holds for $n = 1, 2$.

Now we consider the case $n \geq 3$. Let $\phi(x,y) = \frac{1}{\sqrt{x+y}}$. Then the degree-based topological index $f(G)$ in formula (6) is the sum-connectivity index $X(G)$. By formula (6), we have if $n \geq 3$, then

$$\begin{cases} f(S^n) &= 3f(S^{n-1}) - 12/\sqrt{5} + 15/\sqrt{6}, \\ f(S^2) &= 6(\frac{1}{\sqrt{5}} + \frac{1}{\sqrt{6}}) \end{cases}$$

By solving this recursive formulation, we have

$$X(S^n) = \frac{5\sqrt{6} \times 3^n + 24\sqrt{5} - 25\sqrt{6}}{20} \text{ for } n \geq 2. \square$$

*Theorem 4.* $GA(S^1) = 3$; if $n \geq 2$, we have

$$GA(S^n) = \frac{3(5 \times 3^n - 25 + 8\sqrt{6})}{10}.$$

*Proof.* It can be verified that $GA(S^1) = 3$ and

$GA(S^2) = \frac{12\sqrt{6}}{5} + 6$ thus the theorem holds for $n = 1, 2$. Now

we consider the case $n \geq 3$. Let $\phi(x,y) = \frac{2\sqrt{xy}}{x+y}$. Then the degree-based topological index $f(G)$ in formula (7) is Geometric-Arithmetic index $GA(G)$. By formula (7), we have if $n \geq 3$, then

$$\begin{cases} f(S^n) &= 3f(S^{n-1}) - \frac{24\sqrt{6}}{5} + 15, \\ f(S^2) &= \frac{12\sqrt{6}}{5} + 6 \end{cases}$$

By solving this recursive formulation, we have

$$GA(S^n) = \frac{3(5 \times 3^n - 25 + 8\sqrt{6})}{10} \text{ for } n \geq 2. \square$$

*Theorem 5.* $ABC(S^1) = \frac{3}{\sqrt{2}}$, if $n \geq 2$, we have

$$ABC(S^n) = 3^n - 5 + 3\sqrt{2}.$$

*Proof.* It can be verified that $ABC(S^1) = \frac{3}{\sqrt{2}}$ and

$ABC(S^2) = 6(\frac{1}{\sqrt{2}} + \frac{2}{3})$ thus the theorem holds for $n = 1, 2$.

Now we consider the case $n \geq 3$. Let $\phi(x,y) = \sqrt{\frac{x+y-2}{xy}}$.

Then the degree-based topological index $f(G)$ in formula (8) is ABC index $ABC(G)$. By formula (8), we have if $n \geq 3$, then

$$\begin{cases} f(S^n) &= 3f(S^{n-1}) - 12/\sqrt{2} + 10, \\ f(S^2) &= 6(\frac{1}{\sqrt{2}} + \frac{2}{3}) \end{cases}$$

By solving this recursive formulation, we have $ABC(S^n) = 3^n - 5 + 3\sqrt{2}$ for $n \geq 2$. $\square$

*Theorem 6.* $F(S^n) = 3^{n+3} - 57$

*Proof.* It can be verified that $F(S^1) = 24$ and $F(S^2) = 186$ thus the theorem holds for $n = 1, 2$. Now we consider the case $n \geq 3$. Let $\phi(x,y) = x^2 + y^2$. Then the degree-based topological index $f(G)$ in formula (9) is $F$ index $F(G)$. By formula (9), we have if $n \geq 3$, then

$$\begin{cases} f(S^n) &= 3f(S^{n-1}) - 12 \times 13 + 15 \times 18, \\ f(S^2) &= 186 \end{cases}$$

By solving this recursive formulation, we have $F(S^n) = 3^{n+3} - 57$. $\square$

*Theorem 7.* $H(S^1) = \frac{3}{2}$; if $n \geq 2$, we have

$$H(S^n) = 0.5 \times 3^n - 0.1$$

*Proof.* It can be verified that $H(S^1) = \frac{3}{2}$ and

$H(S^2) = 6(\frac{2}{5} + \frac{2}{6})$ thus the theorem holds for $n = 1, 2$. Now

we consider the case $n \geq 3$. Let $\phi(x,y) = \frac{2}{x+y}$. Then the

degree-based topological index $f(G)$ in formula (10) is $H$

index $H(G)$. By formula (10), we have if $n \geq 3$, then

$$
\begin{cases}
f(S^n) &= 3f(S^{n-1}) - 12 \times \dfrac{2}{5} + 15 \times \dfrac{2}{6}, \\
f(S^2) &= 6(\dfrac{2}{5} + \dfrac{2}{6})
\end{cases}
$$

By solving this recursive formulation, we have $H(S^n) = 0.5 \times 3^n - 0.1$ for $n \geq 2$. $\square$

*Theorem 8.* $\mathcal{S}(S^1) = \dfrac{512}{27}$; if $n \geq 2$, we have

$$
\mathcal{S}(S^n) = \frac{1448292227 \times 3^n - 4965837723}{8429568}
$$

*Proof.* It can be verified that $\mathcal{S}(S^1) = \dfrac{512}{27}$ and $\mathcal{S}(S^2) = \dfrac{328320}{343}$ thus the theorem holds for $n = 1, 2$. Now we consider the case $n \geq 3$. We know that Sankruti index is defined based on $s_G(u)$ which is the summation of the degrees of all the neighbors of a vertex $u$, and by formula (11), we give the recursive formulation as follows which is different as formula (12).

$$
\begin{cases}
\mathcal{S}(S^n) &= 3\mathcal{S}(S^{n-1}) - 12 \times \left(\dfrac{6 \times 8}{6+8-2}\right)^3 + 15 \times \left(\dfrac{9 \times 9}{9+9-2}\right)^3, \\
\mathcal{S}(S^2) &= \dfrac{328320}{343}
\end{cases}
$$

By solving this recursive formulation, we have $\mathcal{S}(S^n) = \dfrac{1448292227 \times 3^n - 4965837723}{8429568}$ for $n \geq 2$. $\square$

Based on the result of Observation 1, we have

*Theorem 9.* If $n \geq 2$, then $Zg_1(S^n, x) = 6x^5 + \left(\dfrac{3^{n+1}-15}{2}\right)x^6$,

$Zg_1(S^n, x) = 6x^6 + \left(\dfrac{3^{n+1}-15}{2}\right)x^9$.

*Proof.* By the definition of the first Zagreb polynomial, we have

$$
\begin{aligned}
Zg_1(G, x) &= \sum_{e = uv \in E(G)} x^{d_u + d_v} \\
&= \sum_{e \in E_{2,3}} x^{d_u + d_v} + \sum_{e \in E_{3,3}} x^{d_u + d_v} \\
&= 6x^5 + \left(\frac{3^{n+1}-15}{2}\right)x^6.
\end{aligned}
$$

By the definition of the second Zagreb polynomial, we have

$$
\begin{aligned}
Zg_2(G, x) &= \sum_{e = uv \in E(G)} x^{d_u d_v} \\
&= \sum_{e \in E_{2,3}} x^{d_u d_v} + \sum_{e \in E_{3,3}} x^{d_u d_v} \\
&= 6x^6 + \left(\frac{3^{n+1}-15}{2}\right)x^9.
\end{aligned}
$$

## 3. Conclusion

In this paper, we study some of the *topostructural indices* of base-3 Sierpiński graphs by analysis a recursive formulation. By using this approach, we derived the formulae of the First Zagreb index $Zg_1(G)$, Second Zagreb index $Zg_2(G)$, the first Zagreb polynomial, the second Zagreb polynomial, sum-connectivity index $X(G)$, Geometric-Arithmetic index $GA(G)$, Atom-Bond Connectivity index $ABC(G)$, forgotten index $F(G)$, harmonic index $H(G)$ and Sankruti index $\mathcal{S}(G)$ of base-3 Sierpiński graphs.

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