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The hexagonal chains with the extremal third-order Randić index☆

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ABSTRACT

The third-order Randić index of a graph G is defined as $R_3(G) = \sum_{u_1u_2u_3u_4} \frac{1}{\sqrt{d(u_1)d(u_2)d(u_3)d(u_4)}}$, where the summation is taken over all possible paths of length three of G. A recursive formula for computing the third-order Randić index of a hexagonal chain is given in this paper, and the hexagonal chains with the extremal third-order Randić index are characterized.

1. Introduction

The connectivity index (or Randić index) of a graph G, denoted by $R(G)$, was introduced by Randić [1] in the study of branching properties of alkanes. It is defined as

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

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 connectivity index can be found in the literature [2–13].

With the intention of extending the applicability of the connectivity index, Randić, Kier, Hall et al. [14,15] considered the higher-order connectivity index of a graph G as

$$R_k(G) = \sum_{u_1u_2\cdots u_{k+1}} \frac{1}{\sqrt{d(u_1)d(u_2)\cdots d(u_{k+1})}}$$

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 $u_{k+1}u_h\cdots u_1$). 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 [14,16]. Results related to the mathematical properties of these indices have been reported in the literature [2,3]. Specifically, Rada [11] 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 [4], the second- and third-order Randić indices of phenylenes have been discussed in [12] and [13]. In this paper, we first give the recursive formulas for computing the third-order Randić indices of hexagonal chains, and then determine the upper and lower bounds of their third-order Randić indices. Finally, we characterize the extremal graphs with the extremal third-order Randić index.

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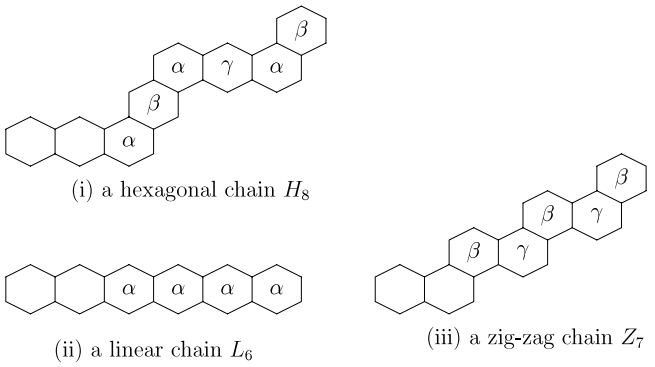

Fig. 1. Single hexagonal chains with different types of fusions.

Table 1
The weights of some paths of length 3 in H_{n+3} (Fig. 2(1)).

$wxyz$	wa_1a_2z	$wa_1a_2b_2$	$wa_1b_1c_1$	$xyza_2$	xwa_1a_2
$\frac{1}{4}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{6}$
xwa_1b_1	$yxwa_1$	yza_2a_1	yza_2b_2	$za_2a_1b_1$	$za_2b_2c_2$
$\frac{1}{2\sqrt{6}}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{6}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{6}$	$\frac{1}{6}$

2. The recursive formulas for computing the third-order Randić indices of hexagonal chains

A hexagonal system is a 2-connected plane graph whose every interior face is bounded by a regular hexagon of unit length 1. The hexagonal systems are of considerable importance in theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbons. A vertex of a hexagonal system belongs to, at most, three hexagons. A vertex shared by three hexagons is called an internal vertex of the respective hexagonal system. A hexagonal system H is said to be catacondensed if it does not possess internal vertices, otherwise H is said to be pericondensed.

A hexagonal chain is a catacondensed hexagonal system which has no hexagon adjacent to more than two hexagons. Some examples of hexagonal chains can be found in Fig. 1.

Now, we first consider the recursive formula for computing the third-order Randić index of a hexagonal chain.

It is easy to see that any hexagonal chains H_{n+1} with $n+1$ hexagons can be obtained from a hexagonal chain H_n with n hexagons by attaching it to a new hexagon. Based on this fact, a hexagonal chain can be constructed inductively. There are three types of fusion for attaching a new hexagon h_{n+1} to a hexagonal chain H_n with n hexagons $h_1, h_2, \ldots, h_n$:

(i) if h_{n+1} is on the line l, it is called α-type fusing;
(ii) if h_{n+1} is on the left-hand side of l, it is called β-type fusing;
(iii) if h_{n+1} is on the right-hand side of l, it is called γ-type fusing

where l is the direct line from the center of h_{n-1} to the center of h_n. Any hexagonal chain H_n $(n \geq 2)$ can be obtained from H_2 by a stepwise fusion of new hexagons, and at each step a θ-type fusion is selected, where $\theta \in \{\alpha, \beta, \gamma\}$.

Let $H_{n+2} = H(\theta_1, \theta_2, \ldots, \theta_n)$ be the hexagonal chain with $n+2$ hexagons obtained from H_2 by θ_1-type, θ_2-type, $\ldots$, θ_n-type fusing, successively. Then $H(\alpha, \alpha, \ldots, \alpha)$ is called a linear chain L_{n+2}. $H(\beta, \gamma, \beta, \gamma, \ldots)$ or $H(\gamma, \beta, \gamma, \beta, \ldots)$ is called a zig-zag chain Z_{n+2}.

Note that $H(\theta_1, \theta_2, \ldots, \theta_n) \cong H(\overline{\theta_1}, \overline{\theta_2}, \ldots, \overline{\theta_n})$ if

$$\overline{\theta} = \begin{cases} \alpha, & \text{if } \theta = \alpha; \\ \beta, & \text{if } \theta = \gamma; \\ \gamma, & \text{if } \theta = \beta. \end{cases}$$

Let $H_{n+3} = H(\theta_1, \theta_2, \ldots, \theta_n, \theta_{n+1})$ be a hexagonal chain, as in Fig. 2.

Case I. $\theta_n = \theta_{n+1} = \alpha$. Then H_{n+3} is obtained from H_{n+2} by an α-type fusing (see Fig. 2(1)). The paths $wxyz$, wa_1a_2z, $wa_1a_2b_2$, $wa_1b_1c_1$, $xyza_2$, xwa_1a_2, xwa_1b_1, $yxwa_1$, yza_2a_1, yza_2b_2, $za_2a_1b_1$, $za_2b_2c_2$ of length 3 are added. Except for the paths $d_1c_1b_1a_1$, $c_2c_1b_1a_1$, $d_2c_2b_2a_2$, $c_1c_2b_2a_2$, $c_1b_1a_1a_2$, $c_2b_2a_2a_1$ and $b_1a_1a_2b_2$, the other paths of length 3 in H_{n+3} contribute the same weight to the sum that defines the third-order Randić index. Let $W_1(P)$ and $W_2(P)$ be the weight $\frac{1}{\sqrt{d(v_1)d(v_2)d(v_3)d(v_4)}}$ of the path $P = v_1v_2v_3v_4$ in H_{n+3} and H_{n+2}, respectively.

By the definition of the third-order Randić index and Tables 1 and 2, we have

$$R_3(H_{n+3}) = R_3(H_{n+2}) + \frac{4}{3} + \frac{2}{9}\sqrt{6}.$$