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Vertex-degree-based topological indices of hexagonal systems with equal number of edges

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ABSTRACT

In this paper, we find extremal values of vertex-degree-based topological indices over Γ_m, the set of hexagonal systems with m edges. The main idea consists in constructing hexagonal systems with maximal number of inlets in Γ_m which have simultaneously minimal number of hexagons. Also we show that the convex spiral S_h has extremal TI -value over $\Gamma_{3h+\lceil\sqrt{12h-3}\rceil}$.

1. Introduction

In the chemical literature, a great variety of topological indices (molecular structure descriptors) have been and are currently considered in applications to QSPR/QSAR studies. Many of them depend only on the degrees of the vertices of the underlying molecular graph and are now called vertex-degree-based topological indices. More precisely, given nonnegative numbers $\{\psi_{ij}\}$, a vertex-degree-based topological index is expressed as

$$TI = TI(G) = \sum_{1\le i\le j\le n-1} m_{ij}\psi_{ij}$$

where G is a (molecular) graph with n vertices and m_{ij} is the number of edges of G connecting a vertex of degree i with a vertex of degree j. For instance, $\psi_{ij} = ij$ pertains to the second Zagreb index [11], $\psi_{ij} = \frac{1}{\sqrt{ij}}$ to the Randić connectivity index [24], whereas $\frac{2\sqrt{ij}}{i+j}$, $\frac{1}{\sqrt{i+j}}$, $\frac{(ij)^3}{(i+j-2)^3}$, and $\frac{2}{i+j}$ pertain, respectively, to the geometric–arithmetic [6,27], sum-connectivity [28], augmented Zagreb [9], and harmonic [29] indices. Details of these and other vertex-degree-based topological indices can be found in the books [13,14,19] and [2,7,8,10,15,16,18,20,25,26].

We are interested in studying vertex-degree-based topological indices over hexagonal systems, graph representations of benzenoid hydrocarbons which are of great importance in chemistry. For the definition of hexagonal systems and details of this theory we refer to [12]. It is well known that numerous topological properties of hexagonal systems are determined by the structural features on their perimeter. These features are shown in Fig. 1.

The numbers of fissures, bays, coves and fjords of a hexagonal system H are denoted by $f = f(H), B = B(H), C = C(H)$, and $F = F(H)$, respectively. The parameter

$$r = r(H) = f(H) + B(H) + C(H) + F(H)$$

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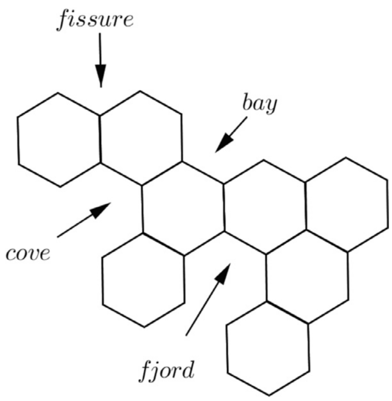

Fig. 1. Different types of inlets in a hexagonal system.

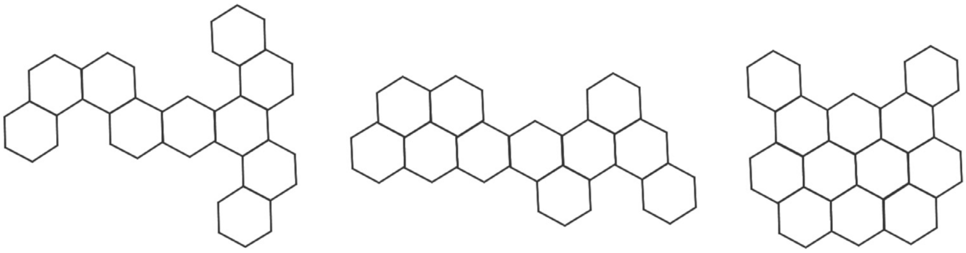

Fig. 2. Hexagonal systems in Γ_{51}.

was introduced in [21] and is called the number of inlets of H. Another quantity much studied in the theory of hexagonal systems is the so-called bay regions of H, denoted by $b = b(H)$, and is defined as

$$b = b(H) = B(H) + 2C(H) + 3F(H)$$

which counts the number of edges on the perimeter, connecting two vertices of degree 3. The relation between the number of inlets and the number of bay regions in a hexagonal system H is given by

$$r(H) = 2h(H) - b(H) - n_i(H) - 2 \quad (1)$$

where $h(H)$ is the number of hexagons and $n_i(H)$ is the number of internal vertices of H [3]. One special class of hexagonal systems is formed by the convex hexagonal systems. These are defined as the hexagonal systems for which $b = 0$ [3].

From a mathematical and chemical point of view, it is of great interest to find the extremal values of *TI* for significant classes of graphs. In the case of hexagonal systems, most of the work has been done over the set of hexagonal systems with equal number of hexagons [3,4,22,23]. In [1] the authors studied extremal values over the set of hexagonal systems with equal number of vertices. So it is natural now to consider the set of hexagonal systems with equal number of edges.

From now on we will denote by Γ_m the set of hexagonal systems with m edges. Fig. 2 shows several hexagonal systems belonging to Γ_{51}.

We note that the number of hexagons in the hexagonal systems of Γ_{51} is variable. In general, given a positive integer m, the variation of the number of hexagons in Γ_m is completely determined by Harary and Harborth [17]: if $H \in \Gamma_m$ then

$$\left\lceil \frac{1}{5}(m-1) \right\rceil \leq h(H) \leq m - \left\lceil \frac{1}{3}\left(2m - 2 + \sqrt{4m+1}\right) \right\rceil. \quad (2)$$

In this paper, we find extremal values of vertex-degree-based topological indices over Γ_m (see Theorem 3.1). The main idea consists in constructing hexagonal systems with maximal number of inlets in Γ_m which have simultaneously minimal number of hexagons $\left\lceil \frac{1}{5}(m-1) \right\rceil$ (Theorem 2.4). Also we show in Theorem 3.3 that the convex spiral S_h has extremal *TI* -value over $\Gamma_{3h+\lceil\sqrt{12h-3}\rceil}$.

2. Maximal number of inlets in the set of hexagonal systems with equal number of edges

The hexagonal systems in Fig. 3 appeared in [1] and the following result was proved.

Proposition 2.1 *[1, Proposition 2.4]. Let H be a hexagonal system with h hexagons. Then*

1. *If* $n_i(H) = 1$ *then* $r(H) \leq r(M_h) = \begin{cases} 3 & if \quad h = 3 \\ 2h - 4 & if \quad h \geq 4 \end{cases}$;