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On topological properties of sierpinski networks

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ABSTRACT

Sierpinski graphs constitute an extensively studied class of graphs of fractal nature applicable in topology, mathematics of Tower of Hanoi, computer science, and elsewhere. A large number of properties like physico-chemical properties, thermodynamic properties, chemical activity, biological activity, etc. are determined by the chemical applications of graph theory. These properties can be characterized by certain graph invariants referred to as topological indices. In QRAR/QSPR study these graph invariants has played a vital role. In this paper, we study the molecular topological properties of Sierpinski networks and derive the analytical closed formulas for the atom-bond connectivity (*ABC*) index, geometric-arithmetic (*GA*) index, and fourth and fifth version of these topological indices for Sierpinski networks denoted by $S(n, k)$.

1. Introduction and preliminary results

The application of molecular structure descriptors is nowadays a standard procedure in the study of structure-property relations, especially in QSPR/QSAR study. In the last few years, the number of proposed molecular descriptors is rapidly growing due to the chemical significance of these descriptors. These descriptors correlate certain chemical and physical properties of chemical compounds. A close correlation of Randić index to the boiling point and Kovats constants has been found. A good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes is provided by the atom-bond connectivity (ABC) index. For certain physico-chemical properties like boiling point, Entropy, Enthalpy of vaporization, Standard enthalpy of vaporization, Enthalpy of formation and Acentric factor, the predictive power of geometric-arithmetic (*GA*) index is better than predictive power of the Randić connectivity index [8]. Topological characterization of chemical structures allows the classification of molecules and modelling unknown structures with desired properties. Molecules and molecular compounds are often modeled by molecular graphs. A model that is used to characterize a chemical compound is called *chemical graph*. 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. The combination of chemistry, mathematics and information science which studies QSAR/QSPR relationships is known as *cheminformatics*. Many chemical and physical properties of the chemical compounds can be found with the help of QSAR /QSPR models. The topological indices such as Wiener index, Szeged index, Randić index, Zagreb indices and *ABC* index are used to correlate different chemical and physical properties like the boiling point, molecular weight, vapour pressure, π-electrom energy etc.

A molecular graph can be described by different ways such as, a drawing, a polynomial, a sequence of numbers, a matrix or by a derived number called a topological index . A topological index is a numeric quantity associated with a graph which characterizes the topology of graph and is invariant under the graph automorphism. To establish a correlation model between the structures of chemical compounds and the coressponding chemical and physical properties it is required to numerically code the structures of chemical compounds. hence in the QSAR/QSPR studied the task is to transfer the graph into numerical format. for this purpose there are many techniques in which the popular one is topological indices. In more precise way, a *topological index* $Top(G)$ of a graph, is a number such that, if H is isomorphic to G, then $Top(H) = Top(G)$. The concept of topological indices came from Wiener [30] while he was working on boiling point of paraffin, named this index as *path number*. Later on, the path number was renamed as *Wiener index* [7]. There are three major classes of topological indices which are distance based topological indices, degree based topological indices and counting

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related. Among these classes degree based topological indices are of great importance and play a vital role in chemical graph theory and particularly in theoretical chemistry.

In this article, G is considered to be a graph with vertex set and edge set $V(G)$ and $E(G)$ respectively. The degree of a vertex $u \in V(G)$ in a graph G is the number of edges which are incident with vertex u. It is denoted by d_u. The notations used in this article are mainly taken from the books [10,15].

Let G be a connected graph. Then the *Wiener index* [30] of G is defined as

$$W(G) = \frac{1}{2}\sum_{(u,v)} d(u,v) \tag{1}$$

where (u, v) is any ordered pair of vertices in G and $d(u, v)$ is the distance between the vertices u and v.

Milan Randić [28] introduced the oldest degree based topological index *Randić* index, denoted by $R_{-\frac{1}{2}}(G)$ and defined as

$$R_{-\frac{1}{2}}(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}} \tag{2}$$

Randić index was then generalized by Bollobás and Erdös [5] for any real number α. The general Randić index, $R_\alpha(G)$, is defined as

$$R_\alpha(G) = \sum_{uv\in E(G)} (d_u d_v)^\alpha \quad \text{for} \quad \alpha \in \mathbb{R} \tag{3}$$

Gutman and Trinajstić [16] introduced the *first and second Zagreb indices*, denoted by $M_1(G)$ and $M_2(G)$, respectively and defined as

$$M_1(G) = \sum_{uv\in E(G)} (d_u + d_v) \tag{4}$$

$$M_2(G) = \sum_{uv\in E(G)} (d_G(u)d_G(v)). \tag{5}$$

The general Randić index for $\alpha = 1$ is the second Zagreb index for any graph. Estrada et al. [11] introduced a well known topological index, called the atom-bond connectivity (*ABC*) index. It is defined as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \tag{6}$$

The degree based topological index *geometric-arithmetic* (*GA*) index was introduced by Vukičević et al. in [29] and defined as

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

Some versions of the atom bond connectivity (*ABC*) index and geometric arithemetic *GA* index was defined recently. Ghorbani et al. [13] introduced the fourth version of *ABC* index and defined as

$$ABC_4(G) = \sum_{uv\in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}, \tag{8}$$

where $S_u = \sum_{v\in N_G(u)} d_v$ where $N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$.

The fifth version of *GA* index is proposed by Graovac et al. [14] and defined as

$$GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v} \tag{9}$$

The eccentric version of atom-bond connectivity idex, ABC_5 and geometric-arithmetic index, GA_4 were introduced by Vukičević et al. [29] and Ghorbani et al. [9] repectively, by using the eccentricity of each vertex of a connected graph. They are defined as

$$ABC_5(G) = \sum_{uv\in E(G)} \sqrt{\frac{e_u + e_v - 2}{e_u e_v}}$$

Where $e_u = \max_{v\in V(G)} d(u, v)$.

$$GA_4(G) = \sum_{uv\in E(G)} \frac{2\sqrt{e_u e_v}}{e_u + e_v}$$

Imran et al. studied various degree based topological indices for various networks like silicates, hexagonal, honeycomb and oxide in [20]. Nowadays there is an extensive research activity on *ABC* and *GA* indices and their variants. For further study of topological indices of various graphs and chemical structures, see [1–4,6,12,17–19,21,22,24–27].

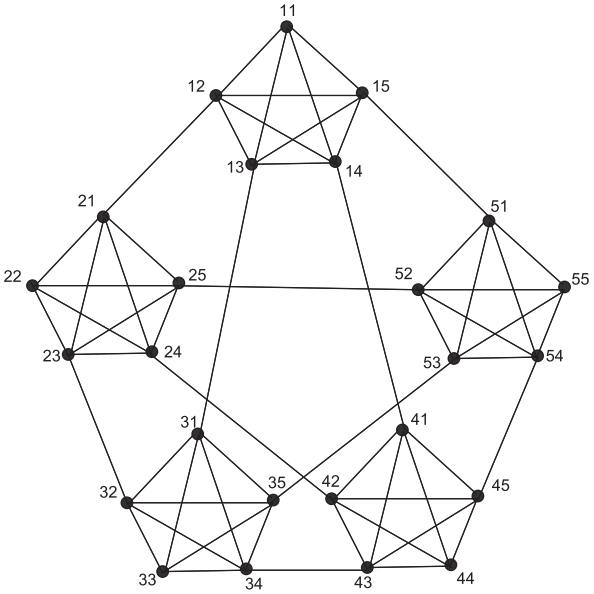

Fig. 1. Sierpinski network $S(3, 4)$

2. On topological indices of sierpinski networks $S(n, k)$

In this paper, we compute the analytical closed formulas for *ABC*, *GA*, ABC_4, ABC_5, GA_4 and GA_5 indices for *Sierpinski networks* denoted by $S(n, k)$. The sierpinski networks $S(n, k)$ are defined on the vertex set $V(S(n, k)) = \{1, 2, \ldots, k\}^n$. We have $|V(S(n, k))| = k^n$ for any $n \geq 1$ and $k \geq 1$ and vertices of these graphs can be written as $u = (u_1, u_2, \ldots u_n)$, where $u_r \in \{1, 2, \ldots\ldots, k\}$ and $r \in \{1, 2, \ldots..n\}$.

Two different vertices $u = (u_1, u_2, \ldots u_n)$ and $v = (v_1, v_2, \ldots v_n)$, where $u_r, v_r \in \{1, 2, \ldots\ldots, k\}$ and $r \in \{1, 2, \ldots..n\}$ of sierpinski network $S(n, k)$ are adjacent iff there exists an $h \in \{1, 2, \ldots., n\}$ such that:

- $u_t = v_t$ for $t = 1, \ldots, h-1$.
- $u_h = v_h$; and
- $u_t = v_h$ and $v_t = u_h$ for $t = h+1, \ldots, n$.

The definition of sierpinski networks $S(n, k)$ originated from the topological studies of the Lipscomb's space and sierpinski network $S(n, k)$ is isomorphic to the graphs of the Tower of Hanoi with n disks [23]. Moreover, sierpinski graphs are the first nontrivial families of graphs of fractal type for which the crossing number is known and several metric invariants such as unique 1-perfect codes, average distance of sierpinski graphs are studied in the literature. The sierpinski networks $S(3, 4)$ and $S(2, 5)$ are depicted in