Catacondensed Benzenoids and Phenylenes with the Extremal Third–order Randić Index

Hanyuan Deng
College of Mathematics and Computer Science,
Hunan Normal University, Changsha, Hunan 410081, P. R. China
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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 $G$. Using the recursive formulas for computing the third-order Randić index of catacondensed benzenoids and phenylenes, we characterize the extremal catacondensed benzenoids and phenylenes with respect to the third-order Randić index, respectively.

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([2-18]).

In 1976, the higher-order connectivity index of a graph $G$ was introduced in [14,15]:
\[ R_k(G) = \sum_{u_1u_2\cdots u_{k+1}} \frac{1}{\sqrt{d(u_1)d(u_2)\cdots d(u_{k+1})}} \]
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 $u_{k+1}u_{h+1}\cdots u_1$). It has been applied successfully

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to an impressive variety of physical, chemical and biological properties which have appeared in many scientific publications and in two books ([14] and [16]). Results related to the mathematical properties of these indices have been reported in the literature([2] and [3]). Specifically, Rada [11] 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, the second-order Randić index and the third-order Randić index of phenylenes have been discussed in [4, 12-13]. Recently, the upper and lower bounds of the third-order Randić indices among all hexagonal chains and double hexagonal chains have been determined and the extremal graphs also have been characterized in [17, 18]. In this paper, we first extend the class of hexagonal chains to the class of catacondensed benzenoids, and characterize the catacondensed benzenoids with the extremal third-order Randić index, and then determine the phenylenes with the extremal third-order Randić index by using a recursive formula different from [13].

2 The recursive formulas for computing the third-order Randić indices of catacondensed benzenoids

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. 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 is said to be catacondensed (or tree-type) if it does not possess internal vertices, otherwise H is said to be pericondensed. The catacondensed hexagonal systems are the graph representations of an important subclass of benzenoid molecules, i.e., catacondensed benzenoids.

Let \( C_n \) denote the set of catacondensed hexagonal systems containing \( n \) hexagons. \( T \in C_n \), and \( H \) is a hexagon of \( T \). Obviously, \( H \) has at most three adjacent hexagons in \( T \). If \( H \) has exactly three adjacent hexagons in \( T \), then \( H \) is called a full-hexagon of \( T \); if \( H \) has two adjacent hexagons in \( T \), and, moreover, if its two vertices with degree two are adjacent, then \( H \) is called a turn-hexagon of \( T \); and if \( H \) has at most one adjacent hexagon in \( T \), then \( H \) is called an end-hexagon of \( T \). It is easy to see that the number of the end-hexagons of a catacondensed hexagonal system with \( n \geq 2 \) hexagons is two more
than the number of its full-hexagons.

A hexagonal chain is a catacondensed hexagonal system without full-hexagons. We denote by $L_n$ and $Z_n$ the linear hexagonal chain and the zigzag hexagonal chain with $n$ hexagons, respectively, see Figure 1.

Let $T$ be a hexagonal chain with $n$ hexagons $H_1, H_2, \ldots, H_n$, where $H_i$ and $H_{i+1}$ have a common edge for each $i = 1, 2, \ldots, n - 1$. We denote this hexagonal chain by $T = H_1H_2\cdots H_n$. A hexagonal chain with at least two hexagons has two end-hexagons. Let $T \in C_n$, if $T$ is a hexagonal chain, then $T$ is the unique branch of itself; otherwise, let $B = H_1H_2\cdots H_k$, $k \geq 2$, be a hexagonal chain of $T$, where the end-hexagon $H_1$ of $B$ is also an end-hexagon of $T$, the other end-hexagon $H_k$ of $B$ is a full-hexagon of $T$, and $H_i$ is not a full-hexagon of $T$ for $2 \leq i \leq k - 1$, then $B$ is called a branch of $T$.

For example, $B = H_1H_2H_3H_4H_5$ is a branch of the catacondensed hexagonal system illustrated in Figure 1.

If $T$ is not a hexagonal chain, then the number of branches of $T$ is equal to the number of end-hexagons of $T$.

In the following, we discuss the recursive formula for computing the third-order Randić index of a catacondensed hexagonal system.

Let $T_n \in C_n$ be a catacondensed hexagonal system with $n$ hexagons. $B = H_1H_2\cdots H_k$ ($k \geq 2$) is a branch of $T_n$, where $H_1 = uvabcd$ is an end-hexagon of $T_n$, $uv$ is the common edge of $H_1$ and $H_2$. Then $T_{n-1} = T_n - \{a, b, c, d\}$ is a catacondensed hexagonal system with $n - 1$ hexagons.
If \( l = v_1v_2v_3v_4 \) is a path of \( T_n \), then \( W_{T_n}(l) = \frac{1}{\sqrt{d(v_1)d(v_2)d(v_3)d(v_4)}} \) is the weight of the path \( l \) in \( T_n \). And \( Q = W_{T_n}(l) - W_{T_{n-1}}(l) \) for a common path \( l \) of \( T_n \) and \( T_{n-1} \).

**Case I.** \( H_2 \) is neither a turn-hexagon nor a full-hexagon, see Figure 2(1).

From \( T_{n-1} \) to \( T_n \), the new added paths of length 3 must contain one of \( a, b, c, d \), they are given in Table 1 and the sum of their weights is \( \frac{2}{\sqrt{6}} + \frac{17}{12} \).

**Table 1.** The new added paths of length 3 in \( T_n \) and their weights.

<table>
<thead>
<tr>
<th>path</th>
<th>weight</th>
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</thead>
<tbody>
<tr>
<td>( avv_1v_2 )</td>
<td>( \frac{5}{6} )</td>
</tr>
<tr>
<td>( avv_1u_1 )</td>
<td>( \frac{1}{6} )</td>
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<tr>
<td>( duu_1v_2 )</td>
<td>( \frac{5}{6} )</td>
</tr>
<tr>
<td>( duv_1v_2 )</td>
<td>( \frac{1}{6} )</td>
</tr>
<tr>
<td>( bavv_1 )</td>
<td>( \frac{1}{2\sqrt{6}} )</td>
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<tr>
<td>( cdvv_1 )</td>
<td>( \frac{1}{2\sqrt{6}} )</td>
</tr>
<tr>
<td>( abcd )</td>
<td>( \frac{1}{4} )</td>
</tr>
<tr>
<td>( avud )</td>
<td>( \frac{1}{6} )</td>
</tr>
<tr>
<td>( bedu )</td>
<td>( \frac{1}{2\sqrt{6}} )</td>
</tr>
<tr>
<td>( bavu )</td>
<td>( \frac{1}{6} )</td>
</tr>
<tr>
<td>( cdv )</td>
<td>( \frac{1}{6} )</td>
</tr>
<tr>
<td>( cbav )</td>
<td>( \frac{1}{2\sqrt{6}} )</td>
</tr>
</tbody>
</table>

Note that the paths of length 3 in \( T_{n-1} \) whose weights are changed must contain \( u \) or \( v \). They are given in Table 2, and

\[
\sum_{i=1}^{7} Q_i = \frac{1}{3\sqrt{6}} - \frac{5}{12} + \left( \frac{1}{3\sqrt{2}} - \frac{1}{2\sqrt{3}} \right) \left( \frac{1}{\sqrt{d(u_3)}} + \frac{1}{\sqrt{d(v_3)}} \right)
\]

**Table 2.** The paths of length 3 in \( T_{n-1} \) whose weights are changed.

<table>
<thead>
<tr>
<th>path</th>
<th>weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>( uu_1u_2u_3 )</td>
<td>( \frac{1}{\sqrt{d(u_3)}} \left( \frac{1}{3\sqrt{2}} - \frac{1}{2\sqrt{3}} \right) )</td>
</tr>
<tr>
<td>( uu_1u_2v_2 )</td>
<td>( \frac{1}{3\sqrt{6}} - \frac{1}{6} )</td>
</tr>
<tr>
<td>( uvv_1v_2 )</td>
<td>( \frac{1}{3\sqrt{6}} - \frac{1}{2\sqrt{6}} )</td>
</tr>
<tr>
<td>( vv_1v_2v_3 )</td>
<td>( \frac{1}{6} - \frac{1}{6} )</td>
</tr>
</tbody>
</table>

So, \( R_3(T_n) - R_3(T_{n-1}) = \left( \frac{2}{\sqrt{6}} + \frac{17}{12} \right) + \left( \frac{1}{3\sqrt{6}} - \frac{5}{12} + \left( \frac{1}{3\sqrt{2}} - \frac{1}{2\sqrt{3}} \right) \left( \frac{1}{\sqrt{d(u_3)}} + \frac{1}{\sqrt{d(v_3)}} \right) \right) \).

Since \( 2 \leq d(u_3) \leq 3, 2 \leq d(v_3) \leq 3, \)

\[
\frac{2}{9} \sqrt{6} + \frac{4}{3} \leq R_3(T_n) - R_3(T_{n-1}) \leq \frac{1}{2} \sqrt{6} + \frac{2}{3}
\]

(1)

**Case II.** \( H_2 \) is a turn-hexagon.

**Subcase I.** \( H_3 \) is neither a turn-hexagon nor a full-hexagon, see Figure 2(2). Then, from \( T_{n-1} \) to \( T_n \), the new added paths of length 3 are given in Table 3. The sum of their weights is \( \frac{4}{9} \sqrt{6} + \frac{5}{4} \).

**Table 3.**

<table>
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<tr>
<th>path</th>
<th>weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>( avv_1v_2 )</td>
<td>( \frac{5}{6} )</td>
</tr>
<tr>
<td>( avv_1u_4 )</td>
<td>( \frac{3}{\sqrt{6}} )</td>
</tr>
<tr>
<td>( avv_1u_1 )</td>
<td>( \frac{1}{6} )</td>
</tr>
<tr>
<td>( duu_1u_2 )</td>
<td>( \frac{5}{6} )</td>
</tr>
<tr>
<td>( duv_1v_2 )</td>
<td>( \frac{1}{2\sqrt{6}} )</td>
</tr>
<tr>
<td>( bavv_1 )</td>
<td>( \frac{1}{2\sqrt{6}} )</td>
</tr>
<tr>
<td>( cdvv_1 )</td>
<td>( \frac{1}{2\sqrt{6}} )</td>
</tr>
<tr>
<td>( abcd )</td>
<td>( \frac{1}{4} )</td>
</tr>
<tr>
<td>( avud )</td>
<td>( \frac{1}{6} )</td>
</tr>
<tr>
<td>( bedu )</td>
<td>( \frac{1}{2\sqrt{6}} )</td>
</tr>
<tr>
<td>( bavu )</td>
<td>( \frac{1}{6} )</td>
</tr>
<tr>
<td>( cdv )</td>
<td>( \frac{1}{6} )</td>
</tr>
<tr>
<td>( cbav )</td>
<td>( \frac{1}{2\sqrt{6}} )</td>
</tr>
</tbody>
</table>
There are eight paths of length 3 in $T_{n-1}$ whose weights are changed. They are given in Table 4, and

$$\sum_{i=1}^{8} Q_i \frac{1}{6\sqrt{6}} - \frac{17}{36} = \frac{1}{36\sqrt{6}} - \frac{17}{36}.$$  

**Table 4.**

<table>
<thead>
<tr>
<th>$P_i$</th>
<th>$uvu_1u_2u_3$</th>
<th>$uvu_1u_3$</th>
<th>$uvu_1v_2$</th>
<th>$uvu_1v_2v_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_i$</td>
<td>$\frac{1}{6} - \frac{1}{2\sqrt{6}}$</td>
<td>$\frac{1}{6} - \frac{1}{6}$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{2\sqrt{6}}$</td>
<td>$\frac{1}{6} - \frac{1}{6}$</td>
</tr>
<tr>
<td>$P_i$</td>
<td>$vvu_1u_4u_1$</td>
<td>$vvu_1u_3u_2$</td>
<td>$vvu_1v_2u_1$</td>
<td>$u_1uvu_1$</td>
</tr>
<tr>
<td>$Q_i$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{6}$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{6}$</td>
<td>$\frac{1}{6} - \frac{1}{4}$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{2\sqrt{6}}$</td>
</tr>
</tbody>
</table>

And,

$$R_3(T_n) - R_3(T_{n-1}) = \left( \frac{4}{9} \sqrt{6} + \frac{5}{4} \right) + \left( \frac{1}{36} \sqrt{6} - \frac{17}{36} \right) = \frac{17}{36} \sqrt{6} + \frac{7}{9}$$  \hspace{1cm} (2)

**Remark.** If $R_3(T_n) - R_3(T_{n-1}) = \frac{17}{36} \sqrt{6} + \frac{7}{9}$, then, since $H_3$ is neither a turn-hexagon nor a full-hexagon in $T_n$ and by the equation (1), it must have $R_3(T_{n-1}) - R_3(T_{n-2}) = \frac{2}{9} \sqrt{6} + \frac{4}{3}$, where $T_{n-2} = T_{n-1} - \{v, u, u_1, u_2\} = T_n - \{a, b, c, d, v, u, u_1, u_2\}$.

**Subcase II.** $H_3$ is a turn-hexagon.

(i) If $d(u_4) = 3$, see Figure 2(3), then $d(v_2) = d(v_3) = 2$ since $H_3$ is not a full-hexagon. From $T_{n-1}$ to $T_n$, the new added paths of length 3 and their weights are the same as in Table 3. Also, there are eight paths of length 3 in $T_{n-1}$ whose weights are changed. They are given in Table 5, and

$$\sum_{i=1}^{8} Q_i = -\frac{4}{3\sqrt{6}} + \frac{5}{36} = -\frac{2}{9} \sqrt{6} + \frac{5}{36}$$  

**Table 5.**

<table>
<thead>
<tr>
<th>$P_i$</th>
<th>$uvu_1u_2u_3$</th>
<th>$uvu_1u_3$</th>
<th>$uvu_1v_2$</th>
<th>$uvu_1v_2v_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_i$</td>
<td>$\frac{1}{6} - \frac{1}{2\sqrt{6}}$</td>
<td>$\frac{1}{6} - \frac{1}{6}$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{2\sqrt{6}}$</td>
<td>$\frac{1}{6} - \frac{1}{6}$</td>
</tr>
<tr>
<td>$P_i$</td>
<td>$vvu_1u_4u_1$</td>
<td>$vvu_1u_3u_2$</td>
<td>$vvu_1v_2u_1$</td>
<td>$u_1uvu_1$</td>
</tr>
<tr>
<td>$Q_i$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{6}$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{6}$</td>
<td>$\frac{1}{6} - \frac{1}{4}$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{2\sqrt{6}}$</td>
</tr>
</tbody>
</table>

So,

$$R_3(T_n) - R_3(T_{n-1}) = \left( \frac{4}{9} \sqrt{6} + \frac{5}{4} \right) + \left( -\frac{2}{9} \sqrt{6} + \frac{5}{36} \right) = \frac{2}{9} \sqrt{6} + \frac{25}{18}$$  \hspace{1cm} (3)

(ii) If $d(u_4) = 2$, see Figure 2(4), then $d(v_2) = d(v_3) = 3$ since $H_3$ is a turn-hexagon. From $T_{n-1}$ to $T_n$, the new added paths of length 3 are given in Table 6. The sum of their weights is $\frac{1}{2} \sqrt{6} + \frac{13}{12}$. 
Also, there are nine paths of length 3 in $T_{n-1}$ whose weights are changed. They are given in Table 7, and

$$\sum_{i=1}^{9} Q_i = -\frac{1}{3\sqrt{6}} - \frac{1}{4} + \frac{1}{d(v_4)} \left( \frac{1}{3\sqrt{3}} - \frac{1}{3\sqrt{2}} \right)$$

Table 7.

<table>
<thead>
<tr>
<th>$P_i$</th>
<th>$uu_1u_2u_3$</th>
<th>$u_1v_1u_3$</th>
<th>$u_1v_1v_2$</th>
<th>$v_1v_2v_4$</th>
<th>$v_1v_2v_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_i$</td>
<td>$\frac{1}{5} - \frac{1}{2\sqrt{6}}$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
<td>$\frac{1}{d(v_4)} \left( \frac{1}{3\sqrt{3}} - \frac{1}{3\sqrt{2}} \right)$</td>
<td>$\frac{1}{9} - \frac{1}{3\sqrt{6}}$</td>
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</tbody>
</table>

So, $R_3(T_n) - R_3(T_{n-1}) = \left( \frac{1}{2} \sqrt{6} + \frac{13}{12} \right) + \left( -\frac{1}{3\sqrt{6}} - \frac{1}{4} + \frac{1}{d(v_4)} \left( \frac{1}{3\sqrt{3}} - \frac{1}{3\sqrt{2}} \right) \right)$.

Since $2 \leq d(v_4) \leq 3$, we have

$$\frac{1}{2} \sqrt{6} + \frac{2}{3} \leq R_3(T_n) - R_3(T_{n-1}) \leq \frac{7}{18} \sqrt{6} + \frac{17}{18} \quad (4)$$

**Subcase III.** $H_3$ is a full-hexagon, see Figure 2(5). Then $k = 3$.

From $T_{n-1}$ to $T_n$, the new added paths of length 3 and their weights are the same as in Table 6. Also, there are nine paths of length 3 in $T_{n-1}$ whose weights are changed. They are given in Table 8, and

$$\sum_{i=1}^{9} Q_i = -\frac{1}{\sqrt{6}} + \frac{1}{36} + \frac{1}{d(v_4)} \left( \frac{1}{3\sqrt{3}} - \frac{1}{3\sqrt{2}} \right)$$

Table 8.

<table>
<thead>
<tr>
<th>$P_i$</th>
<th>$uu_1u_2u_3$</th>
<th>$u_1v_1u_3$</th>
<th>$u_1v_1v_2$</th>
<th>$v_1v_2v_4$</th>
<th>$v_1v_2v_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_i$</td>
<td>$\frac{1}{5} - \frac{1}{2\sqrt{6}}$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
<td>$\frac{1}{d(v_4)} \left( \frac{1}{3\sqrt{3}} - \frac{1}{3\sqrt{2}} \right)$</td>
<td>$\frac{1}{9} - \frac{1}{3\sqrt{6}}$</td>
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</table>

So, $R_3(T_n) - R_3(T_{n-1}) = \left( \frac{1}{2} \sqrt{6} + \frac{13}{12} \right) + \left( -\frac{1}{\sqrt{6}} + \frac{1}{36} + \frac{1}{d(v_4)} \left( \frac{1}{3\sqrt{3}} - \frac{1}{3\sqrt{2}} \right) \right)$.

Since $2 \leq v_4 \leq 3$, we have

$$\frac{7}{18} \sqrt{6} + \frac{17}{18} \leq R_3(T_n) - R_3(T_{n-1}) \leq \frac{5}{18} \sqrt{6} + \frac{11}{9} \quad (5)$$
Case III. $H_2$ is a full-hexagon. Then $k = 2$.

Subcase I. $d(u_3) = d(v_3) = 2$, see Figure 2(6). Then $(d(u_4), d(u_5)) \neq (3, 3)$ and $(d(v_4), d(v_5)) \neq (3, 3)$.

From $T_{n-1}$ to $T_n$, the new added paths of length 3 are given in Table 9 and the sum of their weights is $\frac{7}{18} \sqrt{6} + \frac{17}{12}$.

<table>
<thead>
<tr>
<th>avv_v3</th>
<th>avv_v2</th>
<th>avuu</th>
<th>duu_u3</th>
<th>duu_u2</th>
<th>duv_v1</th>
<th>bavv_v1</th>
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</table>

Also, there are eleven paths of length 3 in $T_{n-1}$ whose weights are changed. They are given in Table 10, and

$$
\sum_{i=1}^{11} Q_i = f(u_4, u_5; v_4, v_5)
$$

$$
= \left( -\frac{1}{6} \sqrt{6} + \frac{1}{18} \right) - \left( \frac{1}{2\sqrt{3}} - \frac{1}{3\sqrt{2}} \right) \left( \frac{1}{\sqrt{d(u_5)}} + \frac{1}{\sqrt{d(v_5)}} \right)
$$

$$
- \left( \frac{1}{3\sqrt{2}} - \frac{1}{3\sqrt{3}} \right) \left( \frac{1}{\sqrt{d(u_4)}} + \frac{1}{\sqrt{d(v_4)}} \right).
$$

Table 10.

<table>
<thead>
<tr>
<th>$u_1 u_3 u_5$</th>
<th>$u_1 u_2 u_4$</th>
<th>$u_1 u_2 v_2$</th>
<th>$u_2 v_1 v_3$</th>
<th>$u_2 v_1 v_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1 / \sqrt{d(u_3)} (1 / 3\sqrt{3} - 1 / 2\sqrt{3})$</td>
<td>$1 / \sqrt{d(u_1)} (1 / 3\sqrt{3} - 1 / 3\sqrt{2})$</td>
<td>$1 / 3\sqrt{6} - 1 / 6$</td>
<td>$1 / 3\sqrt{6} - 1 / 6$</td>
<td>$1 / 3\sqrt{6} - 1 / 6$</td>
</tr>
<tr>
<td>$P_1$</td>
<td>$v_1 v_2 v_3$</td>
<td>$v_1 v_2 v_3$</td>
<td>$v_1 v_2 v_3$</td>
<td>$v_1 v_2 v_3$</td>
</tr>
<tr>
<td>$Q_1$</td>
<td>$1 / \sqrt{d(v_3)} (1 / 3\sqrt{3} - 1 / 2\sqrt{3})$</td>
<td>$1 / \sqrt{d(v_1)} (1 / 3\sqrt{3} - 1 / 3\sqrt{2})$</td>
<td>$1 / 3\sqrt{6} - 1 / 6$</td>
<td>$1 / 3\sqrt{6} - 1 / 6$</td>
</tr>
<tr>
<td>$P_1$</td>
<td>$u_1 u_2 v_1$</td>
<td>$u_1 u_2 v_1$</td>
<td>$u_1 u_2 v_1$</td>
<td>$u_1 u_2 v_1$</td>
</tr>
<tr>
<td>$Q_1$</td>
<td>$1 / 3\sqrt{6} - 1 / 6$</td>
<td>$1 / 3\sqrt{6} - 1 / 6$</td>
<td>$1 / 3\sqrt{6} - 1 / 6$</td>
<td>$1 / 3\sqrt{6} - 1 / 6$</td>
</tr>
</tbody>
</table>

Since $\frac{1}{2\sqrt{3}} - \frac{1}{3\sqrt{2}} > \frac{1}{3\sqrt{3}} > 0$, $(d(u_4), d(u_5)) \neq (3, 3)$ and $(d(v_4), d(v_5)) \neq (3, 3)$,

$$
\frac{-2}{9} \sqrt{6} + \frac{1}{18} = f(2, 2; 2, 2) \leq f(u_4, u_5; v_4, v_5) \leq f(2, 3; 2, 3) = \frac{1}{18} \sqrt{6} - \frac{11}{18}
$$

So, $R_3(T_n) - R_3(T_{n-1}) = \left( \frac{7}{18} \sqrt{6} + \frac{17}{12} \right) + f(u_4, u_5; v_4, v_5)$, and

$$
\frac{1}{6} \sqrt{6} + \frac{53}{36} \leq R_3(T_n) - R_3(T_{n-1}) \leq \frac{4}{9} \sqrt{6} + \frac{29}{36}
$$

(6)

Subcase II. $d(u_3) = 3, d(v_3) = 2$, see Figure 2(7). Then $(d(v_4), d(v_5)) \neq (3, 3)$.

From $T_{n-1}$ to $T_n$, the new added paths of length 3 are given in Table 11 and the sum of their weights is $\frac{5}{18} \sqrt{6} + \frac{1}{2}$. 


Table 11.

<table>
<thead>
<tr>
<th>$avv_1v_3$</th>
<th>$avv_1v_2$</th>
<th>$avuu_1$</th>
<th>$duu_1u_3$</th>
<th>$duu_1u_2$</th>
<th>$duvv_1$</th>
<th>$bavv_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{1}{6}$</td>
<td>$\frac{1}{6}$</td>
<td>$\frac{1}{2\sqrt{6}}$</td>
<td>$\frac{1}{3\sqrt{6}}$</td>
<td>$\frac{1}{3\sqrt{6}}$</td>
<td>$\frac{1}{3\sqrt{6}}$</td>
<td>$\frac{1}{6}$</td>
</tr>
</tbody>
</table>

cdvu 

| $\frac{1}{6}$ | $\frac{1}{3}$ | $\frac{1}{6}$ | $\frac{1}{2\sqrt{6}}$ | $\frac{1}{5}$ | $\frac{1}{6}$ | $\frac{1}{2\sqrt{6}}$ |

\[ \text{Figure 2.} \]
Also, there are twelve paths of length 3 in $T_{n-1}$ whose weights are changed. They are given in Table 12, and

$$
\sum_{i=1}^{12} Q_i = f(u_4, u_6; v_4, v_5)
= \left( -\frac{7}{36} \sqrt{6} + \frac{1}{9} \right) - \left( \frac{1}{2\sqrt{3}} - \frac{1}{3\sqrt{2}} \right) \frac{1}{\sqrt{d(v_5)}}
- \left( \frac{1}{3\sqrt{2}} - \frac{1}{3\sqrt{3}} \right) \left( \frac{1}{\sqrt{d(u_4)}} + \frac{1}{\sqrt{d(u_6)}} + \frac{1}{\sqrt{d(v_4)}} \right).
$$

<table>
<thead>
<tr>
<th>$P_i$</th>
<th>$uu_1u_3u_6$</th>
<th>$uu_1u_3u_5$</th>
<th>$uu_1u_2u_4$</th>
<th>$uu_1u_2v_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_i$</td>
<td>$\frac{1}{\sqrt{d(u_6)}} \left( \frac{1}{3\sqrt{3}} - \frac{1}{3\sqrt{2}} \right)$</td>
<td>$\frac{1}{9} - \frac{1}{3\sqrt{3}}$</td>
<td>$\frac{1}{\sqrt{d(u_4)}} \left( \frac{1}{3\sqrt{3}} - \frac{1}{3\sqrt{2}} \right)$</td>
<td>$\frac{1}{9} - \frac{1}{3\sqrt{3}}$</td>
</tr>
</tbody>
</table>

Since $\frac{1}{2\sqrt{3}} - \frac{1}{3\sqrt{2}} > \frac{1}{3\sqrt{2}} - \frac{1}{3\sqrt{3}} > 0$, and $(d(v_4), d(v_5)) \neq (3, 3)$,

$$
-\frac{1}{9} \sqrt{6} - \frac{2}{9} = f(2, 2; 2, 2) \leq f(u_4, u_6; v_4, v_5) \leq f(3, 3; 2, 3) = -\frac{7}{36} \sqrt{6}
$$

So, $R_3(T_n) - R_3(T_{n-1}) = (\frac{4}{9} \sqrt{6} + \frac{5}{2}) + f(u_4, u_6; v_4, v_5)$, and

$$
\frac{1}{3} \sqrt{6} + \frac{37}{36} \leq R_3(T_n) - R_3(T_{n-1}) \leq \frac{1}{4} \sqrt{6} + \frac{5}{4}
$$

(7)

**Subcase III.** $d(u_3) = 2, d(v_3) = 3$, see Figure 2(8). Then it is symmetric to Subcase II.

**Subcase IV.** $d(u_3) = d(v_3) = 3$, see Figure 2(9). Then, from $T_{n-1}$ to $T_n$, the new added paths of length 3 are given in Table 13 and the sum of their weights is $\frac{1}{2} \sqrt{6} + \frac{13}{11}$.

<table>
<thead>
<tr>
<th>$avv_1v_3$</th>
<th>$avv_1v_2$</th>
<th>$avu_1u_3$</th>
<th>$duu_1u_3$</th>
<th>$duu_1u_2$</th>
<th>$duvv_1$</th>
<th>$bavv_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{1}{3\sqrt{3}}$</td>
<td>$\frac{1}{3\sqrt{3}}$</td>
<td>$\frac{1}{3\sqrt{3}}$</td>
<td>$\frac{1}{3\sqrt{3}}$</td>
<td>$\frac{1}{3\sqrt{3}}$</td>
<td>$\frac{1}{3\sqrt{3}}$</td>
<td>$\frac{1}{3\sqrt{3}}$</td>
</tr>
<tr>
<td>$\frac{1}{3\sqrt{2}}$</td>
<td>$\frac{1}{3\sqrt{2}}$</td>
<td>$\frac{1}{3\sqrt{2}}$</td>
<td>$\frac{1}{3\sqrt{2}}$</td>
<td>$\frac{1}{3\sqrt{2}}$</td>
<td>$\frac{1}{3\sqrt{2}}$</td>
<td>$\frac{1}{3\sqrt{2}}$</td>
</tr>
<tr>
<td>$\frac{1}{\sqrt{6}}$</td>
<td>$\frac{1}{\sqrt{6}}$</td>
<td>$\frac{1}{\sqrt{6}}$</td>
<td>$\frac{1}{\sqrt{6}}$</td>
<td>$\frac{1}{\sqrt{6}}$</td>
<td>$\frac{1}{\sqrt{6}}$</td>
<td>$\frac{1}{\sqrt{6}}$</td>
</tr>
</tbody>
</table>

Also, there are thirteen paths of length 3 in $T_{n-1}$ whose weights are changed. They are given in Table 14, and
$$\sum_{i=1}^{13} Q_i = f(u_4, u_6; v_4, v_6)$$
\[
= \left( \frac{-2}{9} \sqrt{6} + \frac{1}{6} \right) + \left( \frac{1}{3\sqrt{3}} - \frac{1}{3\sqrt{2}} \right) \left( \frac{1}{\sqrt{d(u_4)}} + \frac{1}{\sqrt{d(u_6)}} + \frac{1}{\sqrt{d(v_4)}} + \frac{1}{\sqrt{d(v_6)}} \right).
\]

Table 14.

<table>
<thead>
<tr>
<th>$P_i$</th>
<th>$uu_1u_3u_6$</th>
<th>$uu_1u_3u_5$</th>
<th>$uu_1u_2u_4$</th>
<th>$uu_1u_2u_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_i$</td>
<td>$\frac{1}{d(u_6)} \left( \frac{1}{3\sqrt{3}} - \frac{1}{3\sqrt{2}} \right)$</td>
<td>$\frac{1}{9} - \frac{1}{3\sqrt{6}}$</td>
<td>$\frac{1}{9} - \frac{1}{3\sqrt{6}}$</td>
<td>$\frac{1}{9} - \frac{1}{3\sqrt{6}}$</td>
</tr>
<tr>
<td>$P_i$</td>
<td>$uuv_1v_2$</td>
<td>$uuv_1v_3$</td>
<td>$uuv_1v_3v_6$</td>
<td>$vuv_1v_3v_5$</td>
</tr>
<tr>
<td>$Q_i$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
</tr>
<tr>
<td>$P_i$</td>
<td>$vuv_1v_3v_4$</td>
<td>$vuv_1v_3v_2u_2$</td>
<td>$vuv_1u_2v_2$</td>
<td>$vuv_1u_2v_2$</td>
</tr>
<tr>
<td>$Q_i$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
</tr>
</tbody>
</table>

Since $-\frac{1}{2} = f(2, 2; 2, 2) \leq f(u_4, u_6; v_4, v_6) \leq f(3, 3; 3, 3) = -\frac{4}{9} \sqrt{6} + \frac{11}{18}$, and $R_3(T_n) - R_3(T_{n-1}) = \left( \frac{1}{2} \sqrt{6} + \frac{13}{12} \right) + f(u_4, u_6; v_4, v_6)$, we have
\[
\frac{1}{2} \sqrt{6} + \frac{7}{12} \leq R_3(T_n) - R_3(T_{n-1}) \leq \frac{1}{18} \sqrt{6} + \frac{61}{36} \quad (8)
\]

3 Catacondensed benzenoids chains with the extremal third-order Randić index

In this section, we will give the maximum and minimum third-order Randić indices of catacondensed hexagonal systems and characterize the extremal graphs.

When $n = 1, 2, 3, 4$, the third-order Randić indices of catacondensed hexagonal systems with $n$ hexagons are shown in Figure 3.

**Theorem 1.** Let $T_n \in C_n$ be a catacondensed hexagonal system with $n$ hexagons. Then
\[
R_3(T_n) \leq R_3(Z_n)
\]
with equality if and only if $T_n = Z_n$ is the zigzag hexagonal chain with $n$ hexagons.

**Proof.** The result is true for $n = 1, 2, 3, 4$, see Figure 3.

We suppose that the result is true for $n - 2$ and $n - 1$ ($n \geq 5$).
By the equations (1)-(8) and max \(\frac{1}{3}\sqrt{6} + \frac{5}{18}\sqrt{6} + \frac{29}{36}\), \(\frac{1}{12}\sqrt{6} + \frac{61}{36}\) \(<\frac{2}{5}\sqrt{6} + \frac{25}{18}\), we have

\[R_3(T_n) - R_3(T_{n-1}) \leq \frac{2}{9}\sqrt{6} + \frac{25}{18}\] or \(R_3(T_n) - R_3(T_{n-1}) \leq \frac{17}{36}\sqrt{6} + \frac{7}{9}\).

From the remark in Case II, if \(R_3(T_n) - R_3(T_{n-1}) = \frac{17}{36}\sqrt{6} + \frac{7}{9}\), then it must have \(R_3(T_{n-1}) - R_3(T_{n-2}) = \frac{2}{9}\sqrt{6} + \frac{4}{3}\), and

\[R_3(T_n) - R_3(T_{n-2}) = \left(\frac{2}{9}\sqrt{6} + \frac{4}{3}\right) + \left(\frac{17}{36}\sqrt{6} + \frac{7}{9}\right) < 2\left(\frac{2}{9}\sqrt{6} + \frac{25}{18}\right)\]

So, \(R_3(T_n) - R_3(T_{n-2}) \leq 2\left(\frac{2}{9}\sqrt{6} + \frac{25}{18}\right)\). By the inductive hypothesis and the equation (3), we have

\[R_3(T_n) \leq R_3(Z_n)\]

with equality if and only if \(T_n = Z_n\).

\[R_3 = \frac{3}{2}\]

\[R_3 = \frac{2}{3}\sqrt{6} + \frac{11}{6}\]

\[R_3 = \frac{8}{9}\sqrt{6} + \frac{19}{6}\]

\[R_3 = \frac{10}{9}\sqrt{6} + \frac{9}{2}\]

\[R_3 = \frac{49}{36}\sqrt{6} + \frac{71}{18}\]

\[R_3 = \sqrt{6} + \frac{53}{18}\]

\[R_3 = \frac{11}{9}\sqrt{6} + \frac{13}{3}\]

\[R_3 = \frac{3}{2}\sqrt{6} + \frac{65}{18}\]

\[R_3 = \frac{7}{6}\sqrt{6} + \frac{53}{12}\]

Figure 3.

Similarly, because

\[\min\left\{\frac{2}{9}\sqrt{6} + \frac{4}{3}\cdot\frac{1}{2}\sqrt{6} + \frac{2}{3}\cdot\frac{7}{18}\sqrt{6} + \frac{17}{18} \cdot \frac{1}{6}\sqrt{6} + \frac{53}{36} \cdot \frac{1}{3}\sqrt{6} + \frac{37}{36} \cdot \frac{1}{2}\sqrt{6} + \frac{7}{12}\right\} = \frac{2}{9}\sqrt{6} + \frac{4}{3}\]

by the equations (1)-(8) and the induction on \(n\), we can get
Theorem 2. Let \( T_n \in C_n \) be a catacondensed hexagonal system with \( n \) hexagons. Then
\[
R_3(T_n) \geq R_3(L_n)
\]
with equality if and only if \( T_n = L_n \) is the linear hexagonal chain with \( n \) hexagons.

Theorems 1 and 2 show that the graphs with the maximum and minimum third-order Randić indices in \( C_n \) are \( Z_n \) and \( L_n \), respectively. They are the same as in the hexagonal chains\([17]\), and for \( n \geq 3 \)
\[
R_3(Z_n) = \frac{2n + 3}{9} \sqrt{6} + \frac{25n - 22}{18}, \quad R_3(L_n) = \frac{2n + 2}{9} \sqrt{6} + \frac{8n - 5}{6}.
\]

4 The recursive formulas for computing the third-order Randić indices of phenylenes

Phenylenes are a class of chemical compounds in which the carbon atoms form 6- and 4-membered cycles. Each 4-membered cycle(square) is adjacent to two disjoint 6-membered cycles(hexagons), and no two hexagons are adjacent. Their respective molecular graphs are also referred to as phenylenes.

By eliminating, “squeezing out”, the squares from a phenylene, a catacondensed hexagonal system (which may be jammed) is obtained, called the hexagonal squeeze of the respective phenylene. Clearly, there is a one-to-one correspondence between a phenylene (P) and its hexagonal squeeze (S). Both possess the same number of hexagons. In addition, a phenylene with \( n \) hexagons possesses \( n - 1 \) squares. An example of a phenylene and its hexagonal squeeze is shown in Figure 4.

Figure 4. A phenylene and its hexagonal squeeze.
Let $P_n$ be a phenylene with $n$ hexagons. $S_n$ is its hexagonal squeeze. $H$ is a hexagon of $P_n$. Obviously, $H$ has at most three adjacent hexagons in $S_n$. If $H$ has exactly three adjacent hexagons in $S_n$, then $H$ is called a full-hexagon of $S_n$ and $P_n$; if $H$ has at most one adjacent hexagon in $S_n$, then $H$ is called an end-hexagon of $S_n$ and $P_n$. It is easy to see that the number of the end-hexagons is more two than the number of its full-hexagons.

For the third-order Randić index of phenylenes, a formula was given in [13] by using its inlets.

**Lemma ([13]).** Let $P_n$ be a phenylene with $n$ hexagons. Then

$$R_3(P_n) = \frac{109 + 2\sqrt{6}}{36} h + \frac{14\sqrt{6} - 31}{36} r + \frac{5 - 2\sqrt{6}}{18} f - \frac{27 - 10\sqrt{6}}{72} a - \frac{35 - 2\sqrt{6}}{18}$$

where $r, f$ and $a$ are the numbers of inlets, fissures and pairs of adjacent inlets in $P_n$, respectively.

In the following, we discuss the recursive formula for computing the third-order Randić index of phenylenes.

Let $P_n$ be a phenylene with $n$ hexagons. $H_1 = x_1x_2x_3x_4x_5x_6x_1$ is an end-hexagon of $P_n$. $H_2$ is the hexagon adjacent to $H_1$ in the hexagonal squeeze $S_n$ of $P_n$. $P_{n-1} = P_n - \{x_1, x_2, x_3, x_4, x_5, x_6\}$ is a phenylene with $n - 1$ hexagons.

As in Section 2, if $l = v_1v_2v_3v_4$ is a path of $P_n$, then

$$W_{P_n}(l) = \frac{1}{\sqrt{d(v_1)d(v_2)d(v_3)d(v_4)}}$$

is the weight of the path $l$ in $P_n$. And $Q = W_{P_n}(l) - W_{P_{n-1}}(l)$ for a common path $l$ of $P_n$ and $P_{n-1}$.

**Case I.** $H_2$ is neither a turn-hexagon nor a full-hexagon, see Figure 5(1).

From $P_{n-1}$ to $P_n$, the new added paths of length 3 must contain one of $x_1, \ldots, x_6$, they are given in Table 15 and the sum of their weights is $\frac{13}{3\sqrt{6}} + \frac{67}{36}$. 
(1) \( R_3(P_n) - R_3(P_{n-1}) = \frac{8}{9} \sqrt{6} + \frac{10}{9} \)

(2) \( R_3(P_n) - R_3(P_{n-1}) = \frac{4}{9} \sqrt{6} + \frac{39}{18} \)

(3) \( R_3(P_n) - R_3(P_{n-1}) = \frac{1}{3} \sqrt{6} + \frac{22}{9} \)

(4) \( R_3(P_n) - R_3(P_{n-1}) = \frac{4}{9} \sqrt{6} + \frac{39}{18} \)

(5) \( R_3(P_n) - R_3(P_{n-1}) = \frac{1}{3} \sqrt{6} + \frac{22}{9} \)

(6) (i) \( d(u_5) = d(v_5) = 3, \)
\( R_3(P_n) - R_3(P_{n-1}) = \frac{1}{18} \sqrt{6} + \frac{109}{36} \)
(ii) \( d(u_5) = 3, d(v_5) = 2 \)
\( \text{or } d(u_5) = 2, d(v_5) = 3, \)
\( R_3(P_n) - R_3(P_{n-1}) = \frac{1}{18} \sqrt{6} + \frac{11}{4} \)
(iii) \( d(u_5) = d(v_5) = 2, \)
\( R_3(P_n) - R_3(P_{n-1}) = \frac{5}{18} \sqrt{6} + \frac{89}{36} \)

Figure 5.
Table 15. The new added paths of length 3 in $P_n$ and their weights.

<table>
<thead>
<tr>
<th>Path</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_1x_2x_3x_4$</td>
<td>$\frac{1}{\sqrt{6}}$</td>
</tr>
<tr>
<td>$x_1x_2x_4x_1$</td>
<td>$\frac{1}{2}$</td>
</tr>
<tr>
<td>$x_1x_3x_4x_1$</td>
<td>$\frac{1}{\sqrt{6}}$</td>
</tr>
<tr>
<td>$x_1x_4x_1x_2$</td>
<td>$\frac{1}{2}$</td>
</tr>
<tr>
<td>$x_2x_3x_4x_1$</td>
<td>$\frac{1}{2}$</td>
</tr>
<tr>
<td>$x_3x_4x_1x_2$</td>
<td>$\frac{1}{2}$</td>
</tr>
</tbody>
</table>

Note that the paths of length 3 in $P_{n-1}$ whose weights are changed must contain $u$ or $v$. They are given in Table 16, and

$$\sum_{i=1}^{7} Q_i = \frac{1}{\sqrt{6}} - \frac{3}{4}$$

Table 16. The paths of length 3 in $P_{n-1}$ whose weights are changed.

<table>
<thead>
<tr>
<th>Path</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_1u u_1 u_2 u_3$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{6}$</td>
</tr>
<tr>
<td>$u u_1 u_2 v_2$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{6}$</td>
</tr>
<tr>
<td>$u v v_1 v_2$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{6}$</td>
</tr>
<tr>
<td>$v v_1 v_2 v_3$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{6}$</td>
</tr>
<tr>
<td>$v v_1 v_2 u_2$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{6}$</td>
</tr>
<tr>
<td>$u_1 u v v_1$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{6}$</td>
</tr>
</tbody>
</table>

So,

$$R_3(P_n) - R_3(P_{n-1}) = \left( \frac{13}{3\sqrt{6}} + \frac{67}{36} \right) + \left( \frac{1}{\sqrt{6}} - \frac{3}{4} \right) = \frac{8}{9} \sqrt{6} + \frac{10}{9} \quad (9)$$

Case II. $H_2$ is a turn-hexagon. Let $H_3$ be the hexagon adjacent to $H_2$ in $S_n$ and different from $H_1$.

Subcase I. $H_3$ is neither a turn-hexagon nor a full-hexagon, see Figure 5(2). Then, from $P_{n-1}$ to $P_n$, the new added paths of length 3 are given in Table 17. The sum of their weights is $\frac{5}{9} \sqrt{6} + \frac{83}{36}$.

Table 17.

<table>
<thead>
<tr>
<th>Path</th>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_1x_2x_3x_4$</td>
<td>$\frac{1}{\sqrt{6}}$</td>
</tr>
<tr>
<td>$x_1x_2x_4x_1$</td>
<td>$\frac{1}{\sqrt{6}}$</td>
</tr>
<tr>
<td>$x_1x_3x_4x_1$</td>
<td>$\frac{1}{2}$</td>
</tr>
<tr>
<td>$x_1x_4x_1x_2$</td>
<td>$\frac{1}{2}$</td>
</tr>
<tr>
<td>$x_2x_3x_4x_1$</td>
<td>$\frac{1}{2}$</td>
</tr>
<tr>
<td>$x_3x_4x_1x_2$</td>
<td>$\frac{1}{2}$</td>
</tr>
<tr>
<td>$x_2x_1u u_1 u_2$</td>
<td>$\frac{1}{3\sqrt{6}}$</td>
</tr>
<tr>
<td>$x_2x_1u_1 u_2$</td>
<td>$\frac{1}{3\sqrt{6}}$</td>
</tr>
<tr>
<td>$x_2x_1u_1 u_2$</td>
<td>$\frac{1}{3\sqrt{6}}$</td>
</tr>
<tr>
<td>$x_2x_1u_1 u_2$</td>
<td>$\frac{1}{3\sqrt{6}}$</td>
</tr>
<tr>
<td>$x_2x_1u_1 u_2$</td>
<td>$\frac{1}{3\sqrt{6}}$</td>
</tr>
<tr>
<td>$x_2x_1u_1 u_2$</td>
<td>$\frac{1}{3\sqrt{6}}$</td>
</tr>
</tbody>
</table>

u x_1 x_6 v 

<table>
<thead>
<tr>
<th>Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{1}{3}$</td>
</tr>
</tbody>
</table>
There are nine paths of length 3 in $P_{n-1}$ whose weights are changed. They are given in Table 18, and

$$\sum_{i=1}^{9} Q_i = -\frac{2}{3\sqrt{6}} - \frac{5}{36} = -\frac{1}{9}\sqrt{6} - \frac{5}{36}.$$  

Table 18.

<table>
<thead>
<tr>
<th>$P_i$</th>
<th>$uu_1u_2u_3$</th>
<th>$uuv_1u_3$</th>
<th>$uuv_1v_2$</th>
<th>$vuv_1v_2v_3$</th>
<th>$vv_1v_2u_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_i$</td>
<td>$1 - \frac{1}{2\sqrt{6}}$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{6}$</td>
<td>$\frac{1}{9} - \frac{1}{3\sqrt{6}}$</td>
</tr>
<tr>
<td>$P_i$</td>
<td>$vuv_1u_3u_4$</td>
<td>$vuv_1u_3u_2$</td>
<td>$vuv_1u_2u_2$</td>
<td>$u_1uu_1$</td>
<td></td>
</tr>
<tr>
<td>$Q_i$</td>
<td>$\frac{1}{9} - \frac{1}{3\sqrt{6}}$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{6}$</td>
<td>$\frac{1}{6} - \frac{1}{6}$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{2\sqrt{6}}$</td>
<td></td>
</tr>
</tbody>
</table>

And,

$$R_3(P_n) - R_3(P_{n-1}) = \left(\frac{5}{9}\sqrt{6} + \frac{83}{36}\right) + \left(-\frac{1}{9}\sqrt{6} - \frac{5}{36}\right) = \frac{4}{9}\sqrt{6} + \frac{39}{18} \quad (10)$$

Subcase II. $H_3$ is a turn-hexagon or a full-hexagon.

(i) If $H_3$ is a turn-hexagon and $d(v_3) = 3$, see Figure 5(3); (ii) If $H_3$ is a turn-hexagon and $d(v_3) = 2$, see Figure 5(4); (iii) If $H_3$ is a full-hexagon ($d(v_3) = 3$), see Figure 5(5).

Then, from $P_{n-1}$ to $P_n$, the new added paths of length 3 and their weights are the same as in Table 17. Also, there are nine paths of length 3 in $P_{n-1}$ whose weights are changed.

They are given in Table 19, and

$$\sum_{i=1}^{9} Q_i = -\frac{1}{\sqrt{6}} + \frac{1}{36} + \left(\frac{1}{3\sqrt{3}} - \frac{1}{3\sqrt{2}}\right) \frac{1}{\sqrt{d(v_3)}}$$

Table 19.

<table>
<thead>
<tr>
<th>$P_i$</th>
<th>$uu_1u_2u_3$</th>
<th>$uuv_1u_3$</th>
<th>$uuv_1v_2$</th>
<th>$vuv_1v_2v_3$</th>
<th>$vv_1v_2u_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_i$</td>
<td>$\frac{1}{5} - \frac{1}{2\sqrt{6}}$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
<td>$\frac{1}{9} - \frac{1}{6}$</td>
<td>$\left(\frac{1}{3\sqrt{6}} - \frac{1}{3\sqrt{2}}\right) \frac{1}{\sqrt{d(v_3)}}$</td>
<td>$\frac{1}{9} - \frac{1}{3\sqrt{6}}$</td>
</tr>
<tr>
<td>$P_i$</td>
<td>$vuv_1u_3u_4$</td>
<td>$vuv_1u_3u_2$</td>
<td>$vuv_1u_2u_2$</td>
<td>$u_1uu_1$</td>
<td></td>
</tr>
<tr>
<td>$Q_i$</td>
<td>$\frac{1}{5} - \frac{1}{3\sqrt{6}}$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{6}$</td>
<td>$\frac{1}{6} - \frac{1}{6}$</td>
<td>$\frac{1}{3\sqrt{6}} - \frac{1}{2\sqrt{6}}$</td>
<td></td>
</tr>
</tbody>
</table>

So, $R_3(P_n) - R_3(P_{n-1}) = \left(\frac{5}{9}\sqrt{6} + \frac{83}{36}\right) + \left(-\frac{1}{\sqrt{6}} + \frac{1}{36}\right) + \left(\frac{1}{3\sqrt{3}} - \frac{1}{3\sqrt{2}}\right) \frac{1}{\sqrt{d(v_3)}}$.

Since $2 \leq d(v_3) \leq 3$, we have

$$R_3(P_n) - R_3(P_{n-1}) = \begin{cases} \frac{1}{3}\sqrt{6} + \frac{22}{9}, & d(v_3) = 3; \\ \frac{4}{9}\sqrt{6} + \frac{30}{18}, & d(v_3) = 2. \end{cases} \quad (11)$$

Case III. $H_2$ is a full-hexagon, see Figure 5(6).

From $P_{n-1}$ to $P_n$, the new added paths of length 3 are given in Table 20 and the sum of their weights is $\frac{1}{2}\sqrt{6} + \frac{67}{36}$. 

-486-
Also, there are thirteen paths of length 3 in $T_{n-1}$ whose weights are changed. They are given in Table 21, and
\[
\sum_{i=1}^{13} Q_i = f(u_5, v_5) = \left( -\frac{1}{3} \sqrt{6} + \frac{7}{8} \right) + \left( \frac{1}{3\sqrt{3}} - \frac{1}{2\sqrt{2}} \right) \left( \frac{1}{\sqrt{d(u_5)}} + \frac{1}{\sqrt{d(v_5)}} \right).
\]

<table>
<thead>
<tr>
<th>$x_1x_2x_3x_4$</th>
<th>$x_1x_5x_6x_4$</th>
<th>$x_1x_5x_7u_1$</th>
<th>$x_1u_1x_5x_7$</th>
<th>$x_1u_1x_5u_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{1}{2\sqrt{6}}$</td>
<td>$\frac{1}{5}$</td>
<td>$\frac{1}{5}$</td>
<td>$\frac{1}{5}$</td>
<td>$\frac{1}{5}$</td>
</tr>
<tr>
<td>$x_1u_1u_2$</td>
<td>$x_1u_1u_3$</td>
<td>$x_6x_5x_4x_3$</td>
<td>$x_6x_1x_2x_3$</td>
<td>$x_6x_1u_1$</td>
</tr>
<tr>
<td>$\frac{1}{9}$</td>
<td>$\frac{1}{9}$</td>
<td>$\frac{1}{2\sqrt{6}}$</td>
<td>$\frac{1}{6}$</td>
<td>$\frac{1}{9}$</td>
</tr>
<tr>
<td>$x_6u_1u_1$</td>
<td>$x_6u_1v_2$</td>
<td>$x_6u_1v_3$</td>
<td>$x_2x_3x_4x_5$</td>
<td>$x_2x_1x_6x_5$</td>
</tr>
<tr>
<td>$\frac{1}{9}$</td>
<td>$\frac{1}{9}$</td>
<td>$\frac{1}{2\sqrt{6}}$</td>
<td>$\frac{1}{6}$</td>
<td>$\frac{1}{9}$</td>
</tr>
<tr>
<td>$x_2x_1u_1$</td>
<td>$x_2x_1u_4$</td>
<td>$x_5x_6x_1u$</td>
<td>$x_5x_6u_1$</td>
<td>$x_3x_2x_1u$</td>
</tr>
<tr>
<td>$\frac{1}{3\sqrt{6}}$</td>
<td>$\frac{1}{3\sqrt{6}}$</td>
<td>$\frac{1}{3\sqrt{6}}$</td>
<td>$\frac{1}{3\sqrt{6}}$</td>
<td>$\frac{1}{6}$</td>
</tr>
<tr>
<td>$x_4x_5x_6v$</td>
<td>$ux_1x_6v$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\frac{1}{5}$</td>
<td>$\frac{1}{5}$</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

So, $R_3(P_n) - R_3(P_{n-1}) = \left( \frac{1}{2} \sqrt{6} + \frac{87}{36} \right) + f(u_5, v_5)$, and
\[
R_3(P_n) - R_3(P_{n-1}) = \begin{cases} 
\frac{1}{18} \sqrt{6} + \frac{109}{36}, & d(u_5) = d(v_5) = 3; \\
\frac{5}{18} \sqrt{6} + \frac{89}{36}, & d(u_5) = d(v_5) = 3.
\end{cases}
\] (12)

5 Phenylenes with the extremal third-order Randić index

In this section, we will give the maximum and minimum third-order Randić indices of phenylenes and characterize the extremal graphs.

When $n = 1, 2, 3, 4$, the third-order Randić indices of phenylenes with $n$ hexagons are shown in Figure 6, using Lemma in the section 4.
Theorem 3. Let $P_n$ be a phenylene with $n$ hexagons, $n \geq 2$. Then

$$R_3(P_n) \leq \left(\frac{7}{9} \sqrt{6} + \frac{53}{18}\right) + (n - 2) \left(\frac{8}{9} \sqrt{6} + \frac{10}{9}\right)$$

with equality if and only if $P_n$ is the phenylene with $n$ hexagons whose hexagonal squeeze is the linear hexagonal chain.

Proof. The result is true for $n = 2, 3, 4$, see Figure 6.

We suppose that the result is true for $n - 1$ ($n \geq 5$).

By the equations (9)-(12) and

$$\frac{8}{9} \sqrt{6} + \frac{10}{9} > \frac{1}{3} \sqrt{6} + \frac{22}{9} > \frac{4}{9} \sqrt{6} + \frac{39}{18} > \frac{1}{18} \sqrt{6} + \frac{109}{36} > \frac{1}{6} \sqrt{6} + \frac{11}{4} > \frac{5}{18} \sqrt{6} + \frac{89}{36}$$

we have

$$R_3(P_n) - R_3(P_{n-1}) \leq \frac{8}{9} \sqrt{6} + \frac{10}{9}$$

By the inductive hypothesis,

$$R_3(P_n) \leq R_3(P_{n-1}) + \left(\frac{8}{9} \sqrt{6} + \frac{10}{9}\right) \leq R_3(P_2) + (n - 2) \left(\frac{8}{9} \sqrt{6} + \frac{10}{9}\right)$$

i.e.,

$$R_3(P_n) \leq \left(\frac{7}{9} \sqrt{6} + \frac{53}{18}\right) + (n - 2) \left(\frac{8}{9} \sqrt{6} + \frac{10}{9}\right)$$

and from the equation (9), the equality holds if and only if $P_n$ is the phenylene with $n$ hexagons whose hexagonal squeeze is the linear hexagonal chain.

□

Let $F_n$ denote the set of phenylenes with $n$ hexagons satisfying the following:

(i) if $n$ is even, then each hexagon of the phenylene is a full-hexagon or an end-hexagon;

(ii) if $n \geq 3$ is odd, then there is exactly one turn-hexagon in the phenylene and it is not adjacent to any end-hexagon in its hexagonal squeeze for $n \geq 7$, the other hexagons are full-hexagon or an end-hexagon.

From Figure 6, we can see that $R_3(F_2) = \frac{7}{9} \sqrt{6} + \frac{53}{18}$, $R_3(F_3) = \frac{11}{9} \sqrt{6} + \frac{46}{9}$ and $R_3(F_4) = \frac{3}{2} \sqrt{6} + \frac{91}{12}$. 

By the equations (11) and (12), we can compute recursively that

\[
R_3(F_n) = \begin{cases} 
\frac{7}{5}\sqrt{6} + \frac{53}{18}, & n = 2; \\
\frac{11}{9}\sqrt{6} + \frac{46}{9}, & n = 3; \\
\left(\frac{3}{2}\sqrt{6} + \frac{91}{12}\right) + \frac{n-4}{2} \left(\frac{1}{3}\sqrt{6} + \frac{22}{9}\right) + \frac{1}{6}\sqrt{6} + \frac{11}{4}\right)) , & n \geq 4 \text{ is even}; \\
\left(\frac{3}{2}\sqrt{6} + \frac{91}{12}\right) + \left(\frac{1}{3}\sqrt{6} + \frac{22}{9}\right) , & n=5; \\
\left(\frac{3}{2}\sqrt{6} + \frac{91}{12}\right) + 2 \left(\frac{1}{3}\sqrt{6} + \frac{22}{9}\right) + \left(\frac{5}{18}\sqrt{6} + \frac{89}{36}\right) \\
+ \frac{n-7}{2} \left(\frac{1}{3}\sqrt{6} + \frac{22}{9}\right) + \left(\frac{1}{6}\sqrt{6} + \frac{11}{4}\right)) , & n \geq 7 \text{ is odd}
\end{cases}
\]

for any \( F_n \in \mathcal{F}_n \).

**Theorem 4.** Let \( P_n \) be a phenylenes with \( n \geq 2 \) hexagons. Then \( R_3(P_n) \geq R_3(F_n) \) with equality if and only if \( P_n \in \mathcal{F}_n \).

**Proof.** We prove the result by the induction on \( n \). The result is true for \( n = 2, 3, 4 \) from Figure 6.

Suppose that the result is true for \( n - 1 \) (\( n \geq 5 \)). Let \( P_n \) be a phenylenes with \( n \) hexagons and the minimum third-order Randić index. \( H_1 \) is an end-hexagon which is farthest from the center of \( P_n \), \( H_2 \) is the hexagon adjacent to \( H_1 \) in its hexagonal squeeze. \( P_{n-1} = P_n - H_1 \).

\[
R_3 = \frac{3}{2}, \quad R_3 = \frac{7}{5}\sqrt{6} + \frac{53}{18}, \quad R_3 = \frac{5}{3}\sqrt{6} + \frac{73}{18}, \quad R_3 = \frac{11}{9}\sqrt{6} + \frac{46}{9}, \quad R_3 = \frac{23}{9}\sqrt{6} + \frac{93}{18}, \quad R_3 = \frac{19}{9}\sqrt{6} + \frac{56}{9}, \quad R_3 = \frac{3}{2}\sqrt{6} + \frac{131}{18}, \quad R_3 = \frac{14}{9}\sqrt{6} + \frac{68}{9}, \quad R_3 = \frac{3}{2}\sqrt{6} + \frac{91}{12}
\]

Figure 6.
Case I. $H_2$ is not a full-hexagon, see Figures 5(1)-(5).

(i) If $P_n$ is the phenylene in Figure 5(1), then

$$R_3(P_n) = R_3(P_{n-1}) + \left(\frac{8}{9}\sqrt{6} + \frac{10}{9}\right)$$
(by the equation (9))

$$\geq R_3(F_{n-1}) + \left(\frac{8}{9}\sqrt{6} + \frac{10}{9}\right)$$
(by the inductive hypothesis)

where $F_{n-1} \in \mathcal{F}_{n-1}$. So,

$$R_3(P_n) \geq \begin{cases} 
\left(\frac{3}{2}\sqrt{6} + \frac{91}{12}\right) + \frac{n-5}{2} \left(\frac{1}{3}\sqrt{6} + \frac{22}{9}\right) \\
+ \left(\frac{1}{9}\sqrt{6} + \frac{11}{4}\right) + \left(\frac{8}{9}\sqrt{6} + \frac{10}{9}\right), & n \geq 5 \text{ is odd;} \\
\left(\frac{3}{2}\sqrt{6} + \frac{91}{12}\right) + 2 \left(\frac{1}{3}\sqrt{6} + \frac{22}{9}\right) \\
+ \left(\frac{1}{18}\sqrt{6} + \frac{89}{36}\right) + \frac{n-6}{2} \left(\frac{1}{6}\sqrt{6} + \frac{11}{4}\right) \\
+ \left(\frac{1}{9}\sqrt{6} + \frac{11}{4}\right) + \left(\frac{8}{9}\sqrt{6} + \frac{10}{9}\right), & n \geq 8 \text{ is even}
\end{cases}$$

a contradiction.

(ii) If $P_n$ is the phenylene in Figure 5(2), let $P_{n-2} = P_{n-1} - H_2$. Then

$$R_3(P_n) = R_3(P_{n-1}) + \left(\frac{4}{9}\sqrt{6} + \frac{39}{18}\right)$$
(by the equation (10))

$$= R_3(P_{n-2}) + \left(\frac{8}{9}\sqrt{6} + \frac{10}{9}\right) + \left(\frac{4}{9}\sqrt{6} + \frac{39}{18}\right)$$
(by the equation (9))

$$> R_3(P_{n-2}) + \left(\frac{1}{3}\sqrt{6} + \frac{22}{9}\right) + \left(\frac{1}{6}\sqrt{6} + \frac{11}{4}\right)$$

$$\geq R_3(F_{n-2}) + \left(\frac{1}{3}\sqrt{6} + \frac{22}{9}\right) + \left(\frac{1}{6}\sqrt{6} + \frac{11}{4}\right)$$
(by the inductive hypothesis)

$$\geq R_3(F_n)$$

a contradiction, where $F_{n-2} \in \mathcal{F}_{n-2}$.

(iii) If $P_n$ is the phenylene in Figure 5(4), let $P_{n-2} = P_{n-1} - H_2$. Then

$$R_3(P_n) = R_3(P_{n-1}) + \left(\frac{4}{9}\sqrt{6} + \frac{39}{18}\right)$$
(by the equation (10))

$$\geq R_3(P_{n-2}) + \left(\frac{4}{9}\sqrt{6} + \frac{39}{18}\right) + \left(\frac{4}{9}\sqrt{6} + \frac{39}{18}\right)$$
(by the equation (10))
\[ R_3(P_{n-2}) + \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{1}{6} \sqrt{6} + \frac{11}{4} \right) \geq R_3(F_{n-2}) + \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{1}{6} \sqrt{6} + \frac{11}{4} \right) \text{ (by the inductive hypothesis)} \]
\[ \geq R_3(F_n) \]

a contradiction, where \( F_{n-2} \in F_{n-2} \).

(iv) If \( P_n \) is the phenylene in Figure 5(3) or (5), then

\[ R_3(P_n) = R_3(P_{n-1}) + \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) \text{ (by the equation (11))} \]
\[ \geq R_3(F_{n-1}) + \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) \text{ (by the inductive hypothesis)} \]
\[ \text{ (with equality if and only if } P_{n-1} \in F_{n-1} \) \]

So,

\[
R_3(P_n) \begin{cases} 
\left( \frac{3}{2} \sqrt{6} + \frac{91}{12} \right) + \frac{n-5}{2} \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) \\
+ \left( \frac{1}{6} \sqrt{6} + \frac{11}{4} \right) + \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right), & n \geq 5 \text{ is odd;} \\
\left( \frac{3}{2} \sqrt{6} + \frac{91}{12} \right) + \frac{n}{3} \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) \\
+ \left( \frac{5}{18} \sqrt{6} + \frac{5}{36} \right) + \frac{n-8}{2} \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) \\
+ \left( \frac{1}{6} \sqrt{6} + \frac{11}{4} \right) + \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right), & n \geq 8 \text{ is even} \\
\end{cases}
\]
\[ \geq R_3(F_n), \]

with equality if and only if \( n = 5 \) and \( P_4 \in F_4 \), and then \( P_5 \in F_5 \).

**Case II.** \( H_2 \) is a full-hexagon, see Figure 7.

**Subcase I.** If \( H_4 \) is a full-hexagon, see Figure 7(1), then \( n \geq 6 \). Let \( P_{n-2} = P_{n-1} - H_3 \).

\[ R_3(P_n) = R_3(P_{n-1}) + \left( \frac{1}{6} \sqrt{6} + \frac{11}{4} \right) \text{ (by the equation (12))} \]
\[ = R_3(P_{n-2}) + \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{1}{6} \sqrt{6} + \frac{11}{4} \right) \text{ (by the equation (11))} \]
\[ \geq R_3(F_{n-2}) + \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{1}{6} \sqrt{6} + \frac{11}{4} \right) \text{ (by the inductive hypothesis)} \]
\[ \text{ (with equality if and only if } P_{n-2} \in F_{n-2} \) \]
\[ \geq R_3(F_n) \text{ (with equality if and only if } n \neq 7 \) \]
So, $R_3(P_n) \geq R_3(F_n)$ with equality if and only if $P_n \in F_n$.

**Subcase II.** If $H_4$ is neither a full-hexagon nor a turn-hexagon, see Figure 7(2), let $P_{n-2} = P_{n-1} - H_3$ and $P_{n-3} = P_{n-2} - H_2$. Then

$$R_3(P_n) = R_3(P_{n-1}) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) \quad \text{(by the equation (12))}$$

$$= R_3(P_{n-2}) + \left( \frac{4}{9} \sqrt{6} + \frac{39}{18} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) \quad \text{(by the equation (11))}$$

$$= R_3(P_{n-3}) + \left( \frac{8}{9} \sqrt{6} + \frac{10}{9} \right) + \left( \frac{4}{9} \sqrt{6} + \frac{39}{18} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) \quad \text{(by the equation (9))}$$

$$\geq R_3(F_{n-3}) + \left( \frac{8}{9} \sqrt{6} + \frac{10}{9} \right) + \left( \frac{4}{9} \sqrt{6} + \frac{39}{18} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) \quad \text{(by the inductive hypothesis)}$$

where $F_{n-3} \in F_{n-3}$. So,

$$R_3(P_n) \geq \begin{cases} 
\left( \frac{7}{5} \sqrt{6} + \frac{53}{25} \right) + \left( \frac{8}{9} \sqrt{6} + \frac{10}{9} \right) & n=5; \\
+ \left( \frac{4}{9} \sqrt{6} + \frac{39}{18} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right), \\
\left( \frac{11}{9} \sqrt{6} + \frac{46}{9} \right) + \left( \frac{8}{9} \sqrt{6} + \frac{10}{9} \right) & n=6; \\
+ \left( \frac{4}{9} \sqrt{6} + \frac{39}{18} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right), \\
\left( \frac{3}{2} \sqrt{6} + \frac{91}{12} \right) + \frac{n-7}{2} \left( \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) \\
+ \left( \frac{4}{9} \sqrt{6} + \frac{14}{9} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) \right) & n \geq 7 \text{ is odd}; \\
+ \left( \frac{8}{9} \sqrt{6} + \frac{10}{9} \right) + \left( \frac{3}{2} \sqrt{6} + \frac{91}{12} \right) + 2 \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) & n=8; \\
\left( \frac{3}{2} \sqrt{6} + \frac{91}{12} \right) + 2 \left( \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) \right) \\
+ \frac{n-10}{2} \left( \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{1}{6} \sqrt{6} + \frac{11}{4} \right) \right) & n \geq 10 \text{ is even}; \\
+ \left( \frac{8}{9} \sqrt{6} + \frac{10}{9} \right) + \left( \frac{4}{9} \sqrt{6} + \frac{39}{18} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right), & n \geq 10 \text{ is even} \\
\end{cases} \quad > R_3(F_n),$$

a contradiction.

**Subcase III.** $H_4$ is a turn-hexagon, see Figures 7(3)-(6).
(i) When $H_5$ is not a full-hexagon, see Figures 7(3)-(5), we have $R_3(P_n) > R_3(G_0)$ by Lemma in the section 4, a contradiction.

(ii) When $H_5$ is a full-hexagon, see Figure 7(6), then $n \geq 7$.

$$R_3(P_n) = R_3(P_{n-1}) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) \quad \text{(by the equation (12))}$$

$$= R_3(P_{n-2}) + \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) \quad \text{(by the equation (11))}$$

$$= R_3(P_{n-3}) + 2 \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) \quad \text{(by the equation (11))}$$

$$\geq R_3(F_{n-3}) + 2 \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) \quad \text{(by the inductive hypothesis, and with equality iff $P_{n-3} \in \mathcal{F}_{n-3}$)}$$

where $F_{n-3} \in \mathcal{F}_{n-3}$. So,

$$R_3(P_n) \geq \begin{cases} 
\left( \frac{3}{2} \sqrt{6} + \frac{91}{12} \right) + \frac{n-7}{2} \left( \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{1}{6} \sqrt{6} + \frac{11}{4} \right) \right) \\
+2 \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) \\
\text{(with equality iff $P_{n-3} \in \mathcal{F}_{n-3}$ and $n - 3$ is even),} \\
\text{n \geq 7 is odd;} \\
\left( \frac{3}{2} \sqrt{6} + \frac{91}{12} \right) + \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) \\
+2 \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) \\
\left( \frac{3}{2} \sqrt{6} + \frac{91}{12} \right) + 2 \left( \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{1}{6} \sqrt{6} + \frac{11}{4} \right) \right) = R_3(F_8), \\
\text{n = 8;} \\
\left( \frac{3}{2} \sqrt{6} + \frac{91}{12} \right) + 2 \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) \\
+ \frac{n-10}{2} \left( \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{1}{6} \sqrt{6} + \frac{11}{4} \right) \right) \\
+2 \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{5}{18} \sqrt{6} + \frac{89}{36} \right) \\
\left( \frac{3}{2} \sqrt{6} + \frac{91}{12} \right) + \frac{n-4}{2} \left( \left( \frac{1}{3} \sqrt{6} + \frac{22}{9} \right) + \left( \frac{1}{6} \sqrt{6} + \frac{11}{4} \right) \right) = R_3(P_n), \\
\text{n \geq 10 is even} \\
i.e., R_3(P_n) \geq R_3(F_n) \text{ with equality if and only if } n \geq 7 \text{ is odd and } P_n \in \mathcal{F}_n.$$

\[\square\]

**Remark.** From the theorems 3-4 and the results in [17], we know that

(i) if a phenylene $P_n$ has the maximum third-order Randić index among all phenylenes with $n$ hexagons, then its hexagonal squeeze also has the maximum third-order Randić index among all catacondensed hexagonal systems with $n$ hexagons; but
(ii) if a phenylene $P_n$ has the minimum third-order Randić index among all phenylenes with $n \geq 4$ hexagons, then its hexagonal squeeze needs not to have the minimum third-order Randić index among all catacondensed hexagonal systems with $n$ hexagons.

Figure 7.
References


[18] H. Deng, Double hexagonal chains with the extremal third–order Randić index, *Ars Combin.* ACCEPTED.