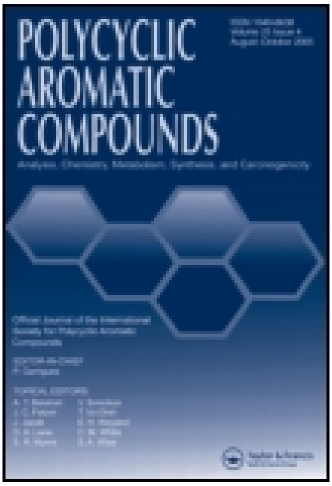

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Atom-bond Connectivity Index of Benzenoid Systems and Fluoranthene Congeners

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The recently introduced atom-bond connectivity (*ABC*) index has been applied to study the stability of alkanes and the strain energy of cycloalkanes. In this article, the *ABC* index of both benzenoid systems and fluoranthene congeners is shown to depend solely on the number of vertices, hexagons and inlets. In addition, the author characterizes the extremal catacondensed benzenoid systems with the maximal and minimal *ABC* index.

Key Words: fluoranthene congener, atom-bond connectivity (ABC) index, benzenoid system, inlet.

INTRODUCTION

Molecular descriptors have found a wide application in the theory of the quantitative structure-property relations (QSPR) and the quantitative structure-activity relations (QSAR). Among them, topological indices have a prominent place (15). One of the best known and widely used is the connectivity index (i.e., Randić index) introduced in 1975 by M. Randić (12), who has shown this index to reflect molecular branching. Some results about branching can be found in Gutman et al. (8), Vukičević (16), Vukičević and Gutman (18), and Vukičević and Žerovnik (20), and in the references cited therein. However, many physico-chemical properties are dependent on factors rather different than branching. In order to take this into account but at the same time to keep the spirit of the Randić index, E. Estrada et al. (5) proposed a new index of graph G, known as

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the *atom-bond connectivity (ABC) index*, which is abbreviated as $ABC(G)$ and defined as follows:

$$ABC(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}$$

where the summation goes over all edges of G, d_i and d_j are the degrees of the terminal vertices v_i and v_j of edge v_iv_j, and $E(G)$ is the edge set of G. The ABC index has been proven to be a valuable predictive index in the study of the heat of formation in alkanes and has been applied up to now to study the stability of alkanes and the strain energy of cycloalkanes (5). Recently, there are some known contributions on the ABC index (2, 4, 6).

A *benzenoid system* (7), also called honeycomb system, is a finite connected subgraph of the infinite hexagonal lattice without cut vertices or non-hexagonal interior faces. Benzenoid systems are widely used because they are the representations of the skeletons of molecules of benzenoid hydrocarbons. More details on this important class of molecular graphs can be found in Gutman and Cyvin (7) and in the references cited therein. Recall that A *catacondensed benzenoid system* is a benzenoid system whose vertices are all on the perimeter. A hexagon of a catacondensed benzenoid system is said to be a *turning hexagon* if it has two or three non-parallel edges which are common edges with other hexagons. A catacondensed benzenoid system without turning hexagon is said to be a *linear chain benzenoid system*, denoted by L_h if it possesses h hexagons. The special graphs mentioned above are depicted as in Figure 1.

Fluoranthene congeners considered in paper (17) consist of two benzenoid fragments, joined so as to form an additional five-membered ring. In other words, the general form of a fluoranthene congener H is obtained by joining two benzenoid systems (X and Y) so as to form a five-membered ring (cf. Figure 2). Thus, the systems are, from a structural point of view, closely similar to

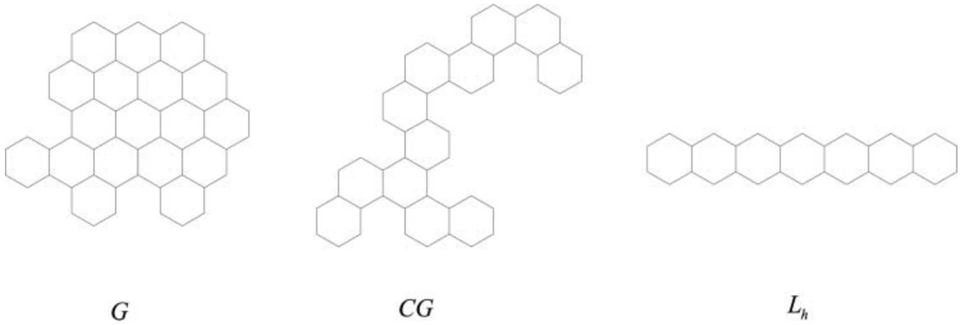
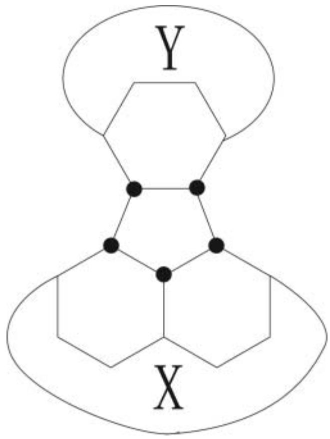


Figure 1: A benzenoid system *G*, a catacondensed benzenoid system *CG* and a linear chain benzenoid system L_h.



H

Figure 2: A general form of a fluoranthene congener H.

benzenoid systems. Many results about fluoranthene congeners can be found in Gutman and Žerovnik (9), Gutman et al. (10, 11), and Vukičević et al. (17).

In this article, we are interested in the *ABC* index of benzenoid systems and fluoranthene congeners. Two formulas (in Theorem 3.2 and 4.2) are obtained for computing the *ABC* index of both a benzenoid system and fluoranthene congener. As a consequence, we characterize the extremal catacondensed benzenoid systems with the maximal and minimal *ABC* index over the set of catacondensed benzenoid systems with a fixed number of hexagons.

DEFINITIONS AND NOTATIONS

Throughout the present paper we use the notations and terminology proposed in Cyvin and Gutman (3) and Gutman and Cyvin (7). For a benzenoid system G, we call a vertex of degree j a *j-vertex*. A *(j, k)-edge* stands for an edge connecting a j-vertex with a k-vertex. The number of j-vertices and (j, k)-edges in the graph will be denoted by n_j and m_{jk}, respectively. If one goes along the perimeter of G, then a *fissure* is a structural feature formed by a 2-vertex, followed by a 3-vertex, followed by a 2-vertex. A simple *bay* is formed by a 2-vertex, followed by two 3-vertices, followed by a 2-vertex. A *cove* and a *fjord* are the features formed, respectively, by three and four consecutive 3-vertices, lying between 2-vertices. An illustrative example is depicted as in Figure 3.

For a benzenoid system G, the number of fissures, simple bays, coves and fjords are respectively denoted by f, B, C and F. The fissures, bays, coves

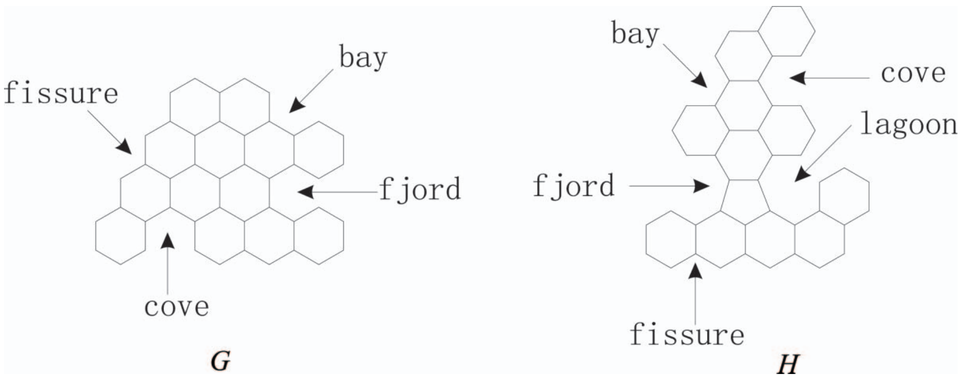


Figure 3: Types of inlets occurring on the perimeter of a benzenoid system *G* and a fluoranthene congener *H*.

and fjords are called various types of *inlets*. The total number of inlets on the perimeter of a benzenoid system will be denoted by r_1, i.e.,

$$r_1 = f + B + C + F. \tag{2.1}$$

For a fluoranthene congener H, a fissure, bay, coves and fjord are defined as in full analogy to the benzenoid systems. Furthermore, we define an additional type of inlet called the *lagoon*, denoted by L. This is a feature of the perimeter, formed by a 2-vertex, followed by five 3-vertices, followed by a 2-vertex (cf. Figure 3). With the inlets defined as above, and the total number of inlets on the perimeter of a fluoranthene congener will be denoted by r_2, we have

$$r_2 = f + B + C + F + L. \tag{2.2}$$

THE *ABC* INDEX OF BENZENOID SYSTEMS

In this section, we obtain the formulas about the ABC index of benzenoid systems and catacondensed benzenoid systems. In the case of a benzenoid system G with n vertices and h hexagons, which possesses only $(2,2)$-, $(2,3)$-, and $(3,3)$-edges, the ABC index of a benzenoid system G reduces to

$$ABC(G) = \frac{\sqrt{2}}{2} m_{22} + \frac{\sqrt{2}}{2} m_{23} + \frac{2}{3} m_{33}. \tag{3.1}$$

Meanwhile, there is the following relations to the parameters such as n, h, r_1, m_{22}, m_{23}, and m_{33} in a benzenoid system.

Lemma 3.1. (13) *Let G be a benzenoid system with n vertices, h hexagons and r_1 inlets. Then:*

$$m_{22} = n - 2h - r_1 + 2$$
$$m_{23} = 2r_1$$
$$m_{33} = 3h - r_1 - 3.$$

By Lemma 3.1 and Eq. (3.1), one can obtain the *ABC* index of benzenoid systems.

Theorem 3.1. *Let G be a benzenoid system with n vertices, h hexagons and r_1 inlets. Then:*

$$ABC(G) = \frac{\sqrt{2}}{2}n + (2 - \sqrt{2})h + \frac{3\sqrt{2} - 4}{6}r_1 + (\sqrt{2} - 2).$$

Proof. Let G be a benzenoid system with n vertices, h hexagons and r_1 inlets. By Lemma 3.1 and Eq. (3.1), we have

$$\begin{aligned} ABC(G) &= \frac{\sqrt{2}}{2}m_{22} + \frac{\sqrt{2}}{2}m_{23} + \frac{2}{3}m_{33} \\ &= \frac{\sqrt{2}}{2}(n - 2h - r_1 + 2) + \frac{\sqrt{2}}{2}(2r_1) + \frac{2}{3}(3h - r_1 - 3) \\ &= \frac{\sqrt{2}}{2}n + (2 - \sqrt{2})h + \frac{3\sqrt{2} - 4}{6}r_1 + (\sqrt{2} - 2). \end{aligned}$$

□

As a consequence, we consider the maximal and minimal *ABC* index over the set of catacondensed benzenoid systems with a fixed number of hexagons. Let $\mathscr{C}_h$ denote the set of all catacondensed benzenoid systems with h hexagons. In order to characterize the extremal catacondensed benzenoid systems, we construct catacondensed benzenoid systems with minimal number of inlets according to the methods in Randić (12). For positive integers k and t, let $H(k, t)$ denote the catacondensed ladder benzenoid systems (cf. Figure 4). If h is even ($h \geq 6$), let E_h be the catacondensed benzenoid system obtained by adding two hexagons (shaded hexagons in Figure 4), one to the angular hexagon of the bottom and the other, to the angular hexagon of the top of the catacondensed ladder benzenoid system $H(2, \frac{h-2}{2})$. Clearly, $E_h \in \mathscr{C}_h$ and $r_1(E_h) = \frac{h}{2} + 1$ since

$$f(E_h) = 0, B(E_h) = 2, C(E_h) = 2, F(E_h) = \frac{h}{2} - 3.$$

If h is odd ($h \geq 5$), let O_h be the catacondensed benzenoid system obtained by adding only one hexagon (shaded hexagon in Figure 4) to the angular hexagon

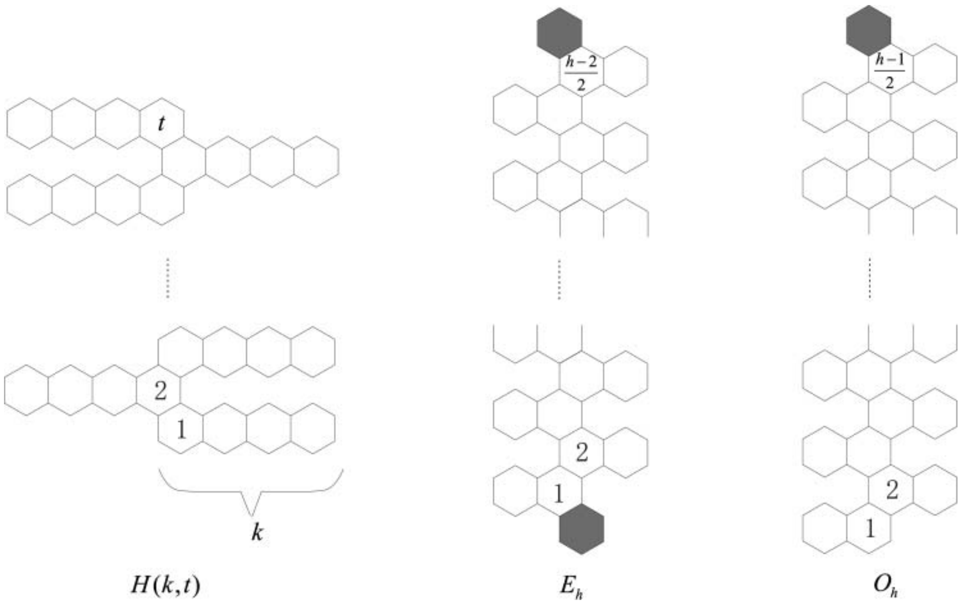


Figure 4: The catacondensed ladder benzenoid system $H(k, t)$ and the extremal catacondensed benzenoid systems E_h and O_h.

located in the bottom of the catacondensed ladder benzenoid system $H(2, \frac{h-1}{2})$. In this case $O_h \in \mathscr{C}_h$ and $r_1(O_h) = \frac{h+1}{2} + 1$ since

$$f(O_h) = 1, B(O_h) = 2, C(O_h) = 1, F(O_h) = \frac{h+1}{2} - 3.$$

In Rada (14), there is the following conclusion to the bound on the parameter r_1.

Lemma 3.2. (14) *Let CG be a catacondensed benzenoid system in $\mathscr{C}_h$. Then:*

$$2(h-1) = r_1(L_h) \geq r_1(CG) \geq \begin{cases} r_1(E_h) = \dfrac{h}{2} + 1 & \textit{if } h \textit{ is even} \\ r_1(O_h) = \dfrac{h+1}{2} + 1 & \textit{if } h \textit{ is odd,} \end{cases}$$

where $L_h \in \mathscr{C}_h$.

Furthermore, for a catacondensed benzenoid system CG, there is a fact (14) that

$$n = 4h + 2. \tag{3.2}$$

From Theorem 3.1, thus we obtain the ABC index of catacondensed benzenoid system and characterize the extremal catacondensed benzenoid systems with the maximal and minimal ABC index.

Theorem 3.2. *Let CG be a catacondensed benzenoid system with fixed h hexagons and r_1 inlets. Then:*

(i) $ABC(CG) = (2+\sqrt{2})h + \frac{3\sqrt{2}-4}{6}r_1 + (2\sqrt{2}-2)$;

(ii) *ABC(CG) is a monotone increasing function about the inlets r_1 of CG;*

(iii)

$$ABC(L_h) \geq ABC(CG) \geq \begin{cases} ABC(E_h), & \text{if } h \text{ is even} \\ ABC(O_h), & \text{if } h \text{ is odd}, \end{cases}$$

where

$$ABC(L_h) = \frac{6\sqrt{2}+2}{3}h + \frac{3\sqrt{2}-2}{3}$$

$$ABC(E_h) = \frac{15\sqrt{2}+20}{12}h + \frac{15\sqrt{2}-16}{6}$$

$$ABC(O_h) = \frac{15\sqrt{2}+20}{12}h + \frac{11\sqrt{2}-12}{4}.$$

Proof. It is obviously true for the conclusions of (i) and (ii) by Theorem 3.1 and Eq. (3.2).

In the following, we consider the conclusion of (iii). From the conclusion of (ii), we must analyze the behavior of r_1 over $\mathscr{C}_h$ in order to have information about the variation of *ABC*(*CG*) over $\mathscr{C}_h$. More precisely, it is our interest to find the maximal and minimal value of r_1 in $\mathscr{C}_h$. Since $r_1(L_h) = 2(h-1)$, $r_1(E_h) = \frac{h}{2}+1$ if h is even and $r_1(O_h) = \frac{h+1}{2}+1$ if h is odd by Lemma 3.2, we have

$$\frac{6\sqrt{2}+2}{3}h + \frac{3\sqrt{2}-2}{3} = ABC(L_h) \geq ABC(CG),$$

$$ABC(CG) \geq ABC(E_h) = \frac{15\sqrt{2}+20}{12}h + \frac{15\sqrt{2}-16}{6}$$

and

$$ABC(CG) \geq ABC(O_h) = \frac{15\sqrt{2}+20}{12}h + \frac{11\sqrt{2}-12}{4}.$$

Thus, the theorem is completely proved. □

THE *ABC* INDEX OF FLUORANTHENE CONGENERS

In the section we consider the *ABC* index of fluoranthene congeners. With the inlets defined as above, Eq. (2.2) remains applicable in the case of fluoranthene congeners. Since a fluoranthene congener possesses only $(2, 2)$-, $(2, 3)$-, and $(3, 3)$-edges, there is a result similar to Lemma 3.1.

Lemma 4.1. *Let H be a fluoranthene congener with n vertices, h hexagons and r_2 inlets. Then:*

$$m_{22} = n - 2h - r_2$$
$$m_{23} = 2r_2$$
$$m_{33} = 3h - r_2.$$

Proof. Let H be a fluoranthene congener with n vertices, h hexagons and r_2 inlets. By the definition of an inlet (i.e., an inlet corresponds to a sequence of vertices on the perimeter, of which the first and the last are 2-vertices and all other are 3-vertices.), it is obvious that

$$m_{23} = 2r_2.$$

From the fact (7) of benzenoid systems and by the construction of fluoranthene congeners, it is easy to see that the number of 3-vertices in H is equal to $2h$, i.e., $n_3 = 2h$. Since $m_{23} + 2m_{33} = 3n_3 = 6h$ and m_{23}, we conclude that

$$m_{33} = 3h - r_2.$$

By Euler's formula (1) which says that for a connected plane graph, the number of vertices plus the number of faces is equal to the number of edges plus two, we have $n + (h + 2) = m + 2 = m_{22} + m_{23} + m_{33} + 2$. Now by substituting the values of m_{23} and m_{33}, one obtains

$$m_{22} = n - 2h - r_2.$$

□

Analogous to the proof of Theorem 3.1, one can easily obtain the *ABC* index of a fluoranthene congener.

Theorem 4.2. *Let H be a fluoranthene congener with n vertices, h hexagons and r_2 inlets. Then:*

$$ABC(H) = \frac{\sqrt{2}}{2}n + (2 - \sqrt{2})h + \frac{3\sqrt{2} - 4}{6}r_2.$$

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