Extremal Polyomino Chains of VDB Topological Indices

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Abstract

We show that the zig-zag chain $Z^3_n$ of segments of length 3 (see Figure 2) has the minimal ABC index among all polyomino chains with $n$ squares. More generally, we give conditions on the numbers $\{\phi_{ij}\}$ under which the zig-zag chain $Z^3_n$ is an extremal value of the induced topological index $T$ defined by

$$T(G) = \sum_{1 \leq i < j \leq n-1} m_{ij}\phi_{ij}$$

where $G$ is a graph with $n$ vertices and $m_{ij}$ is the number of edges of $G$ with terminal vertices of degree $i$ and $j$. We also find extremal values of the general Randić index $R_\alpha$ over the set of all polyomino chains, for some values of $\alpha$.

Mathematics Subject Classification: 05C76, 05C07, 05C35, 05C90

Keywords: Topological indices; Polyomino chains; Extreme values

1 Introduction

A topological index is a molecular-graph-based structure descriptor which plays an important role in QSAR/QSPR research ([3],[15],[16]). A large number of these were conceived, depending on vertex degrees of the molecular
graph, and now are called vertex-degree-based topological indices (VDB for short) [6]. More specifically, given a set of real numbers \(\{\varphi_{ij}\}\), where \(1 \leq i \leq j \leq n-1\), a vertex-degree-based topological index \(T\) is defined for a graph \(G\) with \(n\) vertices as

\[
T(G) = \sum_{1 \leq i \leq j \leq n-1} m_{ij} \varphi_{ij}
\]  

(1)

where \(m_{ij} = m_{ij}(G)\) is the number of edges in \(G\) with terminal vertices of degree \(i\) and \(j\). Different choices of the numbers \(\{\varphi_{ij}\}\) give different topological indices. For instance, the topological index induced by the numbers \(\varphi_{ij} = (ij)^\alpha\), where \(\alpha\) is a real number, is the well-known general Randić index denoted by \(R_\alpha(G)\). We illustrate in Table 1 a list of important VDB topological indices induced by the numbers \(\{\varphi_{ij}\}\).

<table>
<thead>
<tr>
<th>Index</th>
<th>({\varphi_{ij}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Randić [14]</td>
<td>(\frac{1}{\sqrt{ij}})</td>
</tr>
<tr>
<td>Sum-connectivity [24]</td>
<td>(\frac{1}{\sqrt{i+j}})</td>
</tr>
<tr>
<td>Harmonic [23]</td>
<td>(\frac{2}{i+j})</td>
</tr>
<tr>
<td>Geometric-Arithmetic [17]</td>
<td>(\frac{2\sqrt{i+j}}{i+j})</td>
</tr>
<tr>
<td>First Zagreb [10]</td>
<td>(i + j)</td>
</tr>
<tr>
<td>Second Zagreb [10]</td>
<td>(ij)</td>
</tr>
<tr>
<td>Atom-bond-connectivity [4]</td>
<td>(\sqrt{\frac{i+j-2}{ij}})</td>
</tr>
<tr>
<td>Augmented Zagreb [5]</td>
<td>((\frac{ij}{i+j-2})^3)</td>
</tr>
</tbody>
</table>

Table 1: Important VDB topological indices.

In this paper we will study VDB topological indices over a class which has a long and rich history, the polyomino systems [8]. A polyomino system is a finite 2-connected plane graph such that each interior face (also called cell) is surrounded by a regular square of length one. Applications of the polyomino systems to crystal physics can be found in ([7],[9]).

The inner dual graph of a polyomino \(P\) is defined as a plane graph in which the vertex set is the set of all cells of \(P\) and two vertices are adjacent if the corresponding two cells have an edge in common. A polyomino chain is a polyomino system whose inner dual graph is a path. A kink of a polyomino chain is any angularly connected square. A segment of a polyomino chain is a maximal linear chain including the kinks and/or terminal squares at its end. The number of squares in a segment is called the length of the segment. In particular, the linear chain \(L_n\) is a polyomino chain with exactly one segment (of length \(n\)) and the zig-zag chain \(Z_n\) is a polyomino chain in which every segment has length 2 (see Figure 1).
The study of topological indices over polyomino systems have appeared recently in the literature. For instance, Yang et al. ([20],[21]) and Yarahmadi et al. [19] find formulas for the Randić index, the sum-connectivity index and the Zagreb indices of polyomino chains and deduce the extremal values; more recently, An and Xiong [1] generalized some of the previous results to general Randić indices and Deng et al. [2] found formulas for the harmonic indices and deduced the extremal values. Other results can be found in ([18],[22]).

In this paper we study the extremal values of VDB topological indices using transformations of polyomino chains, a technique which was successful in the study of extremal values of VDB topological indices over catacondensed hexagonal systems [11]. This is a natural continuation of the results obtained in ([12],[13]), where conditions on the numbers \{\phi_{ij}\} were given in order to assure that the linear chain or the zig-zag chain are extremal values of the induced VDB topological index \(T\). However, as we shall see in this paper, there are other polyomino chains that are extremal values of VDB topological indices. Namely, we show that the zig-zag chain of segments of length 3, which we denoted by \(Z_3^n\) (see Figure 2), has minimal \(ABC\) index among all polyomino chains with \(n\) squares. Note that for \(n\) odd, all the segments of \(Z_3^n\) are of length 3, whereas for \(n\) even we assume that the last segment of \(Z_3^n\) is of length 4. Actually, we go further and give conditions on the numbers \{\phi_{ij}\} under which the zig-zag chain \(Z_3^n\) is an extremal value of the induced topological index \(T\) defined by (1). As an application of these results, we find values \(\alpha \in \mathbb{R}\) where \(Z_3^n\) is an extremal value of the general Randić index \(R_\alpha\).
2 Transformations of polyomino chains

\( \mathcal{P}_n \) will denote the set of all polyomino chains with \( n \) squares. If \( P \) is any polyomino chain, then we denote by \( |P| \) the number of squares \( P \) has.

Recently several transformations of polyomino chains were introduced in order to determine when the linear chain and the zig-zag chain have extremal values of a VDB topological index over \( \mathcal{P}_n \) ([12], [13]). These transformations are classified as linearizing and angularizing transformations. The linearizing transformations \( L_1 \) and \( L_2 \) are shown in Figure 3, where \( L \) is a linear subchain, \( X \) is a polyomino subchain and \( v \) a vertex with degree 3 or 4.

![Figure 3: Linear operations over a polyomino chain.](image)

The variation of a VDB topological index \( T \) induced by \( \{ \varphi_{ij} \} \) under the linearizing transformations is given as follows [12]:

\[
T(V_1) - T(U_1) = \begin{cases} 
  l_1 = -2 \varphi_{23} + 6 \varphi_{33} - 4 \varphi_{34} & \text{if } |L| \geq 1, \ d(v) = 3 \\
  l_2 = -\varphi_{23} - \varphi_{24} + 5 \varphi_{33} - 3 \varphi_{34} & \text{if } |L| = 0, \ d(v) = 3 \\
  l_3 = -2 \varphi_{23} + 5 \varphi_{33} - 2 \varphi_{34} - \varphi_{44} & \text{if } |L| \geq 1, \ d(v) = 4 \\
  l_4 = -\varphi_{23} - \varphi_{24} + 4 \varphi_{33} - \varphi_{34} - \varphi_{44} & \text{if } |L| = 0, \ d(v) = 4 
\end{cases}
\]

\( l_3 \) and \( l_4 \), corresponding to \( d(v) = 4 \), are missing in [12]. Consequently, if each of the expressions on \( \varphi_{ij} \) given in \( l_1 - l_6 \) are non-negative (resp. non-positive) then the linear chain has maximal (resp. minimal) \( T \)-value over \( \mathcal{P}_n \) [12]. As a consequence of the values given in Table 2, it was deduced that the linear chain has extremal value for important topological indices.

The relations \( l_3 \) and \( l_4 \), corresponding to \( d(v) = 4 \), are missing in [12].

We can go further and determine certain values of \( \alpha \) where the linear chain has extremal value of the generalized Randić index \( R_\alpha \) over \( \mathcal{P}_n \). In Table 3 we show the sign of the expressions on \( R_\alpha \) given in \( l_1 - l_6 \) for each value of \( \alpha \):
Extremal polyomino chains of VDB topological indices

Table 2: VDB topological indices with $L_n$ as extremal polyomino chain.

<table>
<thead>
<tr>
<th></th>
<th>$l_1$</th>
<th>$l_2$</th>
<th>$l_3$</th>
<th>$l_4$</th>
<th>$l_5$</th>
<th>$l_6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Randić</td>
<td>.029</td>
<td>.039</td>
<td>.023</td>
<td>.033</td>
<td>.043</td>
<td>.053</td>
</tr>
<tr>
<td>Sum-connectivity</td>
<td>.043</td>
<td>.052</td>
<td>.037</td>
<td>.046</td>
<td>.055</td>
<td>.063</td>
</tr>
<tr>
<td>Harmonic</td>
<td>.057</td>
<td>.076</td>
<td>.045</td>
<td>.064</td>
<td>.083</td>
<td>.102</td>
</tr>
<tr>
<td>Geometric-arithmetic</td>
<td>.081</td>
<td>.108</td>
<td>.061</td>
<td>.088</td>
<td>.114</td>
<td>.141</td>
</tr>
<tr>
<td>First Zagreb</td>
<td>$-2$</td>
<td>$-2$</td>
<td>$-2$</td>
<td>$-2$</td>
<td>$-2$</td>
<td>$-2$</td>
</tr>
<tr>
<td>Second Zagreb</td>
<td>$-6$</td>
<td>$-5$</td>
<td>$-7$</td>
<td>$-6$</td>
<td>$-5$</td>
<td>$-4$</td>
</tr>
</tbody>
</table>

Table 3: Signs of linearizing operations on $R_\alpha$.

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$l_1$</th>
<th>$l_2$</th>
<th>$l_3$</th>
<th>$l_4$</th>
<th>$l_5$</th>
<th>$l_6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(-\infty, r_5)$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$+$</td>
</tr>
<tr>
<td>$(r_5, r_2)$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$+$</td>
</tr>
<tr>
<td>$(r_2, r_4)$</td>
<td>$-$</td>
<td>$+$</td>
<td>$-$</td>
<td>$-$</td>
<td>$+$</td>
<td>$+$</td>
</tr>
<tr>
<td>$(r_4, -1)$</td>
<td>$-$</td>
<td>$+$</td>
<td>$-$</td>
<td>$+$</td>
<td>$+$</td>
<td>$+$</td>
</tr>
<tr>
<td>$(-1, r_3)$</td>
<td>$+$</td>
<td>$-$</td>
<td>$+$</td>
<td>$+$</td>
<td>$+$</td>
<td>$+$</td>
</tr>
<tr>
<td>$(r_3, 0)$</td>
<td>$+$</td>
<td>$+$</td>
<td>$+$</td>
<td>$+$</td>
<td>$+$</td>
<td>$+$</td>
</tr>
<tr>
<td>$(0, +\infty)$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
</tbody>
</table>

where $r_5 \approx -2.88727$ is a root of the equation $l_5(\alpha) = 0$, $r_2 \approx -1.56204$ is a root of the equation $l_2(\alpha) = 0$, $r_3 \approx -1.23853$ is a root of the equation $l_4(\alpha) = 0$, $r_3 \approx -0.84313$ is a root of the equation $l_3(\alpha) = 0$, $-1$ is a root of the equation $l_1(\alpha) = 0$ and $l_i(0) = 0$ for all $i = 1, \ldots, 6$. Consequently we have the following result:

**Theorem 2.1** The linear chain $L_n$ has maximal $T$-value over $P_n$ for $\alpha \in (r_3, 0)$ and minimal $T$-value over $P_n$ for $\alpha \in (0, +\infty)$.

On the other hand, the angularizing operations $A_1$, $A_2$ and $A_3$ are shown in Figure 4 where $Z$ is a zig-zag subchain, $X$ a polyomino subchain and $v$ a vertex of degree 3 or 4.

The variation of a VDB topological index $T$ induced by $\{\varphi_{ij}\}$ under the angularizing transformations is given as follows [13]:

$$T(V_3) - T(U_3) = \begin{cases} a_1 = -2\varphi_{23} + 4\varphi_{24} - 4\varphi_{34} + 2\varphi_{44} & \text{if } |Z| \geq 1 \\ a_2 = -\varphi_{23} + 3\varphi_{24} - 2\varphi_{33} - \varphi_{34} + \varphi_{44} & \text{if } |Z| = 0 \end{cases} \quad (4)$$

$$T(V_4) - T(U_4) = \begin{cases} a_3 = -2\varphi_{23} + 4\varphi_{24} - \varphi_{33} - 2\varphi_{34} + \varphi_{44} & \text{if } |Z| \geq 1 \\ -\varphi_{23} + 3\varphi_{24} - 2\varphi_{33} - \varphi_{34} + \varphi_{44} & \text{if } |Z| = 0 \end{cases} \quad (5)$$
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$$T(V_5) - T(U_5) = \begin{cases} a_4 = 2\varphi_{24} - 3\varphi_{33} + \varphi_{44} & \text{if } |Z| \geq 1, \ d(v) = 3 \\ a_5 = \varphi_{23} + \varphi_{24} - 5\varphi_{33} + 3\varphi_{34} & \text{if } |Z| = 0, \ d(v) = 3 \\ a_6 = 2\varphi_{24} - 2\varphi_{33} - 2\varphi_{34} + 2\varphi_{44} & \text{if } |Z| \geq 1, \ d(v) = 4 \\ a_7 = \varphi_{23} + \varphi_{24} - 4\varphi_{33} + \varphi_{34} + \varphi_{44} & \text{if } |Z| = 0, \ d(v) = 4 \end{cases}$$

(6)

Note that if $|Z| = 0$ then transformations $A_1$ and $A_2$ are the same and so $T(V_3) - T(U_3) = T(V_4) - T(U_4)$. Also, the relations $a_6$ and $a_7$ obtained from the case $d(v) = 4$ are missing in [13].

Similarly, if each of the expressions on $\varphi_{ij}$ given in $a_1 - a_7$ are non-negative (resp. non-positive) then the zig-zag chain has maximal (resp. minimal) $T$-value over $P_n$ [13]. Table 4 illustrates when the zig-zag chain is an extremal value of important VDB topological indices over $P_n$.

<table>
<thead>
<tr>
<th>Randić</th>
<th>$-0.057$</th>
<th>$-0.053$</th>
<th>$-0.063$</th>
<th>$-0.043$</th>
<th>$-0.039$</th>
<th>$-0.037$</th>
<th>$-0.033$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sum-connectivity</td>
<td>$-0.066$</td>
<td>$-0.063$</td>
<td>$-0.072$</td>
<td>$-0.055$</td>
<td>$-0.052$</td>
<td>$-0.049$</td>
<td>$-0.046$</td>
</tr>
<tr>
<td>Harmonic</td>
<td>$-0.109$</td>
<td>$-0.102$</td>
<td>$-0.121$</td>
<td>$-0.083$</td>
<td>$-0.076$</td>
<td>$-0.071$</td>
<td>$-0.064$</td>
</tr>
<tr>
<td>Geometric-arithmetic</td>
<td>$-0.147$</td>
<td>$-0.141$</td>
<td>$-0.168$</td>
<td>$-0.114$</td>
<td>$-0.108$</td>
<td>$-0.094$</td>
<td>$-0.088$</td>
</tr>
<tr>
<td>First Zagreb</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Second Zagreb</td>
<td>4</td>
<td>4</td>
<td>3</td>
<td>5</td>
<td>5</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>ABC</td>
<td>$0.057$</td>
<td>$0.048$</td>
<td>$0.069$</td>
<td>$0.027$</td>
<td>$0.017$</td>
<td>$0.015$</td>
<td>$0.005$</td>
</tr>
</tbody>
</table>

Table 4: VDB topological indices with $Z_n$ as extremal polyomino chain.

Next we determine certain values of $\alpha$ where the zig-zag chain has extremal value of the generalized Randić index $R_\alpha$ over $P_n$. In Table 5 we show the sign of the expressions on $R_\alpha$ given in $a_1 - a_7$ for each value of $\alpha$: where $t_4 \approx -2.88727$ is a root of the equation $a_4(\alpha) = 0$, $t_6 \approx -1.84071$ is a root of the equation $a_6(\alpha) = 0$, $t_5 \approx -1.56204$ is a root of the equation $a_5(\alpha) = 0$, $t_7 \approx -1.23853$ is a root of the equation $a_7(\alpha) = 0$ and $a_i(0) = 0$ for all $i = 1, \ldots, 7$. Consequently we have the following result:
Table 5: Signs of angularizing operations on $R_\alpha$.

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$a_1$</th>
<th>$a_2$</th>
<th>$a_3$</th>
<th>$a_4$</th>
<th>$a_5$</th>
<th>$a_6$</th>
<th>$a_7$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(-\infty, t_4)$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$+$</td>
<td>$+$</td>
<td>$+$</td>
<td>$-$</td>
</tr>
<tr>
<td>$(t_4, t_6)$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$+$</td>
<td>$+$</td>
<td>$+$</td>
</tr>
<tr>
<td>$(t_6, t_5)$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$+$</td>
<td>$+$</td>
<td>$-$</td>
</tr>
<tr>
<td>$(t_5, t_7)$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$+$</td>
</tr>
<tr>
<td>$(t_7, 0)$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
<td>$-$</td>
</tr>
<tr>
<td>$(0, +\infty)$</td>
<td>$+$</td>
<td>$+$</td>
<td>$+$</td>
<td>$+$</td>
<td>$+$</td>
<td>$+$</td>
<td>$+$</td>
</tr>
</tbody>
</table>

Theorem 2.2 The zig-zag chain $Z_n$ has minimal $T$-value over $\mathcal{P}_n$ for $\alpha \in (t_7, 0)$ and maximal $T$-value over $\mathcal{P}_n$ for $\alpha \in (0, +\infty)$.

An interesting problem would be to find the extremal values of $R_\alpha$ for the values of $\alpha$ that do not satisfy the hypothesis of our results.

3 Polyomino chains with minimal atom-bond connectivity index.

We already know by the previous section that the maximal value of the ABC index is the zig-zag chain $Z_n$ (see Figure 1). However the techniques used to show that the linear chain is an extremal value of ABC fails, as we can see in Table 6.

Table 6: Values of linearizing operations on ABC index.

<table>
<thead>
<tr>
<th></th>
<th>$l_1$</th>
<th>$l_2$</th>
<th>$l_3$</th>
<th>$l_4$</th>
<th>$l_5$</th>
<th>$l_6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABC</td>
<td>.004</td>
<td>-.017</td>
<td>.016</td>
<td>-.005</td>
<td>-.027</td>
<td>-.048</td>
</tr>
</tbody>
</table>

In fact, note that

$$10.927 = ABC \left( \begin{array}{c|c} \hline \ 1 \ 3 \\ \hline \ 1 \\ \hline \end{array} \right) < ABC \left( \begin{array}{c|c} \hline \ 2 \ 3 \\ \hline \ 2 \\ \hline \end{array} \right) = 12.243$$

so the linear chain is not the minimal value of ABC over $\mathcal{P}_5$.

The main result in this section shows that the zig-zag chain $Z_3^n$ of segments of length 3 (see Figure 2) is the minimal value of the ABC over $\mathcal{P}_n$. More generally, we give conditions on the number $\{\varphi_{ij}\}$ under which $Z_3^n$ is an extremal value of the induced $T$ defined by (1).

Lemma 3.1 Let $T$ be a topological index induced by $\{\varphi_{ij}\}$ such that $l_1 \geq 0$, $l_3 \geq 0$ and $l_i \leq 0$ for $i = 2, 4, 5$ and 6. Then for each $P \in \mathcal{P}_n$ ($n \geq 5$) there exists $Q \in \mathcal{P}_n$ such that the first segment of $Q$ has length 3 and $T(P) \geq T(Q)$. 
**Proof.** Clearly, $P = U_1$ or $P = U_2$ as in Figure 3.
Assume first that $P = U_1$. We consider the different possibilities for $|L|$.

a) $|L| = 0$. Since $l_2 \leq 0$ and $l_4 \leq 0$ then by (2)

$$T\left(\begin{array}{c} x \end{array}\right) \geq T\left(\begin{array}{c} \circ \end{array}\right)$$

If $\begin{array}{c} \circ \end{array} = \begin{array}{c} \circ \end{array}$ then again by (2)

$$T\left(\begin{array}{c} x \end{array}\right) = T\left(\begin{array}{c} \circ \end{array}\right) \geq T\left(\begin{array}{c} \circ \end{array}\right)$$

since $l_1 \geq 0$ and $l_3 \geq 0$, and we are done.

Otherwise $\begin{array}{c} x \end{array}$ is of the form $\begin{array}{c} \circ \end{array}$ or $\begin{array}{c} \circ \end{array}$. In the first case, bearing in mind that $l_5 \leq 0$ and $l_6 \leq 0$ we deduce by (3)

$$T\left(\begin{array}{c} x \end{array}\right) = T\left(\begin{array}{c} \circ \end{array}\right) \geq T\left(\begin{array}{c} \circ \end{array}\right) \geq T\left(\begin{array}{c} \circ \end{array}\right)$$

In the latter case clearly

$$T\left(\begin{array}{c} x \end{array}\right) = T\left(\begin{array}{c} \circ \end{array}\right) = T\left(\begin{array}{c} \circ \end{array}\right)$$

b) $|L| = 1$. Then $P$ already has its first segment of length 3.

c) $|L| = 2$. Then $P = \begin{array}{c} \circ \end{array}$ and clearly

$$T\left(\begin{array}{c} \circ \end{array}\right) = T\left(\begin{array}{c} \circ \end{array}\right)$$

d) $|L| \geq 3$. Then clearly $P$ is of the form $\begin{array}{c} \circ \end{array}$ and since $l_1 \geq 0$ and $l_3 \geq 0$ then by (2)

$$T(P) \geq T\left(\begin{array}{c} \circ \end{array}\right)$$
Next we assume that $P = U_2$.

a’) $|L| = 0$. Since $l_5 \leq 0$ and $l_6 \leq 0$ then by (3)

$$T \left( \begin{array}{c}
  \text{x} \\
  \text{x}
\end{array} \right) \geq T \left( \begin{array}{c}
  \text{x} \\
  \text{x}
\end{array} \right)$$

b’) $|L| = 1$. In this case $P$ already has its first segment of length 3.

c’) $|L| = 2$. Then $P$ is of the form

$$\begin{array}{c}
  \text{x} \\
  \text{x}
\end{array}$$

Since $l_5 \leq 0$ and $l_6 \leq 0$ then by (3)

$$T \left( \begin{array}{c}
  \text{x} \\
  \text{x}
\end{array} \right) \geq T \left( \begin{array}{c}
  \text{x} \\
  \text{x}
\end{array} \right)$$

Now

$$\begin{array}{c}
  \text{x} \\
  \text{x}
\end{array}$$

and since $l_1 \geq 0$ and $l_3 \geq 0$ we deduce by (2)

$$T \left( \begin{array}{c}
  \text{x} \\
  \text{x}
\end{array} \right) = T \left( \begin{array}{c}
  \text{x} \\
  \text{x}
\end{array} \right) \geq T \left( \begin{array}{c}
  \text{x} \\
  \text{x}
\end{array} \right)$$

d’) $|L| \geq 3$. Similar to the case d).

Note that the ABC index satisfies the hypothesis of Lemma 3.1 (see Table 6).

In our next results we introduce several transformations of polyomino chains that preserve order relations with respect to a VDB topological index $T$ induced by $\{\varphi_{ij}\}$. The following numbers will be used in the sequel

$$z_1 = 2\varphi_{33} + 2\varphi_{34} - 2\varphi_{24} - 2\varphi_{44}$$
$$z_2 = 2\varphi_{44} + 2\varphi_{23} - 4\varphi_{33}$$
$$z_3 = \varphi_{44} + \varphi_{33} - 2\varphi_{34}$$
$$z_4 = 2\varphi_{23} + 4\varphi_{34} - 6\varphi_{33}$$

and the following polyomino chains will appear in the process:
In general, $S_k$ is the coalescence of $S_{k-1}$ with $\square$ for $k \geq 2$. In our next results $S = S_k$ for some $k \geq 2$.

**Lemma 3.2** Let $T$ be a VDB topological index induced by the numbers $\{\varphi_{ij}\}$ such that $l_5 \leq 0$ and $z_1 \leq 0$. Then for each each $P \in \mathcal{P}_n$ of the form $P = \square \square \cdots$ with $|X| \neq 2$, there exists $U \in \mathcal{P}_n$ of the form $U = \square \cdots$ such that $T(P) \geq T(U)$.

**Proof.** Note that $P$ is one of the following polyomino chains:

We will show that $T(V) \geq T(U)$. If we denote by $M_U$ (resp. $M_V$) the set of edges in bold of $U$ (resp. $V$) then there exists a one-to-one correspondence between the set of edges $E(U) \setminus M_U$ and $E(V) \setminus M_V$, in such a way that the degrees of the end vertices of every edge in $E(U) \setminus M_U$ are equal to those of the corresponding edge in $E(V) \setminus M_V$. Since $M_U$ consists of one 23-edge, two 33-edges, two 34-edges, one $3d(u)$-edge and one 3$d(v)$-edge, and $M_V$ consists of one 23-edge, two 24-edges, one 34-edge, one 44-edge, one 3$d(u)$-edge and one 4$d(v)$-edge, then

$$T(U) - T(V) = \left[ \varphi_{23} + 2\varphi_{33} + 2\varphi_{34} + \varphi_{3d(u)} + \varphi_{3d(v)} \right]$$

$$- \left[ \varphi_{23} + 2\varphi_{24} + \varphi_{34} + \varphi_{44} + \varphi_{3d(u)} + \varphi_{4d(v)} \right]$$

$$= 2\varphi_{33} + \varphi_{34} + \varphi_{3d(v)} - 2\varphi_{24} - \varphi_{44} - \varphi_{4d(v)}$$

$$= \begin{cases} l_5 & \text{if } d(v) = 3 \\ z_1 & \text{if } d(v) = 4 \\ 0 & \end{cases}$$

Consequently $T(U) \leq T(V)$.
**Lemma 3.3** Let \( T \) be a VDB topological index induced by the numbers \( \{\varphi_{ij}\} \) such that \( l_3 \geq 0 \), \( z_2 \leq 0 \) and \( z_3 \leq 0 \). Then for each each \( P \in P_n \) of the form \( P \) with \( |X| \neq 2 \), there exists \( U \in P_n \) of the form \( U \) such that \( T(P) \geq T(U) \).

**Proof.** Note that \( P \) is of the form

\[
U = \begin{array}{c}
\includegraphics{image1}
\end{array}
\quad \text{or} \quad
V = \begin{array}{c}
\includegraphics{image2}
\end{array}
\quad \text{or} \quad
W = \begin{array}{c}
\includegraphics{image3}
\end{array}
\]

We will show that \( T(V) \geq T(U) \) and \( T(W) \geq T(U) \). We first compare

\[
U = \begin{array}{c}
\includegraphics{image4}
\end{array}
\quad \text{and} \quad
V = \begin{array}{c}
\includegraphics{image5}
\end{array}
\]

As in the our previous theorem, looking at the edges in bold in \( U \) and \( V \), we conclude that

\[
T(U) - T(V) = \left[ \varphi_{44} + 2\varphi_{34} + 2\varphi_{23} + \varphi_{4d(u)} + \varphi_{3d(v)} \right] - \left[ 4\varphi_{34} + 2\varphi_{23} + \varphi_{4d(u)} + \varphi_{3d(v)} \right]
\]

\[
= \varphi_{44} + 2\varphi_{34} + \varphi_{23} + \varphi_{4d(u)} - 4\varphi_{33} - \varphi_{3d(u)}
\]

\[
= \begin{cases} 
-l_3 & \text{if } d(u) = 3 \\
-3 & \text{if } d(u) = 4 
\end{cases}
\]

Since \( l_3 \geq 0 \) and \( z_2 \leq 0 \) it follows that \( T(U) \leq T(V) \).

On the other hand, comparing

\[
U = \begin{array}{c}
\includegraphics{image6}
\end{array}
\quad \text{and} \quad
W = \begin{array}{c}
\includegraphics{image7}
\end{array}
\]

we deduce

\[
T(U) - T(W) = \left[ \varphi_{44} + 2\varphi_{34} + 2\varphi_{23} + \varphi_{33} + \varphi_{4d(u)} + \varphi_{3d(v)} \right] - \left[ 4\varphi_{34} + 2\varphi_{23} + \varphi_{4d(u)} + \varphi_{3d(v)} \right]
\]

\[
= z_3 \leq 0
\]
Hence $T(U) \leq T(W)$. ■

**Lemma 3.4** Let $T$ be a VDB topological index induced by the numbers $\{\phi_{ij}\}$ such that $l_5 \leq 0$ and $z_1 \leq 0$. Then for each each $P \in \mathcal{P}_n$ of the form $P = \begin{array}{c} S \hline X \end{array}$ with $|X| \neq 2$, there exists $U \in \mathcal{P}_n$ of the form $U = \begin{array}{c} S \hline V \end{array}$ such that $T(P) \geq T(U)$.

**Proof.** We can write $P$ as

$$U = \begin{array}{c} S \hline U \hline V \end{array} 	ext{ or } V = \begin{array}{c} S \hline V \hline U \end{array}$$

Then

$$T(U) - T(V) = \left[ \phi_{23} + 2\phi_{33} + 2\phi_{34} + \phi_{3d(u)} + \phi_{3d(v)} \right]$$

$$- \left[ \phi_{23} + 2\phi_{24} + \phi_{34} + \phi_{44} + \phi_{3d(u)} + \phi_{4d(v)} \right]$$

$$= 2\phi_{33} + \phi_{34} + \phi_{3d(v)} - \phi_{44} - 2\phi_{24} - \phi_{4d(v)}$$

$$= \begin{cases} l_5 & \text{if } d(v) = 3 \\ z_1 & \text{if } d(v) = 4 \end{cases}$$

$$\leq 0$$

Consequently $T(U) \leq T(V)$. ■

**Lemma 3.5** Let $T$ be a VDB topological index induced by the numbers $\{\phi_{ij}\}$ such that $l_3 \geq 0$ and $z_4 \leq 0$. Then for each each $P \in \mathcal{P}_n$ of the form $P = \begin{array}{c} 3 \hline X \end{array}$ with $|X| \neq 2$, there exists $U \in \mathcal{P}_n$ of the form $U = \begin{array}{c} S \hline V \end{array}$ such that $T(P) \geq T(U)$.

**Proof.** We can write $P$ as

$$U = \begin{array}{c} S \hline U \hline V \end{array} 	ext{ or } V = \begin{array}{c} S \hline V \hline U \end{array}$$
Then

\[ T(U) - T(V) = \left[ 3\varphi_{34} + 2\varphi_{23} + \varphi_{3d(u)} + \varphi_{d(v)} \right] - \left[ 5\varphi_{33} + \varphi_{3d(u)} + \varphi_{3d(v)} \right] = 2\varphi_{23} + 3\varphi_{34} + \varphi_{4d(v)} - 5\varphi_{33} - \varphi_{3d(v)} \]

\[ \leq 0 \]

and so \( T(U) \leq T(V). \)

We can now state and prove the main result of this paper.

**Theorem 3.6** Let \( T \) be a VDB topological index induced by the numbers \( \{\varphi_{ij}\} \) such that \( z_i \leq 0 \) for all \( i = 1, 2, 3, 4 \), \( l_i \leq 0 \) for all \( i = 2, 4, 5, 6 \), \( l_1 \geq 0 \) and \( l_3 \geq 0 \). Then the zig-zag chain \( Z^3_n \) of segments of length 3 has minimal value among all polyomino chains in \( \mathcal{P}_n \).

**Proof.** Let \( P \in \mathcal{P}_n \). By Lemma 3.1 there exists a polyomino chain of the form [image] such that

\[ T(P) \geq T\left( \begin{array}{c}
\end{array}\right). \]

Now we apply Lemmas 3.2 - 3.5 to find polyomino chains in \( \mathcal{P}_n \) such that

\[ T(P) \geq T\left( \begin{array}{c}
\end{array}\right) \geq T\left( \begin{array}{c}
\end{array}\right) \geq T\left( \begin{array}{c}
\end{array}\right) \geq T\left( \begin{array}{c}
\end{array}\right) \geq T\left( \begin{array}{c}
\end{array}\right) \]

Note that the last polyomino chain in the previous sequence of inequalities is of the form [image]

Applying Lemmas 3.2 - 3.5 again we find polyomino chains in \( \mathcal{P}_n \) such that

\[ T\left( \begin{array}{c}
\end{array}\right) \geq T\left( \begin{array}{c}
\end{array}\right) \geq T\left( \begin{array}{c}
\end{array}\right) \geq T\left( \begin{array}{c}
\end{array}\right) \geq T\left( \begin{array}{c}
\end{array}\right) \]
Note now that the last polyomino chain in the previous sequence of inequalities is of the form

Continuing this way and bearing in mind that $S_k$ is a polyomino chain with $4k - 2$ squares, we clearly arrive at one of the following four cases:

If $n = 4k - 2$ then $T(P) \geq T \left( \begin{array}{c} S_k \end{array} \right)$ where $|X| = 2$. It is easy to see that

$$T \left( \begin{array}{c} S_k \end{array} \right) - T \left( \begin{array}{c} \circ \end{array} \right) = l_4 \leq 0$$

$$T \left( \begin{array}{c} \circ \end{array} \right) - T \left( \begin{array}{c} S_k \end{array} \right) = z_3 \leq 0$$

Since $\begin{array}{c} S_k \end{array} = Z_3^n$ we obtain $T(P) \geq T(Z_3^n)$.

If $n = 4k - 1$ then $T(P) \geq T \left( \begin{array}{c} \circ \end{array} \right)$ where $|X| = 2$. It is easy to see that

$$T \left( \begin{array}{c} \circ \end{array} \right) - T \left( \begin{array}{c} S_k \end{array} \right) = l_6 \leq 0$$

Since $\begin{array}{c} \circ \end{array} = Z_3^n$ we obtain $T(P) \geq T(Z_3^n)$.

If $n = 4k$ then $T(P) \geq T \left( \begin{array}{c} \circ \end{array} \right)$ where $|X| = 2$. It is easy to see that

$$T \left( \begin{array}{c} \circ \end{array} \right) - T \left( \begin{array}{c} S_k \end{array} \right) = l_2 \leq 0$$
Since $Z_n^3 = Z_n^3$ we obtain $T(P) \geq T(Z_n^3)$. 

If $n = 4k + 1$ then $T(P) \geq T\left(\begin{array}{c}
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Since $Z_n^3 = Z_n^3$ we obtain $T(P) \geq T(Z_n^3)$. 

Dually we can prove the following result by simply reversing all inequalities.

**Theorem 3.7** Let $T$ be a VDB topological index induced by the numbers $\{\varphi_{ij}\}$ such that $z_i \geq 0$ for all $i = 1, 2, 3, 4$, $l_i \geq 0$ for all $i = 2, 4, 5, 6$, $l_1 \leq 0$ and $l_3 \leq 0$. Then the zig-zag chain $Z_n^3$ of segments of length 3 has maximal value among all polyomino chains in $P_n$.

**Example 3.8** The signs of the numbers $l_i$ ($i = 1, \ldots, 6$) and $z_i$ ($i = 1, \ldots, 4$) are given in Table 7 for the ABC index.

<table>
<thead>
<tr>
<th></th>
<th>$l_1$</th>
<th>$l_2$</th>
<th>$l_3$</th>
<th>$l_4$</th>
<th>$l_5$</th>
<th>$l_6$</th>
<th>$z_1$</th>
<th>$z_2$</th>
<th>$z_3$</th>
<th>$z_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABC</td>
<td>+</td>
<td>-</td>
<td>+</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 7: Signs of the numbers $l_1 - l_6$ and $z_1 - z_4$ for the ABC index.

Hence, by Theorem 3.6, $Z_n^3$ has minimal ABC index among all polyomino chains in $P_n$.

Next we determine the values of $\alpha$ where $Z_n^3$ has extremal value of the generalized Randić index $R_\alpha$ over $P_n$. In Table 3 we can see that for $\alpha \in (r_4, -1)$, $l_i(\alpha) \geq 0$ for all $i = 2, 4, 5, 6$, $l_1(\alpha) \leq 0$ and $l_3(\alpha) \leq 0$ where $r_4 \approx -1.23853$. On the other hand, in Table 8 we show the sign of the numbers $z_1 - z_4$ corresponding to $R_\alpha$:

where $\xi_1 \approx -1.84071$ is a root of the equation $z_1(\alpha) = 0$, $\xi_2 \approx -0.72096$ is a root of the equation $z_2(\alpha) = 0$, $-1$ is a root of the equation $z_4(\alpha) = 0$ and $z_i(0) = 0$ for all $i = 1, \ldots, 4$. Note that for $\alpha \in (\xi_1, -1)$, $z_i \geq 0$ for all $i = 1, \ldots, 4$. Since $\xi_1 < r_4$, by Theorem 3.7 we obtain the following result:

**Theorem 3.9** The zigzag chain $Z_n^3$ of segments of length 3 has maximal $R_\alpha$ value among all polyomino chains in $P_n$ for any $\alpha \in (r_4, -1)$.
Table 8: Signs of the numbers $z_1 - z_4$ corresponding to $R_\alpha$

As we mentioned in our previous section, an interesting problem is to determine the extremal value of $R_\alpha$ over $P_n$ for those $\alpha$ that do not satisfy the hypothesis of our results.

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References


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