Applied Mathematics and Computation 268 (2015) 534–546

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Second order Randić index of fluoranthene-type benzenoid systems

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ARTICLE INFO

Keywords:
Second order Randić index
Inlet
F-benzenoid system
Cata-catacondensed f-benzenoid system

ABSTRACT

Fluoranthene-type benzenoid system are polycyclic conjugated molecules consisting of two benzenoid fragments, connected by two carbon–carbon bonds so as to form a five-membered ring. fluoranthene-type benzenoid system and its congeners are compounds which, in view of their chemical and physical properties, belong among benzenoid hydrocarbons. Let F denotes a fluoranthene-type benzenoid system, whose second order Randić index is denoted by $R_2(F)$. In this paper, we give the expression of $R_2(F)$ in terms of their inlet features. And we find the minimal and maximal value of the second order Randić index over the set of cata-catacondensed fluoranthene-type benzenoid systems, and characterize their corresponding graphs.

1. Introduction

The Randić index (now also called the branching index or the connectivity index) of a graph G, denoted by $R(G)$, invented by the chemist M. Randić [1] in 1975, is the graph-based molecular structure descriptor that is most frequently applied in quantitative structure-property and structure-activity studies [2–6]. For a simple undirected graph $G = (V, E)$, its Randić index $R(G)$ is defined as

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

where $d(u)$ denotes the degree of the vertex u and the summation is taken over all pairs of adjacent vertices of the graph G. Some publications related to the Randić index can be found in the literature [7–16,30]. With the intention of extending the applicability of the Randić index, Randić, Kier, Hall et al. [4,6] considered the higher-order Randić index of a graph G as

$$R_k(G) = \Sigma_{u_1 u_2 \cdots u_{k+1}} \frac{1}{\sqrt{d(u_1)d(u_2)\cdots d(u_{k+1})}},$$

where the summation is taken over all possible paths of length k of G (we do not distinguish between the paths $u_1u_2\cdots u_{k+1}$ and $u_{k+1}\cdots u_2u_1$). This new approach has been applied successfully to an impressive variety of physical, chemical and biological properties (boiling points, solubilities, densities, anesthetic, toxicities etc.) which have appeared in many scientific publications and in two books [4,5]. Results related to the mathematical properties of these indices have been reported in the literature

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http://dx.doi.org/10.1016/j.amc.2015.06.056
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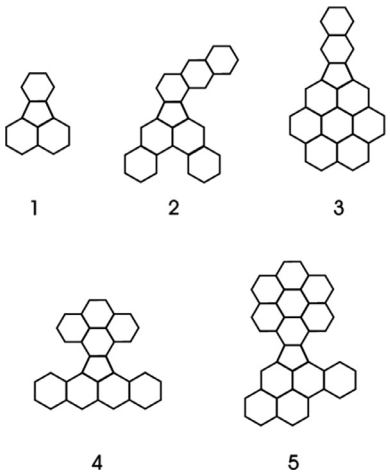

Fig. 1. Examples of fluoranthene-type benzenoid systems. 1 and 2 are cata-catacondensed, 3 is peri-catacondensed, 4 is cata-pericondensed, and 5 is peri-pericondensed.

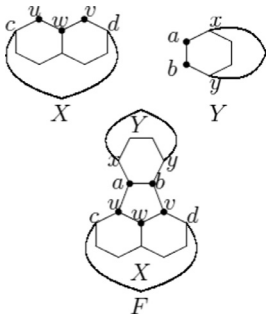

Fig. 2. The general form of an f-benzenoid system (F) and its construction from two benzenoid systems X and Y.

[17–22,28,29]. Specifically, Rada [19] gave an expression of the second-order Randić index of benzenoid systems and found the minimal and maximal values over the set of catacondensed systems. The Randić index of phenylenes has been discussed in [16], the second-order and third-order Randić indices of phenylenes have been discussed in [20] and [22].

Our main concern is the class of the fluoranthene-type benzenoid systems. Fluoranthene is a well-known tetracyclic conjugated hydrocarbon, present in large amounts in coal tar [23,57]. It consists of a benzene and a naphthalene unit, joined through a five-membered ring. Other polycyclic conjugated hydrocarbon, consisting of two benzenoid units joined through a five-membered ring are referred as fluoranthene-type benzenoid system (or fluoranthenes) [25,26]. A few examples of fluoranthene-type benzenoid systems are presented in Fig. 1.

In what follows we will represent the fluoranthene-type benzenoid system by means of their molecular graphs [25]. This, in particular, means that the carbon atoms are represented by vertices, and the carbon–carbon bonds by edges. The molecular graphs of fluoranthene-type benzenoid system are then defined in the following manner. Let X be a benzenoid system [27]. Let u and v be two vertices of X whose degree is two, and which both are adjacent to a vertex w of degree 3. Let Y be another benzenoid system. Let a and b be two adjacent vertices of Y whose degree is two. The fluoranthene-type benzenoid system F is obtained by joining (with a new edge) the vertices u and a , and by joining (with a new edge) the vertices v and b (see Fig. 2).

What first needs to be noticed is that the vertices a, b, v, w, u of F form a five-membered cycle. Each fluoranthene-type benzenoid system possesses (by definition) exactly one five-membered cycle.

Although the structures of fluoranthene-type benzenoid systems and benzenoid hydrocarbons are evidently similar, fluoranthene-type benzenoid systems were excluded from the chemical graph theoretical consideration of benzenoid systems because of the presence of a five-membered ring. As a result, while the topological theory of benzenoid molecules is nowadays one of the most thoroughly elaborated aspect of chemical graph theory [53–56], the first attempts to develop an analogous theory of fluoranthene-type benzenoid systems started only very recently [25].

The fluoranthene-type benzenoid systems considered by us must pertain to plane graphs composed of regular hexagonals and a regular pentagon, all having the same edge lengths. Non-adjacent hexagon and hexagon-pentagon pairs must neither tough nor overlap (we exclude the helicenic and other geometrically non-plane species from the class of fluoranthene-type benzenoid systems). Fluoranthene-type benzenoid systems are compounds which, in view of their chemical and physical properties, belong among benzenoid hydrocarbons. For more about fluoranthene-type benzenoid system, one can see [25,26].