

# Double 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  $R_3(G) = \sum_{u_1 u_2 u_3 u_4} \frac{1}{\sqrt{d(u_1)d(u_2)d(u_3)d(u_4)}}$ , where the summation is taken over all possible paths of length three of  $G$ . In this paper, we first give a recursive formula for computing the third order Randić index of a double hexagonal chain. And then we determine the upper and lower bounds of the third order Randić index and characterize the double hexagonal chains with the extremal third order Randić index.

## 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([5,8-14,21-23]).

With the intention of extending the applicability of the connectivity index, Randić, Kier, Hall and co-workers([2] and [3]) considered the higher-order con-

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nectivity index of a graph  $G$  as

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

where the summation is taken over all possible paths of length  $k$  of  $G$  (we do not distinguish between the paths  $u_1 u_2 \dots u_{k+1}$  and  $u_{k+1} u_h \dots u_1$ ). 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 ([2] and [4]). Results related to the mathematical properties of these indices have been reported in the literature([5] and [6]). Specifically, Rada [15] gave an expression of the second order Randić index of benzenoid systems and found the minimal and maximal value over the set of catacondensed systems. The Randić index of phenylenes has been discussed in [7], the second and the third order Randić indices of phenylenes have been discussed in [16,17]. A recursive formula for computing the third order Randić index of a hexagonal chain is given and the hexagonal chains with the extremal third order Randić index are characterized in [18]. In this paper, we will consider a type of the pericondensed hexagonal system. The double hexagonal chains with the extremal third order Randić index are determined.

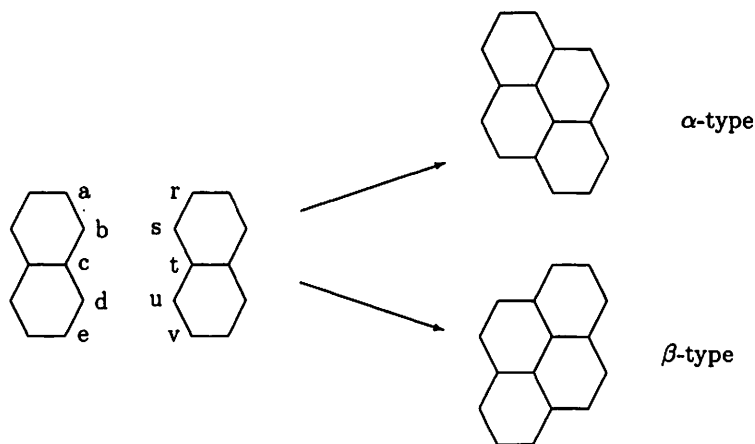


Figure 1.  $\alpha$ -type fusing,  $\beta$ -type fusing.

A hexagonal system is a 2-connected plane graph whose every interior face is bounded by a regular hexagon of unit length 1. Hexagonal systems are of considerable importance in theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbons [19]. 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. An  $n$ -tuple hexagonal chain consists of  $n$  condensed identical hexagonal chains. When  $n = 2$ , we call it a double hexagonal chain [19-20].

A double hexagonal chain can be constructed inductively. Let us orient the naphthalene so that its interior edges is horizontal. There are two types of fusion of two naphthalenes: (i)  $b \equiv r, c \equiv s, d \equiv t, e \equiv u$ ; (ii)  $a \equiv s, b \equiv t, c \equiv u, d \equiv v$  as shown in Figure 1. We call them  $\alpha$ -type and  $\beta$ -type fusing, respectively. Any double hexagonal chain can be obtained from a naphthalene  $B$  by a stepwise fusion of new naphthalene, and at each step a  $\theta$ -type fusion is selected, where  $\theta \in \{\alpha, \beta\}$ .

Let  $B(\theta_1, \theta_2, \dots, \theta_n)$  be the double hexagonal chain with  $2(n + 1)$  hexagons obtained from a naphthalene  $B$  by  $\theta_1$ -type,  $\theta_2$ -type,  $\dots$ ,  $\theta_n$ -type fusing, successively.  $B(\alpha, \alpha, \dots, \alpha)$  or  $B(\beta, \beta, \dots, \beta)$ , i.e.,  $\theta_i = \theta_{i+1}$  for each  $i$ , is called the double linear hexagonal chain and denoted by  $DL_n$ ; if  $\theta_i \neq \theta_{i+1}$  for each  $i$ , then  $B(\theta_1, \theta_2, \dots, \theta_n)$  is called the double zig-zag hexagonal chain and denoted by  $DZ_n$  (see Figure 2).

Let

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

Then  $B(\theta_1, \theta_2, \dots, \theta_n) \cong B(\bar{\theta}_1, \bar{\theta}_2, \dots, \bar{\theta}_n)$ . If  $n \geq 1$ , the double hexagonal chain  $B(\theta_1, \theta_2, \dots, \theta_n)$  is a pericondensed hexagonal system.

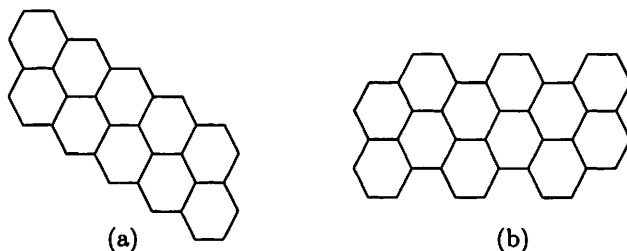


Figure 2. (a) The double linear hexagonal chain  $DL_4 = B(\alpha, \alpha, \alpha, \alpha)$ ;  
 (b) The double zig-zag hexagonal chain  $DZ_5 = B(\beta, \alpha, \beta, \alpha, \beta)$ .

## 2 A recursive formula for computing the third order Randić index of a double hexagonal chain

In this section, we give a recursive formula for computing the third order Randić index of a double hexagonal chain  $B(\theta_1, \theta_2, \dots, \theta_n)$ .

Let  $B_n = B(\theta_1, \theta_2, \dots, \theta_n)$  be a double hexagonal chain with  $2(n + 1)$  hexagons, as in Figure 3.

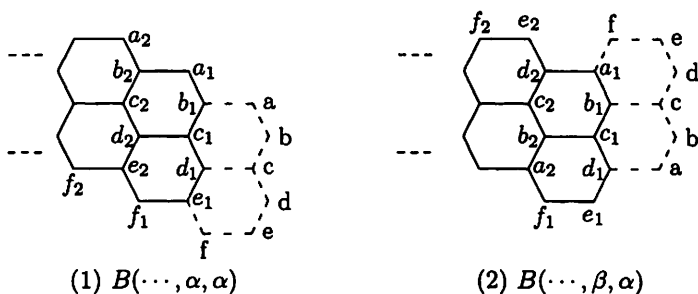


Figure 3.

**Case I.**  $\theta_n = \theta_{n-1} = \alpha$ . Then  $B_n$  is obtained from  $B_{n-1}$  by a  $\alpha$ -type fusing (see Figure 3 (1)). The following paths of length 3 are added:

$abcd, abcd_1, ab_1a_1b_2, ab_1c_1d_2, ab_1c_1d_1, bcde, bcd_1c_1, bcd_1e_1, bab_1a_1, bab_1c_1, cdef, cd_1e_1f, cd_1e_1f_1, cd_1c_1d_2, cd_1c_1b_1, cbab_1, defe_1, dcd_1c_1, dcd_1e_1, efe_1f_1, efe_1d_1, edcd_1, fe_1f_1e_2, fe_1d_1c_1$ .

Table 1. The weights of some paths of length 3 in  $B_n$ .

$abcd$	$abcd_1$	$ab_1a_1b_2$	$ab_1c_1d_2$	$ab_1c_1d_1$	$bcde$
$\frac{1}{2\sqrt{6}}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{2\sqrt{6}}$
$bcd_1c_1$	$bcd_1e_1$	$bab_1a_1$	$bab_1c_1$	$cdef$	$cd_1e_1f$
$\frac{1}{3\sqrt{6}}$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{6}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{3\sqrt{6}}$
$cd_1e_1f_1$	$cd_1c_1d_2$	$cd_1c_1b_1$	$cbab_1$	$defe_1$	$dcd_1c_1$
$\frac{1}{3\sqrt{6}}$	$\frac{1}{9}$	$\frac{1}{9}$	$\frac{1}{6}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{3\sqrt{6}}$
$dcd_1e_1$	$efe_1f_1$	$efe_1d_1$	$edcd_1$	$fe_1f_1e_2$	$fe_1d_1c_1$
$\frac{1}{3\sqrt{6}}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{3\sqrt{6}}$

Table 2. The weights of some paths of length 3 in  $B_n$  and  $B_{n-1}$ .

	$a_2b_2a_1b_1$	$b_2a_1b_1c_1$	$c_2b_2a_1b_1$	$c_2d_2c_1b_1$	$c_2d_2c_1d_1$
$W_1$	$\frac{1}{6}$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{9}$
$W_2$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{9}$	$\frac{1}{3\sqrt{6}}$
	$d_2c_1b_1a_1$	$d_2c_1d_1e_1$	$d_2e_2f_1e_1$	$e_2d_2c_1b_1$	$e_2d_2c_1d_1$
$W_1$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{9}$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{9}$	$\frac{1}{9}$
$W_2$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{3\sqrt{6}}$
	$e_2f_1e_1d_1$	$f_2e_2f_1e_1$	$a_1b_1c_1d_1$	$b_1c_1d_1e_1$	$c_1d_1e_1f_1$
$W_1$	$\frac{1}{3\sqrt{6}}$	$\begin{cases} \frac{1}{6}, & \text{if } d(f_2) = 2; \\ \frac{1}{3\sqrt{6}}, & \text{if } d(f_2) = 3 \end{cases}$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{9}$	$\frac{1}{3\sqrt{6}}$
$W_2$	$\frac{1}{2\sqrt{6}}$	$\begin{cases} \frac{1}{2\sqrt{6}}, & \text{if } d(f_2) = 2; \\ \frac{1}{6}, & \text{if } d(f_2) = 3 \end{cases}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{2\sqrt{6}}$

Except for the paths:

$a_2b_2a_1b_1, b_2a_1b_1c_1, c_2b_2a_1b_1, c_2d_2c_1b_1, c_2d_2c_1d_1, d_2c_1b_1a_1, d_2c_1d_1e_1, d_2e_2f_1e_1, e_2d_2c_1b_1, e_2d_2c_1d_1, e_2f_1e_1d_1, f_2e_2f_1e_1, a_1b_1c_1d_1, b_1c_1d_1e_1, c_1d_1e_1f_1,$   
the other paths of length 3 in  $B_n$  are the same in  $B_{n-1}$ .

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  $B_n$  and  $B_{n-1}$ , respectively.

Note that  $d(f_2) = 2$  if  $\theta_{n-2} = \alpha$  and  $d(f_2) = 3$  if  $\theta_{n-2} = \beta$ . By the definition of the third order Randić, we have

$$R_3(B_n) = R_3(B_{n-1}) + \begin{cases} \frac{4}{3} + \frac{7}{9}\sqrt{6}, & \text{if } \theta_{n-2} = \theta_{n-1} = \theta_n = \alpha; \\ 1 + \frac{11}{12}\sqrt{6}, & \text{if } \theta_{n-2} = \beta \text{ and } \theta_{n-1} = \theta_n = \alpha. \end{cases}$$

And

$$R_3(B_n) = R_3(B_{n-1}) + \begin{cases} \frac{4}{3} + \frac{7}{9}\sqrt{6}, & \text{if } \theta_{n-2} = \theta_{n-1} = \theta_n = \beta; \\ 1 + \frac{11}{12}\sqrt{6}, & \text{if } \theta_{n-2} = \alpha \text{ and } \theta_{n-1} = \theta_n = \beta \end{cases}$$

since  $B(\theta_1, \theta_2, \dots, \theta_n) \cong B(\bar{\theta}_1, \bar{\theta}_2, \dots, \bar{\theta}_n)$ .

**Case II.**  $\theta_{n-1} = \alpha$  and  $\theta_n = \beta$ . Then  $B_n$  is obtained from  $B_{n-1}$  by a  $\beta$ -type fusing (see Figure 3 (2)). The following paths of length 3 are added:

$abcd, abc b_1, ad_1e_1f_1, ad_1c_1b_2, ad_1c_1b_1, bad_1e_1, bad_1c_1, bcd_1c_1, bcb_1a_1, bcde, cbad_1, cb_1c_1d_1, cb_1c_1b_2, cb_1a_1d_2, cb_1a_1f, cdef, dcb_1c_1, dcb_1a_1, defa_1, edcb_1, efa_1b_1, efa_1d_2, fa_1b_1c_1, fa_1d_2c_2, fa_1d_2e_2.$

Table 3. The weights of some paths of length 3 in  $B_n$ .

$\frac{abcd}{2\sqrt{6}}$	$\frac{abcb_1}{6}$	$\frac{ad_1e_1f_1}{2\sqrt{6}}$	$\frac{ad_1c_1b_2}{3\sqrt{6}}$	$\frac{ad_1c_1b_1}{3\sqrt{6}}$	$\frac{bad_1e_1}{2\sqrt{6}}$	$\frac{bad_1c_1}{6}$
$\frac{bcd_1c_1}{3\sqrt{6}}$	$\frac{bcb_1a_1}{3\sqrt{6}}$	$\frac{bcde}{2\sqrt{6}}$	$\frac{cbad_1}{6}$	$\frac{cb_1c_1d_1}{9}$	$\frac{cb_1c_1b_2}{9}$	$\frac{cb_1a_1d_2}{9}$
$\frac{cb_1a_1f}{3\sqrt{6}}$	$\frac{cdef}{2\sqrt{6}}$	$\frac{dcb_1c_1}{3\sqrt{6}}$	$\frac{dcb_1a_1}{3\sqrt{6}}$	$\frac{defa_1}{2\sqrt{6}}$	$\frac{edcb_1}{6}$	$\frac{efa_1b_1}{6}$
$\frac{efa_1d_2}{6}$	$\frac{fa_1b_1c_1}{3\sqrt{6}}$	$\frac{fa_1d_2c_2}{3\sqrt{6}}$	$\frac{fa_1d_2e_2}{6}$			

Table 4. The weights of some paths of length 3 in  $B_n$  and  $B_{n-1}$ .

	$f_2e_2d_2a_1$	$e_2d_2a_1b_1$	$d_2a_1b_1c_1$	$c_2d_2a_1b_1$	$c_2b_2c_1a_1$
$W_1$	$\begin{cases} \frac{1}{6}, & \text{if } d(f_2) = 2; \\ \frac{1}{3\sqrt{6}}, & \text{if } d(f_2) = 3 \end{cases}$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{9}$	$\frac{1}{9}$	$\frac{1}{9}$
$W_2$	$\begin{cases} \frac{1}{2\sqrt{6}}, & \text{if } d(f_2) = 2; \\ \frac{1}{6}, & \text{if } d(f_2) = 3 \end{cases}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{3\sqrt{6}}$
	$c_2b_2c_1d_1$	$b_2c_1b_1a_1$	$b_2c_2d_2a_1$	$b_2c_1d_1e_1$	$a_2b_2c_1b_1$
$W_1$	$\frac{1}{9}$	$\frac{1}{9}$	$\frac{1}{9}$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{9}$
$W_2$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{6}$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{6}$	$\frac{1}{3\sqrt{6}}$
	$a_2b_2c_1d_1$	$a_2f_1e_1d_1$	$a_1b_1c_1d_1$	$b_1c_1d_1e_1$	$c_1d_1e_1f_1$
$W_1$	$\frac{1}{9}$	$\frac{1}{6}$	$\frac{1}{9}$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{6}$
$W_2$	$\frac{1}{3\sqrt{6}}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{2\sqrt{6}}$	$\frac{1}{2\sqrt{6}}$

Except for the paths:

$f_2e_2d_2a_1, e_2d_2a_1b_1, d_2a_1b_1c_1, c_2d_2a_1b_1, c_2b_2c_1a_1, c_2b_2c_1d_1, b_2c_1b_1a_1, b_2c_2d_2a_1, b_2c_1d_1e_1, a_2b_2c_1b_1, a_2b_2c_1d_1, a_2f_1e_1d_1, a_1b_1c_1d_1, b_1c_1d_1e_1, c_1d_1e_1f_1$ ,  
the other paths of length 3 in  $B_n$  are the same in  $B_{n-1}$ .

The weight of these paths are given in Tables 3 and 4, where  $W_1(P)$  and  $W_2(P)$  are the weight of the path  $P$  in  $B_n$  and  $B_{n-1}$ , respectively.

Note that  $d(f_2) = 2$  if  $\theta_{n-2} = \beta$  and  $d(f_2) = 3$  if  $\theta_{n-2} = \alpha$ . By the definition of the third order Randić, we have

$$R_3(B_n) = R_3(B_{n-1}) + \begin{cases} \frac{7}{3} + \frac{7}{18}\sqrt{6}, & \text{if } \theta_{n-2} = \beta, \theta_{n-1} = \alpha, \theta_n = \beta; \\ 2 + \frac{19}{36}\sqrt{6}, & \text{if } \theta_{n-2} = \theta_{n-1} = \alpha, \theta_n = \beta. \end{cases}$$

And

$$R_3(B_n) = R_3(B_{n-1}) + \begin{cases} \frac{7}{3} + \frac{7}{18}\sqrt{6}, & \text{if } \theta_{n-2} = \alpha, \theta_{n-1} = \beta, \theta_n = \alpha; \\ 2 + \frac{19}{36}\sqrt{6}, & \text{if } \theta_{n-2} = \theta_{n-1} = \beta, \theta_n = \alpha. \end{cases}$$

since  $B(\theta_1, \theta_2, \dots, \theta_n) \cong B(\overline{\theta_1}, \overline{\theta_2}, \dots, \overline{\theta_n})$ .

So, we have the following recursive formula

**Theorem 1.** Let  $B_n = B(\theta_1, \theta_2, \dots, \theta_n)$  and  $B_{n-1} = B(\theta_1, \theta_2, \dots, \theta_{n-1})$  be double hexagonal chains,  $n \geq 3$ . Then

$$R_3(B_n) = R_3(B_{n-1}) + \begin{cases} \frac{4}{3} + \frac{7}{9}\sqrt{6}, & \begin{array}{l} \theta_{n-2} = \theta_{n-1} = \theta_n = \alpha \\ \text{or } \theta_{n-2} = \theta_{n-1} = \theta_n = \beta; \end{array} \\ 1 + \frac{11}{12}\sqrt{6}, & \begin{array}{l} \theta_{n-2} = \beta, \theta_{n-1} = \theta_n = \alpha \\ \text{or } \theta_{n-2} = \alpha, \theta_{n-1} = \theta_n = \beta; \end{array} \\ \frac{7}{3} + \frac{7}{18}\sqrt{6}, & \begin{array}{l} \theta_{n-2} = \beta, \theta_{n-1} = \alpha, \theta_n = \beta \\ \text{or } \theta_{n-2} = \alpha, \theta_{n-1} = \beta, \theta_n = \alpha; \end{array} \\ 2 + \frac{19}{36}\sqrt{6}, & \begin{array}{l} \theta_{n-2} = \theta_{n-1} = \alpha, \theta_n = \beta \\ \text{or } \theta_{n-2} = \theta_{n-1} = \beta, \theta_n = \alpha. \end{array} \end{cases}$$

### 3 The extremal double hexagonal chains with respect to the third order Randić index

In this section, we will give the upper and lower bounds on the third order Randić indices of double hexagonal chains and characterize the extremal graphs.

**Theorem 2.** Let  $B_n = B(\theta_1, \theta_2, \dots, \theta_n)$  be a double hexagonal chain with  $2(n+1)$  hexagons. Then

(i)  $R_3(B_n) \geq \frac{12n+7}{9} + \frac{7n+10}{9}\sqrt{6}$

with equality if and only if  $(\theta_1, \theta_2, \dots, \theta_n) = (\alpha, \alpha, \dots, \alpha)$ , or  $(\beta, \beta, \dots, \beta)$ , i.e.,  $B_n$  is the double linear hexagonal chain  $DL_n$ ;

(ii)  $R_3(B_n) \leq \frac{21n-2}{9} + \frac{7n+27}{18}\sqrt{6}$

with equality if and only if  $(\theta_1, \theta_2, \dots, \theta_n) = (\beta, \alpha, \beta, \alpha, \dots)$  or  $(\alpha, \beta, \alpha, \beta, \dots)$ , i.e.,  $B_n$  is the double zig-zag hexagonal chain  $DZ_n$ .

**Proof.** It can be computed out directly that

$$R_3(B) = \frac{11}{6} + \frac{2}{3}\sqrt{6};$$

$$R_3(B_1) = R_3(B(\alpha)) = R_3(B(\beta)) = \frac{19}{9} + \frac{17}{9}\sqrt{6};$$

$$R_3(B_2) = \begin{cases} R_3(B(\alpha, \alpha)) = R_3(B(\beta, \beta)) = \frac{31}{9} + \frac{8}{3}\sqrt{6} \\ R_3(B(\alpha, \beta)) = R_3(B(\beta, \alpha)) = \frac{40}{9} + \frac{41}{18}\sqrt{6} \end{cases}$$

and

$$\frac{31}{9} + \frac{8}{3}\sqrt{6} < \frac{40}{9} + \frac{41}{18}\sqrt{6};$$

$$R_3(B_3) = \begin{cases} R_3(B(\alpha, \alpha, \alpha)) = R_3(B(\beta, \beta, \beta)) = \frac{43}{9} + \frac{31}{9}\sqrt{6} \\ R_3(B(\alpha, \alpha, \beta)) = R_3(B(\beta, \beta, \alpha)) = \frac{49}{9} + \frac{115}{36}\sqrt{6} \\ R_3(B(\alpha, \beta, \alpha)) = R_3(B(\beta, \alpha, \beta)) = \frac{61}{9} + \frac{8}{3}\sqrt{6} \\ R_3(B(\alpha, \beta, \beta)) = R_3(B(\beta, \alpha, \alpha)) = \frac{49}{9} + \frac{115}{36}\sqrt{6} \end{cases}$$

and

$$\frac{43}{9} + \frac{31}{9}\sqrt{6} < \frac{49}{9} + \frac{115}{36}\sqrt{6} < \frac{61}{9} + \frac{8}{3}\sqrt{6}.$$

From Theorem 1 and  $R_3(B_1) = \frac{19}{9} + \frac{17}{9}\sqrt{6}$ , it can be computed out easily that

$$R_3(DL_n) = \frac{12n+7}{9} + \frac{7n+10}{9}\sqrt{6}$$

$$R_3(DZ_n) = \frac{21n-2}{9} + \frac{7n+27}{18}\sqrt{6}.$$

In the following, using the inductive method on  $n$ , we prove that  $R_3(DL_n) \leq R_3(B_n) \leq R_3(DZ_n)$  with the left (or right) equality if and only if  $B_n$  is  $DL_n$  (or  $DZ_n$ ).

The result is true for  $n = 1, 2$  from above.

We suppose that the result is true for  $n$  and  $n - 1$  ( $n \geq 2$ ), i.e.,

$R_3(DL_{n-1}) \leq R_3(B_{n-1}) \leq R_3(DZ_{n-1})$  with the left (or right) equality if and only if  $B_{n-1}$  is  $DL_{n-1}$  (or  $DZ_{n-1}$ ) and  $R_3(DL_n) \leq R_3(B_n) \leq R_3(DZ_n)$  with the left (or right) equality if and only if  $B_n$  is  $DL_n$  (or  $DZ_n$ ).

Let  $B_{n+1} = B(\theta_1, \theta_2, \dots, \theta_n, \theta_{n+1})$  be a double hexagonal chain with  $2(n+2)$  hexagons. Note that

$$\frac{4}{3} + \frac{7}{9}\sqrt{6} < 1 + \frac{11}{12}\sqrt{6} < \frac{7}{3} + \frac{7}{18}\sqrt{6} < 2 + \frac{19}{36}\sqrt{6}.$$

By Theorem 1, we have

(i)  $R_3(B_{n+1}) \geq R_3(B_n) + \frac{4}{3} + \frac{7}{9}\sqrt{6}$  with equality if and only if  $\theta_{n-1} = \theta_n = \theta_{n+1} = \alpha$  or  $\theta_{n-1} = \theta_n = \theta_{n+1} = \beta$ . By the inductive hypothesis,  $R_3(B_n) \geq R_3(DL_n)$  with equality if and only if  $B_n$  is  $DL_n$ . So,  $R_3(B_{n+1}) \geq R_3(DL_{n+1})$  with equality if and only if  $B_{n+1}$  is  $DL_{n+1}$ .

(ii)

$$R_3(B_{n+1}) \leq \begin{cases} R_3(B_n) + (2 + \frac{19}{36}\sqrt{6}), & \text{if } \theta_{n-1} = \theta_n = \alpha, \theta_{n+1} = \beta \\ & \text{or } \theta_{n-1} = \theta_n = \beta, \theta_{n+1} = \alpha; \\ R_3(B_n) + (\frac{7}{3} + \frac{7}{18}\sqrt{6}), & \text{if } \theta_{n-1} = \alpha, \theta_n = \beta, \theta_{n+1} = \alpha \\ & \text{or } \theta_{n-1} = \beta, \theta_n = \alpha, \theta_{n+1} = \beta. \end{cases}$$

$$\leq \begin{cases} R_3(B_{n-1}) + (1 + \frac{11}{12}\sqrt{6}) + (2 + \frac{19}{36}\sqrt{6}), & \text{if } \theta_{n-1} = \theta_n = \alpha, \theta_{n+1} = \beta \\ & \text{or } \theta_{n-1} = \theta_n = \beta, \theta_{n+1} = \alpha; \\ R_3(B_{n-1}) + 2(\frac{7}{3} + \frac{7}{18}\sqrt{6}), & \text{if } \theta_{n-1} = \alpha, \theta_n = \beta, \theta_{n+1} = \alpha \\ & \text{or } \theta_{n-1} = \beta, \theta_n = \alpha, \theta_{n+1} = \beta. \end{cases}$$

Since  $(1 + \frac{11}{12}\sqrt{6}) + (2 + \frac{19}{36}\sqrt{6}) < 2(\frac{7}{3} + \frac{7}{18}\sqrt{6})$ , we have



$$R_3(B_{n+1}) \leq R_3(B_{n-1}) + 2\left(\frac{7}{3} + \frac{7}{18}\sqrt{6}\right)$$

with the equality if and only if  $(\theta_{n-2}, \theta_{n-1}, \theta_n, \theta_{n+1}) = (\beta, \alpha, \beta, \alpha)$  or  $(\alpha, \beta, \alpha, \beta)$ .

By the inductive hypothesis,  $R_3(B_{n-1}) \leq R_3(DZ_{n-1})$  with equality if and only if  $B_{n-1}$  is  $DZ_{n-1}$ . So,  $R_3(B_{n+1}) \leq R_3(DZ_{n+1})$  with equality if and only if  $B_{n+1}$  is  $DZ_{n+1}$ .

Therefore, the result is true for  $n \geq 1$  by the inductive method and the proof of Theorem 2 is completed.

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