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# Convex Hexagonal Systems and Their Topological Indices

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**Abstract**

Convex hexagonal systems (CHS) i. e., hexagonal systems with no bay regions are studied. Among CHS with a fixed number of hexagons, the species with minimal/maximal number of inlets have minimal/maximal or maximal/minimal values for a variety of vertex–degree-based topological indices. These extremal CHS are characterized.

## 1 Convex hexagonal systems

In this paper we study a special class of hexagonal systems [1] in which there are no bay regions. These will be referred to as *convex hexagonal systems* and will be abbreviated by CHS. Their general form is depicted in Fig. 1.

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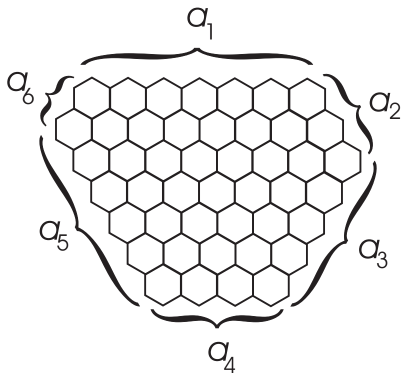


**Fig. 1.** The general form of a convex hexagonal system (CHS). The parameters $a_i \geq 1$ , $i = 1, 2, \ldots, 6$, count the hexagons on the respective side of CHS. For details see text.

The definition of hexagonal systems and details of their theory can be found in the book [1]. Recall that hexagonal systems provide the natural graph representation of benzenoid hydrocarbons. A hexagonal system with $h$ hexagons and $n_i$ internal vertices represents a benzenoid hydrocarbon of the formula $C_{4h+2-n_i}H_{2h+4-n_i}$. For this reason, hexagonal systems with equal number of hexagons and equal number of internal vertices will be said to be *isomeric*. Isomeric hexagonal systems have also equal number of vertices and equal number of edges.

When going along the perimeter of a hexagonal system, then certain features may be encountered, called [1] fissure, bay, cove, and fjord, see Fig. 2. These, respectively, correspond to vertex degree sequences

$$(2,3,2)\ ,\ (2,3,3,2)\ ,\ (2,3,3,3,2)\ ,\ (2,3,3,3,3,2)\ . \tag{1}$$

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

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

was introduced in [2], and is called the number of inlets of $S$.

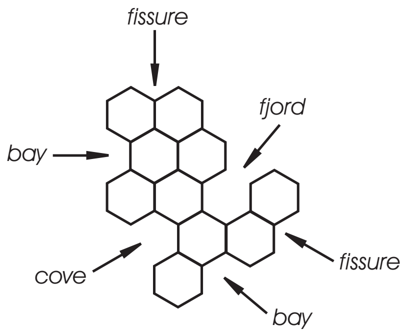


**Fig. 2.** Features lying on the perimeter of a hexagonal system, corresponding to sequences of vertex degrees specified in (1).

The following relations are well known [2] for a hexagonal system $S$ with $n$ vertices, $h$ hexagons, $r$ inlets and $m_{ij}$ edges between vertices of degree $i$ and degree $j$:

$$m_{22} = n - 2h - r + 2 \tag{2}$$

$$m_{23} = 2r \tag{3}$$

$$m_{33} = 3h - r - 3 \tag{4}$$

Another quantity much studied in the theory of benzenoid systems [1] is the number of bay regions $b = b(S)$ defined as $b = B + 2C + 3F$. It is easy to recognize that $b(S)$ counts the number of edges on the perimeter, connecting two vertices of degree 3.

One special class of hexagonal systems is formed by the convex hexagonal systems (CHS). These are defined as the hexagonal systems for which $b = 0$ i. e., $B = C = F = 0$. The motivation for their study is explained in a subsequent section. Here we first establish a few basic properties of CHS, noting that these hexagonal systems were previously considered by one of the present authors [3].

At the first glance, a CHS is determined by the six parameters $a_1, a_2, a_3, a_4, a_5, a_6$ indicating the length of its six sides, cf. Fig. 2. However, these parameters are not all mutually independent.

From the fact that the sides 1 and 4 are parallel, it follows that condition (6) must be obeyed. In a fully analogous manner we arrive also at (5) and (7):

$$a_1 + a_2 = a_4 + a_5 \tag{5}$$

$$a_2 + a_3 = a_5 + a_6 \tag{6}$$

$$a_3 + a_4 = a_6 + a_1 \ . \tag{7}$$

Of these relations only two are linearly independent, e. g., (5) and (6), and then the values of $a_5$ and $a_6$ can be expressed in terms of $a_1, a_2, a_3, a_4$:

$$a_5 = a_1 + a_2 - a_4 \tag{8}$$

$$a_6 = a_3 + a_4 - a_1 \ . \tag{9}$$

We thus arrive at the following:

**Theorem 1.** *Let $H(a_1, a_2, a_3, a_4, a_5, a_6)$ be a convex hexagonal system, cf. Fig. 2. Four parameters among $a_1, a_2, a_3, a_4, a_5, a_6$ fully determine this CHS. Of these four parameters only two can correspond to opposite sides of the CHS. In particular, the structure of the CHS is fully determined by $a_1, a_2, a_3, a_4$.*

From Fig. 2 one may get the impression that the shape of any CHS is hexagonal and that any CHS has six sides. Although this is correct from a formal point of view, some noteworthy special cases need to be pointed out. These are depicted in Fig. 3.

In view of Theorem 1 we may ask how the basic structural parameters of a CHS are determined by the parameters $a_1, a_2, a_3, a_4$. A partial answer to this question is given in Theorem 2.

**Theorem 2.** *Let $H = H(a_1, a_2, a_3, a_4, a_5, a_6)$ be a convex hexagonal system, cf. Fig. 2. Let $r(H)$, $h(H)$, and $n_i(H)$ be the number of inlets, hexagons, and internal vertices of $H$. Then*

$$r(H) = a_1 + 2a_2 + 2a_3 + a_4 - 6 \tag{10}$$

$$\begin{aligned} h(H) &= a_1\, a_3 + a_1\, a_4 + a_2\, a_3 + a_2\, a_4 - a_2 - a_3 \\ &- \frac{1}{2}\, a_1(a_1+1) - \frac{1}{2}\, a_4(a_4+1) + 1 \end{aligned} \tag{11}$$

$$\begin{aligned} n_i(H) &= 2(a_1\, a_3 + a_1\, a_4 + a_2\, a_3 + a_2\, a_4) \\ &- a_1(a_1+2) - a_4(a_4+2) - 4(a_2+a_3) + 6 \ . \end{aligned} \tag{12}$$

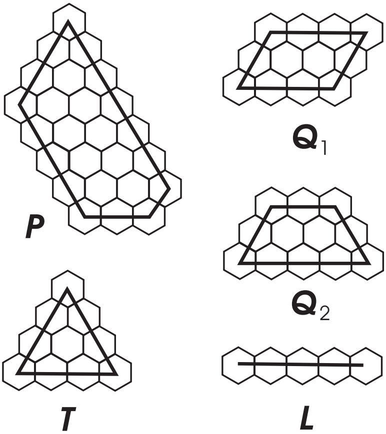


**Fig. 3.** Special cases of the CHS $H(a_1, a_2, a_3, a_4, a_5, a_6)$ from Fig. 2, when some of the parameters $a_i$ are equal to unity: pentagon-shaped $\mathbf{P}$ $(a_1 = 1,\ a_2, a_3, a_4, a_5, a_6 > 1)$, quadrangle-shaped $\mathbf{Q}_1$ $(a_2 = a_5 = 1,\ a_1 = a_4,\ a_3 = a_6)$ and $\mathbf{Q}_2$ $(a_2 = a_5 = 1,\ a_2 = a_6)$, triangle-shaped $\mathbf{T}$ $(a_1 = a_3 = a_5 = 1,\ a_2 = a_4 = a_6)$, and linear $\mathbf{L}$ $(a_2 = a_3 = a_5 = a_6 = 1,\ a_1 = a_4)$.

*Proof.* Eq. (10) follows from the fact that the $i$-th side of $H$ has $a_i - 1$ inlets. Therefore $r(H) = a_1 + a_2 + a_3 + a_4 + a_5 + a_5 + a_6 - 6$. Eq. (10) is then obtained by taking into the relations (8) and (9). $\square$

Eq. (11) is deduced by counting the hexagons in the auxiliary hexagonal system depicted in Fig. 4, and subtracting the number of shaded hexagons. By taking into account that a triangle-shaped hexagonal system (cf. $\mathbf{T}$ in Fig. 3) of size $k$ has $k(k-1)/2$ hexagons, and using the relations (8) and (9), after a lengthy calculation we arrive at Eq. (11). $\square$

Eq. (12) is deduced in an analogous manner as Eq. (11), bearing in mind that a triangle-shaped hexagonal systems of size $k$ has $(k-1)^2$ internal vertices. $\square$

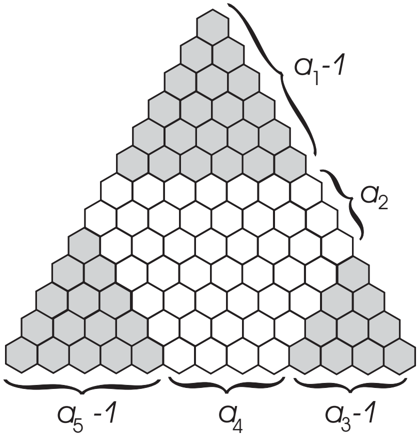


**Fig. 4.** An auxiliary triangle-shaped hexagonal systems used in the proof of Theorem 2. For notation see Fig. 2.

**Remark 3.** *From Theorem 2, expressions for other structural parameters of a CHS directly follow: The numbers of vertices and edges are obtained from* $n = 4h + 2 - n_i$ *and* $m = 5h + 1 - n_i$*. The number of edges of various types can then be computed by using Eqs.* (2)–(4).

**Remark 4.** *A convex hexagonal system* $H(a_1, a_2, a_3, a_4, a_5, a_6)$ *is Kekuléan if and only if* $a_1 = a_4$, $a_2 = a_5$, *and* $a_3 = a_6$*. Details on various classes of Kekuléan CHS, their names, and their Kekulé structure counts can be found in the book* [4].

## 2 Randić connectivity index and its congeners

In 1975, Randić [5] introduced one of the graph–based molecular structure descriptors most widely used in applications to physical and chemical properties, which is now called the Randić index or connectivity index. It is defined for a graph $G$ as

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

where $d(u)$ denotes the degree of the vertex $u$ of $G$ and the summation goes over all edges $uv$ of $G$.

In 1998 Bollobás and Erdős [6] considered the generalized version of the connectivity index

$$R_\alpha(G) = \sum_{uv} [d(u)\, d(v)]^\alpha$$

defined for every $\alpha \in \mathbb{R}$. For $\alpha = -1/2$ one recovers the ordinary connectivity index.

Literature on the connectivity index over the set of hexagonal systems can be found in [2,3]. Recently, Wu and Deng [7] extended the results of [3] to the generalized connectivity indices. Particularly, they found the hexagonal system with maximal $R_\alpha$ for every $\alpha \in \mathbb{R}$ such that $2^{\alpha+1} - 3^\alpha > 0$. Naturally, the following question arises: which hexagonal systems have maximal $R_\alpha$ for $\alpha \in \mathbb{R}$ such that $2^{\alpha+1} - 3^\alpha \leq 0$? Apparently, a solution to this problem is complicated when considering the set of all hexagonal systems with a fixed number of hexagons. However, when we restrict the consideration to convex hexagonal systems, then the solution can be found, applicable not only to the generalized connectivity index, but to all indices of the form (13) (see below).

The connectivity and generalized connectivity indices are two special cases of the expression

$$TI = TI(G) = \sum_{uv} \Psi(d(u), d(v)) \tag{13}$$

when $\Psi(x,y) = 1/\sqrt{x\,y}$ and $\Psi(x,y) = [x\,y]^\alpha$, respectively. In the meantime, a great variety of other analogous vertex–degree–based topological indices (molecular structure descriptors) has been considered in the mathematico–chemical literature [8]. Of these we mention the topological indices in which the function $\Psi$ is defined in the following manner:

| | |
|---|---|
| $\Psi(x,y) = x\,y$ | second Zagreb index [9] |
| $\Psi(x,y) = \sqrt{(x+y-2)/(x\,y)}$ | atom–bond connectivity index [10] |
| $\Psi(x,y) = 1/\sqrt{x+y}$ | sum-connectivity index [11] |
| $\Psi(x,y) = 2\,\sqrt{x\,y}/(x+y)$ | geometric–arithmetic index [12] |
| $\Psi(x,y) = [x\,y/(x+y-2)]^3$ | augmented Zagreb index [13] |
| $\Psi(x,y) = 2/(x+y)$ | harmonic index [14] |

Since any hexagonal system $S$ possesses only vertices of degree 2 and 3, the general expression for the above listed topological indices reads

$$TI(S) = m_{22}\,\Psi(2,2) + m_{23}\,\Psi(2,3) + m_{33}\,\Psi(3,3)$$

which in view of the relations (2)–(4) yields:

$$\begin{aligned} TI(S) &= \Psi(2,2)\,n + \Big[3\,\Psi(3,3) - 2\,\Psi(2,2)\Big]h + \Big[2\,\Psi(2,3) - \Psi(2,2) - \Psi(3,3)\Big]r \\ &+ \Big[2\,\Psi(2,2) - 3\,\Psi(3,3)\Big] \qquad (14) \\ &= \Big[3\,\Psi(3,3) + 2\,\Psi(2,2)\Big]h - \Psi(2,2)\,n_i + \Big[2\,\Psi(2,3) - \Psi(2,2) - \Psi(3,3)\Big]r \\ &+ \Big[4\,\Psi(2,2) - 3\,\Psi(3,3)\Big]\ . \qquad (15) \end{aligned}$$

From Eqs. (14) or (15) we conclude the following general property of the vertex–degree–based topological indices of hexagonal systems:

**Theorem 5.** (a) *If* $2\,\Psi(2,3) - \Psi(2,2) - \Psi(3,3) > 0$, *then among isomeric hexagonal systems, those having smallest (resp. greatest) number of inlets have smallest (resp. greatest) topological index* $TI$, *Eq.* (13).
(b) *If* $2\,\Psi(2,3) - \Psi(2,2) - \Psi(3,3) < 0$, *then among isomeric hexagonal systems, those having smallest (resp. greatest) number of inlets have greatest (resp. smallest) topological index* $TI$.
(c) *If* $2\,\Psi(2,3) - \Psi(2,2) - \Psi(3,3) = 0$, *then all isomeric hexagonal systems have equal values of the topological index* $TI$.

# 3 Estimating the number of inlets

From Theorem 5 it should be evident why we are interested in the number of inlets and its maximal and minimal possible value. We begin this section with a sharp upper bound for the number of inlets in a hexagonal system.

**Lemma 6.** *If* $S$ *is a hexagonal system with* $h$ *hexagons and* $r$ *inlets, then* $r \leq 2(h-1)$.

*Proof.* It is well known [1] that

$$m_{23} = 4h - 4 - 2b - 2n_i$$

where $n_i$ denotes the number of internal vertices of $S$. Using relation (3) we get

$$r = 2(h-1) - (n_i + b)\ .$$

Since $n_i + b \geq 0$, Lemma 6 immediately follows. □

Note that $r(L_h) = 2(h-1)$, where $L_h$ is the linear hexagonal chain (cf. **L** in Fig. 3). Hence, Lemma 6 states that the linear hexagonal chain has the maximal number of inlets among all hexagonal systems with $h$ hexagons. The following question arises naturally:

**Problem 7.** *Which are the hexagonal systems with $h$ hexagons with minimal number of inlets?*

As far as we can see, this problem is not easy to solve. At the moment we can present only a partial answer to this question, namely for convex hexagonal systems. Thus, we consider the following special cases of Problem 7.

**Problem 8.** (a) *Which are the convex hexagonal systems with $h$ hexagons with minimal number of inlets?*
(b) *Which are the convex hexagonal systems with $h$ hexagons and $n_i$ internal vertices with minimal number of inlets?*

We first try to solve Problem 8 by a standard analytical approach – the method of Lagrange multipliers.

Let $H = H(a_1, a_2, a_3, a_4, a_5, a_5, a_6)$ be a convex hexagonal system with $h$ hexagons and $n_i$ internal vertices, whose $r$-value we want to minimize. In view of Eqs. (10)–(12), consider the expression

$$\begin{aligned}\rho &= \Big[a_1 + 2a_2 + 2a_3 + a_4 - 6\Big] + \lambda\Big[a_1\, a_3 + a_1\, a_4 + a_2\, a_3 + a_2\, a_4 - a_2 - a_3 \\ &- \frac{1}{2}\, a_1(a_1+1) - \frac{1}{2}\, a_4(a_4+1) + 1 - h\Big] + \mu\Big[2(a_1\, a_3 + a_1\, a_4 + a_2\, a_3 + a_2\, a_4) \\ &- a_1(a_1+2) - a_4(a_4+2) - 4(a_2+a_3) + 6 - n_i\Big]\end{aligned}$$

and impose the conditions

$$\frac{\partial \rho}{\partial a_i} = 0 \quad , \quad i = 1, 2, 3, 4\ .$$

After appropriate calculation, a system of four linear equations is obtained:

$$\begin{pmatrix} -1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = \Gamma \begin{pmatrix} 1 \\ 2 \\ 2 \\ 1 \end{pmatrix}$$

where $\Gamma = (\lambda + 4\mu - 2)/(2\lambda + 4\mu)$. By solving this system we obtain $a_1 = a_2 = a_3 = a_4$, which together with Eqs. (8) and (9) yields

$$a_1 = a_2 = a_3 = a_4 = a_5 = a_6 = k\ .$$

Thus, by the Lagrange multiplier method we find that the convex hexagonal systems with minimal number of inlets are the members of the circumcoronene series (benzene, $k = 1$, coronene, $k = 2$, circumcoronene, $k = 3$, circumcircumcoronene, $k = 4$, $\ldots$) [15, 16]. This result is of little use, because it restricts us to CHS with $3k(k-1)+1$ hexagons and $6(k-1)^2$ internal vertices. For all other possible values of $h$ and $n_i$ the Lagrange multiplier method fails to yield a solution.

The solution of Problem 8 can be obtained in another, somewhat simpler, manner.

From Eqs. (11) and (12) we directly obtain $2h(S) - n_i(S) = a_1 + 2\,a_2 + 2\,a_3 + a_4 + 4$, which combined with Eq. (10) yields

$$r(S) = 2h(S) - n_i(S) - 2\ . \tag{16}$$

This implies the following remarkable answer to question (b) of Problem 8:

**Theorem 9.** *All isomeric convex hexagonal systems have equal number of inlets.*

**Corollary 10.** *All isomeric convex hexagonal systems have equal topological indices $TI$ defined via Eq.* (13).

Remains part (a) of Problem 8. The answer to it was obtained long time ago by Harary and Harborth [17]. Namely, from Eq. (16) we see that for a fixed value of $h$, the number of inlets will be minimal if the number of internal vertices is maximal. Hexagonal systems with maximal number of internal vertices are constructed by the “spiral” method illustrated in Fig. 5.

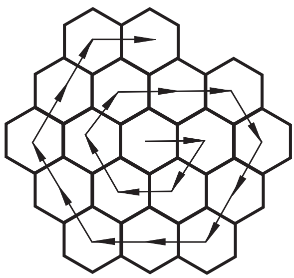

**Fig. 5.** The Harary–Harborth construction of hexagonal systems with maximal number of internal vertices [17]. Hexagons have to be added one-by-one, going along the indicated spiral line.

The hexagonal systems constructed by the "spiral" method are not necessarily convex (and may have a single bay, $B = 1$). If this happens, then the newly added hexagon has to be removed to another position, without altering the number of internal vertices. This is illustrated in Fig. 6.

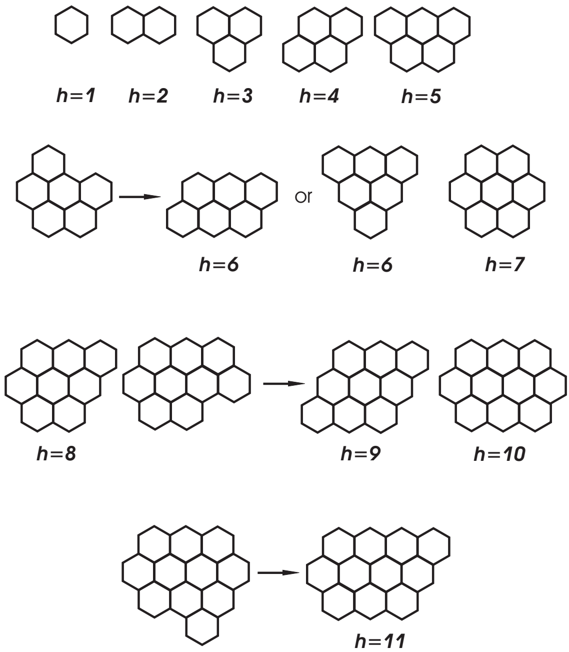


**Fig. 6.** The convex hexagonal systems with the first few $h$-values, possessing minimal number of inlets. These are constructed by the Harary–Harborth "spiral" method (see Fig. 5), with amendments when necessary (moving one or more hexagons so as not to change the $n_i$-value). The case $h = 6$ illustrates the fact that the CHS with minimal number of inlets needs not be unique.

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