Fourth Order Connectivity Index of Hexagonal Chains

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Summary: The higher order connectivity index is a graph invariant defined as ${}^{h}X(G)=\Sigma u_1 u_2 \ldots u_{h+1}(d_{u1} d_{u2} \ldots d_{uh+1})^{-1/2}$, where the summation is taken over all possible paths of length h, and d_{ui} denotes the degree of the vertex u_i of the graph G. In this paper, we stick to researching the fourth order connected index of hexagonal chains and give a calculation formula and we characterize the extremal graphs with the extremal fourth-order Randi¢ index.

Keywords: Connectivity Index; Hexagonal chain; Extreme situation; Randi¢ index.

Introduction

A topological index of molecules is a numeric quantity. It is structure invariant. The first reported use of a topological index in chemistry was studied by Wiener [1] in the study of paraffin boiling points. In chemical language, the Wiener index is equal to the sum of all shortest Carbon-Carbon bond paths in molecule. In graph theoretical language, it is equal to the number of all shortest distances in a graph. Since then, in order to model various molecular properties, many topological index have been designed [2].

In 1975 M. Randi& [3] introduced Randi& index (also called connectivity index) and defined as: $\chi(G)=\sum_{uv}(d_u d_v)^{-\frac{1}{2}}$, where d_u denotes the degree of the vertex u and $E(G)$ the set of edges of graph G. Connectivity index is one of the most important topological indices in Chemical Graph Theory. There is a good correlation between it and several physicochemical properties of alkanes: boiling points，surface areas，energy levels, etc. Connectivity index has been extensively investigated and applied in mathematics and chemistry. In [4], Rada, Araujo and Gutman first studied the Randi& index of benzanoid systems and phenylenes. After that, in [5] Kier and Hall considered the higher order connectivity indices of a general graph G as: ${}^{h}\chi(G)=\sum_{u_1u_2\ldots u_{h+1}}\frac{1}{\sqrt{d_{u_1}d_{u_2}\ldots d_{u_{h+1}}}}$, where the summation is taken over all possible paths of length h of graph G and approved that higher order connectivity indices have widely practice meaning in physics and chemistry. In [6], Rada gave an expression of the second-order Randi& index of benzenoid systems. Deng and Zhang researched the second order Randi& index of phenylenes in [7]. After that in [8], authors gave a calculation formula of the third-order Randi& index of phenylenes. In this paper, we study the fourth-order connected index of hexagonal chains and find their calculation formula and characterize the extremal graphs with the extremal fourth-order Randic index.

Hexagonal chain

Hexagonal chain is a hexagonal system in which each hexagon is only adjacent to at most two hexagons. We write a hexagonal chain with $n(n>2)$ hexagons H_n. It is easy to know any hexagonal

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chain H_{n+1} with n+1 *(n>1)* hexagons can be got by sticking a hexagon to hexagonal chain H_n, which implies any hexagonal chain can be got through the recursive structure. There are three ways to stick a hexagonal to a hexagonal chain H_n,:(1) if h_{n+1} in straight lines l, is called α type adhesion; (2) if h_{n+1} in straight lines l left, is called the β type adhesion; (3) if h_{n+1} on the right side of the linear l, called γ type adhesion. Here l refers to the straight linear connecting the center of h_{n-1} and of h_n. Any a hexagonal chain $H_n(n>2)$ can be got, through bonding some hexagons step by step into the H_2, where each step is a type θ, here $\theta=\{\alpha,\beta,\gamma\}$. Let H_{n+2} is a hexagonal chain with $n+2$ hexagons, which is got by binder a sequence of hexagons with type $\theta_1,\theta_2,\cdots,\theta_n$ to H_2. We call the $H(\alpha,\alpha,\cdots,\alpha)$ linear chain $L(n+2)$, and the $H(\beta,\gamma,\beta,\gamma,\cdots)$ or $H(\gamma,\beta,\gamma,\beta,\cdots)$ zig-zag chain $Z(n+2)$. Some examples of hexagonal chain saw as Fig. 1.

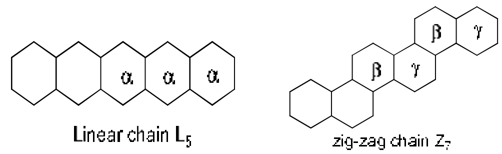

Fig. 1: Hexagonal Chain.

By H_n bond three hexagons getting H_{n+3} has the following twelve cases:

Case 1. $\theta_{n-1}=\alpha$ or $=\beta$ or and $\theta_n=\theta_{n+1}=\alpha$, see Fig. 2 (1), (15) and (19). Among these roads with long size 4, bcdew, cdewx, cdeEz, cCDEz, dewxy, deEzy, ewxyz, eEzyx, wedcC, weEDC, weEzy, wxyzE, xweED, xweEz, xyzED, yxweE, yzEDC, zEDCB is new. Except roads abcde, bcdeE, bcCDE, cdeED, cCDEe, dcCDE, deEDC, edcCB, edcCD, eEDCB, EedcC and EDCBA, other roads with long size 4 in H_{n+3} is the same as in H_{n+2}. Write $W_1(P)$ and $W_2(P)$ as the weight, $(d_{v_1}d_{v_2}d_{v_3}d_{v_4}d_{v_5})^{-\frac{1}{2}}$, of road $P=v_1v_2v_3v_4v_5$ in H_{n+2} and H_{n+3} respectively. We calculate the weight of these roads as following Table-1 and Tuble-2.

Table-1: The weight of new roads with long 4 in H_{n+3}.

bcdew	cdewx	cdeEz	cCDEz	dewxy	deEzy	ewxyz	eEzyx	wedcC
$\frac{1}{6\sqrt{2}}$	$\frac{1}{6\sqrt{2}}$	$\frac{1}{6\sqrt{3}}$	$\frac{1}{6\sqrt{3}}$	$\frac{1}{4\sqrt{3}}$	$\frac{1}{6\sqrt{2}}$	$\frac{1}{4\sqrt{3}}$	$\frac{1}{6\sqrt{2}}$	$\frac{1}{6\sqrt{3}}$
weEDC	**weEzy**	**wxyzE**	**xweED**	**xweEz**	**xyzED**	**yxweE**	**yzEDC**	**zEDCB**
$\frac{1}{6\sqrt{3}}$	$\frac{1}{6\sqrt{2}}$	$\frac{1}{4\sqrt{3}}$	$\frac{1}{6\sqrt{2}}$	$\frac{1}{6\sqrt{2}}$	$\frac{1}{4\sqrt{3}}$	$\frac{1}{6\sqrt{2}}$	$\frac{1}{6\sqrt{2}}$	$\frac{1}{6\sqrt{2}}$

The Fourth Order Connectivity Index of Hexagonal Chain

Let $H_{n+3} = H(\theta_1, \theta_2, \cdots, \theta_n, \theta_{n+1})$ be one of following hexagonal chains:

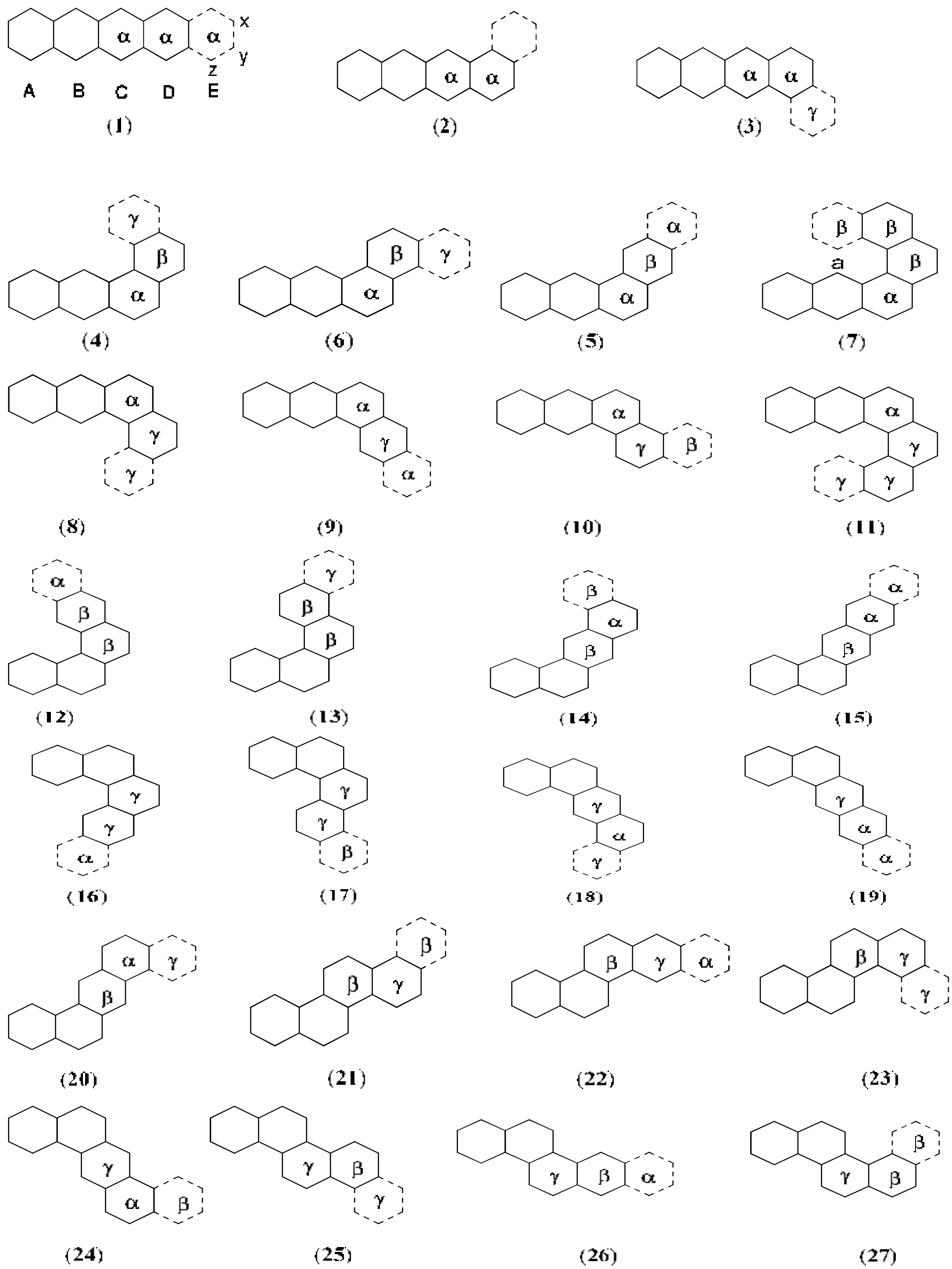

Fig. 2: Hexagonal Chain H_{n+3}.

Table-2: The weight of roads with long 4 in H_{n+2} and H_{n+3}.

	abcde	bcdeE	bcCDE	cdeED	cCDEe	dcCDE
W₁	$\frac{1}{6\sqrt{2}}$	$\frac{1}{4\sqrt{3}}$	$\frac{1}{6\sqrt{2}}$	$\frac{1}{4\sqrt{3}}$	$\frac{1}{6\sqrt{2}}$	$\frac{1}{6\sqrt{2}}$
W₂	$\frac{1}{6\sqrt{3}}$	$\frac{1}{6\sqrt{3}}$	$\frac{1}{6\sqrt{3}}$	$\frac{1}{6\sqrt{3}}$	$\frac{1}{9\sqrt{2}}$	$\frac{1}{6\sqrt{3}}$
	deEDC	**edcCB**	**edcCD**	**eEDCB**	**EedcC**	**EDCBA**
W₁	$\frac{1}{4\sqrt{3}}$	$\frac{1}{6\sqrt{2}}$	$\frac{1}{6\sqrt{2}}$	$\frac{1}{4\sqrt{3}}$	$\frac{1}{6\sqrt{2}}$	$\frac{1}{6\sqrt{2}}$
W₂	$\frac{1}{6\sqrt{3}}$	$\frac{1}{6\sqrt{3}}$	$\frac{1}{6\sqrt{3}}$	$\frac{1}{6\sqrt{3}}$	$\frac{1}{9\sqrt{2}}$	$\frac{1}{6\sqrt{3}}$

By the definition of the fourth order connectivity index and the values in Table-1 and Tuble-2, we have:

$$^4\chi(\mathrm{H}_{n+3}) = {}^4\chi(\mathrm{H}_{n+2}) + \frac{5}{18}\sqrt{2} + \frac{7}{9}\sqrt{3}$$

Case 2. $\theta_{n-1}=\theta_n=\alpha$, $\theta_{n+1}=\beta$ or $\theta_{n+1}=\gamma$, see Fig. 2 (2) and (3). Similar to case 1, we have:

$$^4\chi(\mathrm{H}_{n+3}) = {}^4\chi(\mathrm{H}_{n+2}) + \frac{23}{36}\sqrt{2} + \frac{7}{9}\sqrt{3}$$

Case 3. $\theta_{n-1}=\alpha$, $\theta_n=\theta_{n+1}=\beta$ or $\theta_n=\theta_{n+1}=\gamma$, see figure 2 (4), (8). Similar to case 1, we have:

$$^4\chi(\mathrm{H}_{n+3}) = {}^4\chi(\mathrm{H}_{n+2}) + \frac{13}{18}\sqrt{2} + \frac{55}{108}\sqrt{3}$$

Case 4. $\theta_{n-1}=\alpha$, $\theta_n=\beta$, $\theta_{n+1}=\alpha$ or $\theta_{n-1}=\alpha$, $\theta_n=\gamma$, $\theta_{n+1}=\alpha$ or $\theta_{n-1}=\beta$, $\theta_n=\gamma$, $\theta_{n+1}=\alpha$ or $\theta_{n-1}=\gamma$, $\theta_n=\beta$, $\theta_{n+1}=\alpha$, see Fig. 2 (5), (9), (22) and (26). Similar to case 1, we have:

$$^4\chi(\mathrm{H}_{n+3}) = {}^4\chi(\mathrm{H}_{n+2}) + \frac{19}{36}\sqrt{2} + \frac{17}{27}\sqrt{3}$$

Case 5. $\theta_{n-1}=\alpha$, $\theta_n=\beta$, $\theta_{n+1}=\gamma$ 或 $\theta_{n-1}=\alpha$, $\theta_n=\gamma$, $\theta_{n+1}=\beta$, , see Fig. 2 (6) and (10). Similar to case 1,

we have: $^4\chi(\mathrm{H}_{n+3}) = {}^4\chi(\mathrm{H}_{n+2}) + \frac{5}{9}\sqrt{2} + \frac{17}{27}\sqrt{3}$

Case 6. $\theta_{n-1}=\theta_n=\theta_{n+1}=\beta$ or $\theta_{n-1}=\theta_n=\theta_{n+1}=\gamma$, , see Fig. 2 (7) and (11). Similar to case 1, we have:

$$^4\chi(\mathrm{H}_{n+3}) = {}^4\chi(\mathrm{H}_{n+2}) + \begin{cases} \frac{13}{18}\sqrt{2} + \frac{17}{36}\sqrt{3} & \text{if degree}(a) = 2, \\ \frac{11}{18}\sqrt{2} + \frac{61}{108}\sqrt{3} & \text{if degree}(a) = 3 \end{cases}$$

Case 7. $\theta_{n-1}=\theta_n=\beta$, $\theta_{n+1}=\alpha$ or $\theta_{n-1}=\theta_n=\gamma$, $\theta_{n+1}=\alpha$, see Fig. 2 (12) and (16). Similar to case 1, we have:

$$^4\chi(\mathrm{H}_{n+3}) = {}^4\chi(\mathrm{H}_{n+2}) + \frac{19}{36}\sqrt{2} + \frac{22}{27}\sqrt{3}$$

Case 8. $\theta_{n-1}=\theta_n=\beta$, $\theta_{n+1}=\gamma$ or $\theta_{n-1}=\theta_n=\gamma$, $\theta_{n+1}=\beta$, see Fig. 2 (13) and (17). Similar to case 1, we have:

$$^4\chi(\mathrm{H}_{n+3}) = {}^4\chi(\mathrm{H}_{n+2}) + \frac{4}{9}\sqrt{2} + \frac{13}{18}\sqrt{3}$$

Case 9. $\theta_{n-1}=\beta$, $\theta_n=\alpha$, $\theta_{n+1}=\beta$ or $\theta_{n-1}=\gamma$, $\theta_n=\alpha$, $\theta_{n+1}=\gamma$, see Fig. 2 (14) and (18). Similar as case 1, we have:

$$^4\chi(\mathrm{H}_{n+3}) = {}^4\chi(\mathrm{H}_{n+2}) + \frac{29}{36}\sqrt{2} + \frac{4}{9}\sqrt{3}$$

Case 10. $\theta_{n-1}=\beta$, $\theta_n=\alpha$, $\theta_{n+1}=\gamma$ or $\theta_{n-1}=\gamma$, $\theta_n=\alpha$, $\theta_{n+1}=\beta$, see Fig. 2 (20) and (24). Similar as case 1, we have:

$$^4\chi(\mathrm{H}_{n+3}) = {}^4\chi(\mathrm{H}_{n+2}) + \frac{7}{12}\sqrt{2} + \frac{11}{18}\sqrt{3}$$

Case 11. $\theta_{n-1}=\beta$, $\theta_n=\gamma$, $\theta_{n+1}=\beta$ or $\theta_{n-1}=\gamma$, $\theta_n=\beta$, $\theta_{n+1}=\gamma$, see Fig. 2 (21) and (25). Similar as case 1, we have:

$$^4\chi(\mathrm{H}_{n+3}) = {}^4\chi(\mathrm{H}_{n+2})+\frac{5}{9}\sqrt{2}+\frac{2}{3}\sqrt{3}$$

Case 12. $\theta_{n-1}=\beta$, $\theta_n=\gamma$, $\theta_{n+1}=\gamma$ or $\theta_{n-1}=\gamma$, $\theta_n=\beta$, $\theta_{n+1}=\beta$, see Fig. 2 (23) and (27). Similar as case 1, we have:

$$^4\chi(\mathrm{H}_{n+3}) = {}^4\chi(\mathrm{H}_{n+2})+\frac{4}{9}\sqrt{2}+\frac{77}{108}\sqrt{3}$$

Sum up the above 12 cases, we can get the following theorem:

Theorem 1 Let $H_{n+2}=H(\theta_1, \theta_2, \ldots \theta_n)$ and $H_{n+3}=H(\theta_1, \theta_2, \ldots \theta_n, \theta_{n+1})$, then

$$\begin{cases}
\frac{5}{18}\sqrt{2}+\frac{7}{9}\sqrt{3}, & \text{if } (\theta_{n-1},\theta_n,\theta_{n+1})=(\alpha,\alpha,\alpha),(\beta,\alpha,\alpha) \text{ or } (\gamma,\alpha,\alpha); \\
\frac{23}{36}\sqrt{2}+\frac{7}{9}\sqrt{3}, & \text{if } (\theta_{n-1},\theta_n,\theta_{n+1})=(\alpha,\alpha,\beta) \text{ or } (\alpha,\alpha,\gamma) \\
\frac{13}{18}\sqrt{2}+\frac{55}{108}\sqrt{3}, & \text{if } (\theta_{n-1},\theta_n,\theta_{n+1})=(\alpha,\beta,\beta) \text{ or } (\alpha,\gamma,\gamma); \\
\frac{19}{36}\sqrt{2}+\frac{17}{27}\sqrt{3}, & \text{if } (\theta_{n-1},\theta_n,\theta_{n+1})=(\alpha,\beta,\alpha),(\alpha,\gamma,\alpha),(\beta,\gamma,\alpha) \text{ or } (\gamma,\beta,\alpha); \\
\frac{5}{9}\sqrt{2}+\frac{17}{27}\sqrt{3}, & \text{if } (\theta_{n-1},\theta_n,\theta_{n+1})=(\alpha,\beta,\gamma) \text{ or } (\alpha,\gamma,\beta); \\
\frac{13}{18}\sqrt{2}+\frac{17}{36}\sqrt{3} \text{ or } \frac{11}{18}\sqrt{2}+\frac{61}{108}\sqrt{3}, & \text{if } (\theta_{n-1},\theta_n,\theta_{n+1})=(\beta,\beta,\beta) \text{ or } (\gamma,\gamma,\gamma); \\
\frac{19}{36}\sqrt{2}+\frac{22}{27}\sqrt{3}, & \text{if } (\theta_{n-1},\theta_n,\theta_{n+1})=(\beta,\beta,\alpha) \text{ or } (\gamma,\gamma,\alpha); \\
\frac{4}{9}\sqrt{2}+\frac{13}{18}\sqrt{3}, & \text{if } (\theta_{n-1},\theta_n,\theta_{n+1})=(\beta,\beta,\gamma) \text{ or } (\gamma,\gamma,\beta); \\
\frac{7}{12}\sqrt{2}+\frac{11}{18}\sqrt{3}, & \text{if } (\theta_{n-1},\theta_n,\theta_{n+1})=(\beta,\alpha,\gamma) \text{ or } (\gamma,\alpha,\beta); \\
\frac{29}{36}\sqrt{2}+\frac{4}{9}\sqrt{3}, & \text{if } (\theta_{n-1},\theta_n,\theta_{n+1})=(\beta,\alpha,\beta) \text{ or } (\gamma,\alpha,\gamma); \\
\frac{5}{9}\sqrt{2}+\frac{2}{3}\sqrt{3}, & \text{if } (\theta_{n-1},\theta_n,\theta_{n+1})=(\beta,\gamma,\beta) \text{ or } (\gamma,\beta,\gamma); \\
\frac{4}{9}\sqrt{2}+\frac{77}{108}\sqrt{3}, & \text{if } (\theta_{n-1},\theta_n,\theta_{n+1})=(\beta,\gamma,\gamma) \text{ or } (\gamma,\beta,\beta);
\end{cases}$$

The Extremal Graphs of Hexagonal Chain

By the recursive formula of the fourth order connectivity index of hexagonal chain, we deduce the extreme values of fourth order connectivity index, and depict their extremal graphs.

Theorem 2 Let $H_{n+3}=H(\theta_1, \theta_2, \ldots \theta_n, \theta_{n+1})$ be a hexagonal chain with $n+3\,(n\geq 2)$ hexagons, then the following results hold:

(1) $^4\chi(H_{n+3})\geq\frac{5n+29}{18}\sqrt{2}+\frac{7n+12}{9}\sqrt{3}$. If and only if $(\theta_1,\theta_2,\cdots,\theta_n)=(\alpha,\alpha,\cdots,\alpha)$, the equality holds. That is, H_{n+3} is a linear chain.(2)

$^4\chi(H_{n+3})\leq\frac{10n+41}{18}\sqrt{2}+\frac{18n+35}{108}\sqrt{3}$, If and only if $(\theta_1,\theta_2,\cdots\theta_n)=(\beta,\gamma,\beta,\gamma,\ldots)$ or $(\gamma,\beta,\gamma,\beta\cdots)$, the equality holds. That is, H_{n+3} is a Zig-Zag chain Z_{n+3}.

Proof: By theorem 1 and

$^{4}\chi(H(\alpha,\alpha,\alpha))=\frac{13}{6}\sqrt{2}+\frac{26}{9}\sqrt{3}$, $^{4}\chi(\mathrm{H}(\beta,\gamma,\beta))={}^{4}\chi(\mathrm{H}(\gamma,\beta,\gamma))=\frac{16}{6}\sqrt{2}+\frac{71}{27}\sqrt{3}$,

we can get

$$^{4}\chi(\mathrm{L}_{n+3})=\frac{5(n\text{-}2)+39}{18}\sqrt{2}+\frac{7(n\text{-}2)+26}{9}\sqrt{3}=\frac{5n+29}{18}\sqrt{2}+\frac{7n+12}{9}\sqrt{3},$$

$$^{4}\chi(\mathrm{Z}_{n+3})=\frac{10(n-2)+51}{18}\sqrt{2}+\frac{18(n-2)+71}{27}\sqrt{3}=\frac{10n+41}{18}\sqrt{2}+\frac{18n+35}{108}\sqrt{3}$$

Next, we prove our theorem by inductive method. By a series of direct calculation, we can get:

$$^{4}\chi(\mathrm{H}_2)=\sqrt{2}+\frac{5}{6}\sqrt{3} \qquad ^{4}\chi(\mathrm{H}_3)=\begin{cases} ^{4}\chi(\mathrm{H}(\alpha))=\frac{29}{18}\sqrt{2}+\frac{4}{3}\sqrt{3}, \\ ^{4}\chi(\mathrm{H}(\beta))={}^{4}\chi(\mathrm{H}(\gamma))=\frac{31}{18}\sqrt{2}+\frac{4}{3}\sqrt{3}. \end{cases}$$

$$^{4}\chi(\mathrm{H}_4)=\begin{cases} ^{4}\chi(\mathrm{H}(\alpha,\alpha))=\frac{17}{9}\sqrt{2}+\frac{19}{9}\sqrt{3} \\ ^{4}\chi(\mathrm{H}(\alpha,\beta))={}^{4}\chi(\mathrm{H}(\alpha,\gamma))=\frac{9}{4}\sqrt{2}+\frac{17}{9}\sqrt{3} \\ ^{4}\chi(\mathrm{H}(\beta,\alpha))={}^{4}\chi(\mathrm{H}(\gamma,\alpha))=\frac{9}{4}\sqrt{2}+\frac{17}{9}\sqrt{3} \\ ^{4}\chi(\mathrm{H}(\beta,\beta))={}^{4}\chi(\mathrm{H}(\gamma,\gamma))=\frac{41}{18}\sqrt{2}+\frac{211}{108}\sqrt{3} \\ ^{4}\chi(\mathrm{H}(\beta,\gamma))={}^{4}\chi(\mathrm{H}(\gamma,\beta))=\frac{41}{18}\sqrt{2}+\frac{53}{27}\sqrt{3} \end{cases}$$

From the above we can see, the theorem holds for $n=0,1,2$.

$$\frac{5}{18}\sqrt{2}+\frac{7}{9}\sqrt{3}<\frac{19}{36}\sqrt{2}+\frac{17}{27}\sqrt{3}<\frac{19}{36}\sqrt{2}+\frac{22}{27}\sqrt{3}<\frac{3}{18}\sqrt{2}+\frac{17}{36}\sqrt{3}<\frac{11}{18}\sqrt{2}+\frac{61}{108}\sqrt{3}<\frac{5}{9}\sqrt{2}+\frac{17}{27}\sqrt{3}$$

$$<\frac{4}{9}\sqrt{2}+\frac{11}{18}\sqrt{3}<\frac{7}{12}\sqrt{2}+\frac{11}{18}\sqrt{3}<\frac{13}{18}\sqrt{2}+\frac{55}{108}\sqrt{3}<\frac{23}{36}\sqrt{2}+\frac{7}{9}\sqrt{3}<\frac{29}{36}\sqrt{2}+\frac{4}{9}\sqrt{3}<\frac{5}{9}\sqrt{2}+\frac{2}{3}\sqrt{3}$$

(1) Now we assume the case (1) of the theorem holds for n, that is $^{4}\chi(H_{n+2})\geq {}^{4}\chi(L_{n+2})$

Let $\mathrm{H}_{n+3}=\mathrm{H}(\theta_1, \theta_2, \ldots \theta_n, \theta_{n+1})$ be a hexagonal chain with $n+3$ hexagons. By Theorem 1, we can get $^{4}\chi(\mathrm{H}_{n+3})\geq {}^{4}\chi(\mathrm{H}_{n+2})+\frac{5}{18}\sqrt{2}+\frac{7}{9}\sqrt{3}$. The equation hold iff $(\theta_{n-1},\theta_n,\theta_{n+1})=(\alpha,\alpha,\alpha)$. By the inductive hypothesis, $^{4}\chi(H_{n+3})\geq {}^{4}\chi(L_{n+3})$. The equation hold if and only if H_{n+3} is L_{n+3} . Therefore the theorem (1) holds.

(2) Now we assume the case (2) of the

theorem holds for *n*, that is $^4\chi(H_{n+2}) \le {^4\chi}(Z_{n+2})$

By Theorem 1, $^4\chi(\mathrm{H}_{n+3}) \le {^4\chi}(\mathrm{H}_{n+2}) + \frac{5}{9}\sqrt{2} + \frac{2}{3}\sqrt{3}$.

Therefore, by the inductive hypothesis, $^4\chi(\mathrm{H}_{n+3}) \le {^4\chi}(\mathrm{Z}_{n+2}) + \frac{5}{9}\sqrt{2} + \frac{2}{3}\sqrt{3}$ if and only if H_{n+3} is Z_{n+3} , the equation holds. Therefore, the theorem (2) holds.

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