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Extremal Polyomino Chains of VDB Topological Indices

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Abstract

We show that the zig-zag chain Z_n^3 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 $\{\varphi_{ij}\}$ under which the zig-zag chain Z_n^3 is an extremal value of the induced topological index T defined by

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

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_α over the set of all polyomino chains, for some values of α.

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 QSPR/QSAR 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

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

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 α 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 $\{\varphi_{ij}\}$.

Index	$\{\varphi_{ij}\}$
Randić [14]	$\frac{1}{\sqrt{ij}}$
Sum-connectivity [24]	$\frac{1}{\sqrt{i+j}}$
Harmonic [23]	$\frac{2}{i+j}$
Geometric-Arithmetic [17]	$\frac{2\sqrt{ij}}{i+j}$
First Zagreb [10]	$i+j$
Second Zagreb [10]	ij
Atom-bond-connectivity [4]	$\sqrt{\frac{i+j-2}{ij}}$
Augmented Zagreb [5]	$\left(\frac{ij}{i+j-2}\right)^3$

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 its 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]).

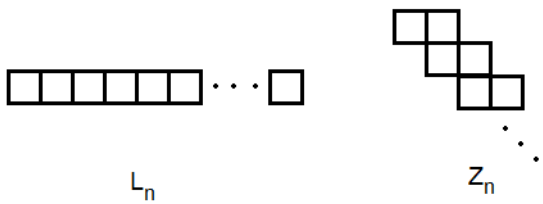


Figure 1: Linear chain L_n and Zig-zag chain Z_n.

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 $\{\varphi_{ij}\}$ 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_n^3 (see Figure 2), has minimal ABC index among all polyomino chains with n squares. Note that for n odd, all the segments of Z_n^3 are of length 3, where as for n even we assume that the last segment of Z_n^3 is of length 4. Actually, we go further and give conditions on the numbers $\{\varphi_{ij}\}$ under which the zig-zag chain Z_n^3 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_n^3 is an extremal value of the general Randić index R_α.

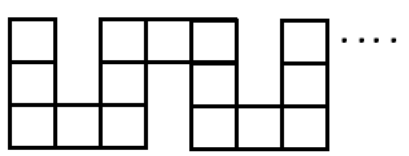


Figure 2: Polyomino chain Z_n^3.

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.

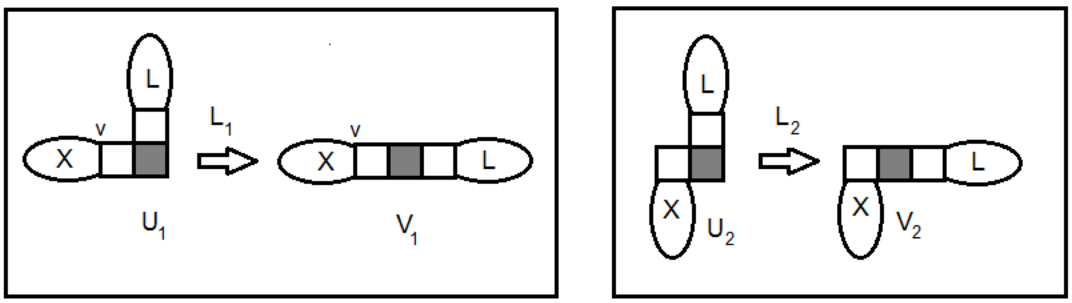


Figure 3: Linear operations over a polyomino chain.

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

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

$$T(V_2)-T(U_2)=\begin{cases} l_5=-2\varphi_{24}+3\varphi_{33}-\varphi_{44} & if \quad |L|\geq 1 \\ l_6=\varphi_{23}-3\varphi_{24}+2\varphi_{33}+\varphi_{34}-\varphi_{44} & if \quad |L|=0 \end{cases} \tag{3}$$

Consequently, if each of the expressions on φ_{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 α where the linear chain has extremal value of the generalized Randić index R_α over $\mathcal{P}_n$. In Table 3 we show the sign of the expressions on R_α given in l_1-l_6 for each value of α:

	l_1	l_2	l_3	l_4	l_5	l_6
Randić	.029	.039	.023	.033	.043	.053
Sum-connectivity	.043	.052	.037	.046	.055	.063
Harmonic	.057	.076	.045	.064	.083	.102
Geometric-arithmetic	.081	.108,	.061	.088	.114	.141
First Zagreb	−2	−2	−2	−2	−2	−2
Second Zagreb	−6	−5	−7	−6	−5	−4

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

α	l_1	l_2	l_3	l_4	l_5	l_6
$(-\infty, r_5)$	−	−	−	−	−	+
(r_5, r_2)	−	−	−	−	+	+
(r_2, r_4)	−	+	−	−	+	+
$(r_4, -1)$	−	+	−	+	+	+
$(-1, r_3)$	+	−	+	+	+	+
$(r_3, 0)$	+	+	+	+	+	+
$(0, +\infty)$	−	−	−	−	−	−

Table 3: Signs of linearizing operations on R_α.

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 $l_2(\alpha) = 0$, $r_4 \approx -1.23853$ 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 $\mathcal{P}_n$ for $\alpha \in (r_3, 0)$ and minimal T-value over $\mathcal{P}_n$ 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]:

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

$$T(V_4) - T(U_4) = \begin{cases} a_3 = -2\varphi_{23} + 4\varphi_{24} - \varphi_{33} - 2\varphi_{34} + \varphi_{44} & if \quad |Z| \geq 1 \\ -\varphi_{23} + 3\varphi_{24} - 2\varphi_{33} - \varphi_{34} + \varphi_{44} & if \quad |Z| = 0 \end{cases} \tag{5}$$

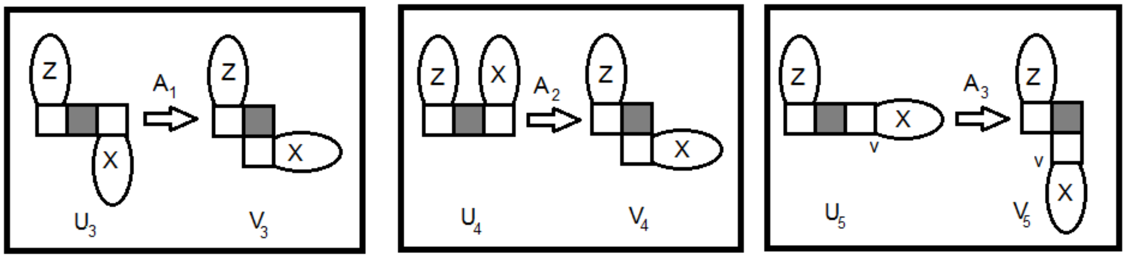


Figure 4: Angular operations over a polyomino chain.

$$T(V_5)-T(U_5)=\begin{cases} a_4=2\varphi_{24}-3\varphi_{33}+\varphi_{44} & if \quad |Z|\geq 1,\ d(v)=3\\ a_5=\varphi_{23}+\varphi_{24}-5\varphi_{33}+3\varphi_{34} & if \quad |Z|=0,\ d(v)=3\\ a_6=2\varphi_{24}-2\varphi_{33}-2\varphi_{34}+2\varphi_{44} & if \quad |Z|\geq 1,\ d(v)=4\\ a_7=\varphi_{23}+\varphi_{24}-4\varphi_{33}+\varphi_{34}+\varphi_{44} & if \quad |Z|=0,\ d(v)=4 \end{cases} \tag{6}$$

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 φ_{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 $\mathcal{P}_n$ [13]. Table 4 illustrates when the zig-zag chain is an extremal value of important VDB topological indices over $\mathcal{P}_n$.

	a_1	a_2	a_3	a_4	a_5	a_6	a_7
Randić	$-.057$	$-.053$	$-.063$	$-.043$	$-.039$	$-.037$	$-.033$
Sum-connectivity	$-.066$	$-.063$	$-.072$	$-.055$	$-.052$	$-.049$	$-.046$
Harmonic	$-.109$	$-.102$	$-.121$	$-.083$	$-.076$	-071	$-.064$
Geometric-arithmmetic	$-.147$	$-.141$	$-.168$	$-.114$	$-.108$	$-.094$	$-.088$
First Zagreb	2	2	2	2	2	2	2
Second Zagreb	4	4	3	5	5	6	6
ABC	.057	.048	.069	.027	.017	.015	.005

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

Next we determine certain values of α where the zig-zag chain has extremal value of the generalized Randić index R_α over $\mathcal{P}_n$. In Table 5 we show the sign of the expressions on R_α given in a_1-a_7 for each value of α:
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:

α	a_1	a_2	a_3	a_4	a_5	a_6	a_7
$(-\infty, t_4)$	$-$	$-$	$-$	$+$	$+$	$+$	$+$
(t_4, t_6)	$-$	$-$	$-$	$-$	$+$	$+$	$+$
(t_6, t_5)	$-$	$-$	$-$	$-$	$+$	$-$	$+$
(t_5, t_7)	$-$	$-$	$-$	$-$	$-$	$-$	$+$
$(t_7, 0)$	$-$	$-$	$-$	$-$	$-$	$-$	$-$
$(0, +\infty)$	$+$	$+$	$+$	$+$	$+$	$+$	$+$

Table 5: Signs of angularizing operations on R_α.

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_α for the values of α that do not satisfy the hypothesis of our results.

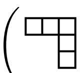
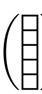
3 Polyomino chains with minimal atom-bond connectivity index.

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.

	l_1	l_2	l_3	l_4	l_5	l_6
ABC	.004	$-.017$	.016	$-.005$	$-.027$	$-.048$

Table 6: Values of linearizing operations on ABC index.

In fact, note that

$10.927 = ABC\,($  $) < ABC\,($  $) = 12.243$

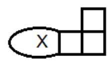
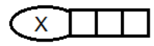
so the linear chain is not the minimal value of ABC over $\mathcal{P}_5$.

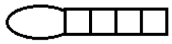
The main result in this section shows that the zig-zag chain Z_n^3 of segments of length 3 (see Figure 2) is the minimal value of the ABC over $\mathcal{P}_n$. More generally, we give conditions on the number $\{\varphi_{ij}\}$ under which Z_n^3 is an extremal value of the induced T defined by (1).

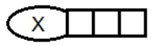
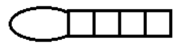
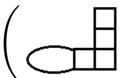
Lemma 3.1 *Let T be a topological index induced by $\{\varphi_{ij}\}$ such that $l_1 \geq 0$, $l_3 \geq 0$ and $l_i \leq 0$ for $i = 2, 4, 5$ and 6. Then for each $P \in \mathcal{P}_n$ $(n \geq 5)$ there exists $Q \in \mathcal{P}_n$ such that the first segment of Q has length 3 and $T(P) \geq T(Q)$.*

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 $|L|$.

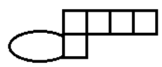
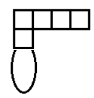
a) $|L| = 0$. Since $l_2 \leq 0$ and $l_4 \leq 0$ then by (2)

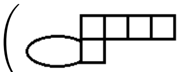
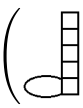
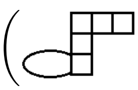
$T\Big($  $\Big) \geq T\Big($  $\Big)$

If  =  then again by (2)

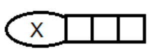
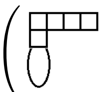
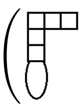
$T\Big($  $\Big) = T\Big($  $\Big) \geq T\Big($  $\Big)$

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

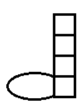
Otherwise  is of the form  or . In the first case, bearing in mind that $l_5 \leq 0$ and $l_6 \leq 0$ we deduce by (3)

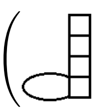
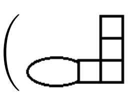
$T\Big($  $\Big) = T\Big($  $\Big) \geq T\Big($  $\Big) \geq T\Big($  $\Big)$

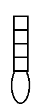
In the latter case clearly

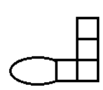
$T\Big($  $\Big) = T\Big($  $\Big) = T\Big($  $\Big)$

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

c) $|L| = 2$. Then $P =$  and clearly

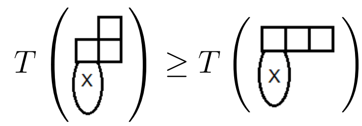
$T\Big($  $\Big) = T\Big($  $\Big)$

d) $|L| \geq 3$. Then clearly P is of the form  and since $l_1 \geq 0$ and $l_3 \geq 0$ then by (2)

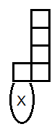
$T(P) \geq T\Big($  $\Big)$

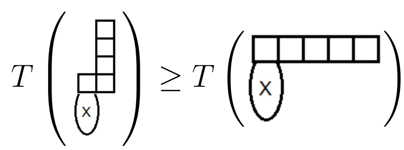
Next we assume that $P = U_2$.

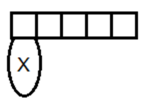
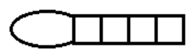
a') $|L| = 0$. Since $l_5 \leq 0$ and $l_6 \leq 0$ then by (3)

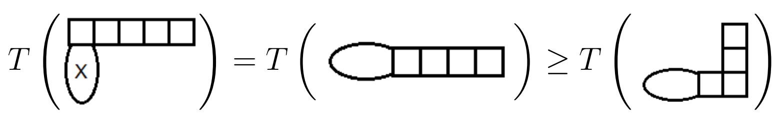


b') $|L| = 1$. In this case P already has its first segment of length 3.

c') $|L| = 2$. Then P is of the form . Since $l_5 \leq 0$ and $l_6 \leq 0$ then by (3)



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



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

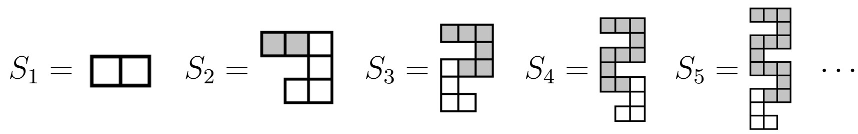
■

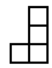
Note that the ABC index satisfies the hypothesis of Lemma 3.1 (see Table 6).

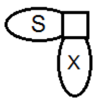
In our next results we introduce several transformations of polyomino chains that preserve order relations with respect to a VDB topological index T induced by $\{\varphi_{ij}\}$. The following numbers will be used in the sequel

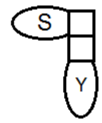
$$\begin{aligned} z_1 &= 2\varphi_{33} + 2\varphi_{34} - 2\varphi_{24} - 2\varphi_{44} \\ z_2 &= 2\varphi_{44} + 2\varphi_{23} - 4\varphi_{33} \\ z_3 &= \varphi_{44} + \varphi_{33} - 2\varphi_{34} \\ z_4 &= 2\varphi_{23} + 4\varphi_{34} - 6\varphi_{33} \end{aligned}$$

and the following polyomino chains will appear in the process:



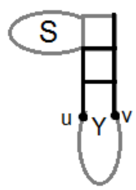
In general, S_k is the coalescence of S_{k-1} with  for $k \geq 2$. In our next results $S = S_k$ for some $k \geq 2$.

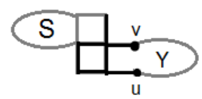
Lemma 3.2 *Let T be a VDB topological index induced by the numbers $\{\varphi_{ij}\}$ such that $l_5 \leq 0$ and $z_1 \leq 0$. Then for each each $P \in \mathcal{P}_n$ of the form $P =$* 

with $|X| \neq 2$, there exists $U \in \mathcal{P}_n$ of the form $U =$ 

such that $T(P) \geq T(U)$.

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

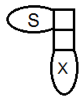
$U =$ 

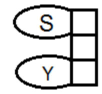
or $V =$ 

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 $3d(v)$-edge, and M_V consists of one 23-edge, two 24-edges, one 34-edge, one 44-edge, one $3d(u)$-edge and one $4d(v)$-edge, then

$$\begin{aligned} T(U) - T(V) &= \left[\varphi_{23} + 2\varphi_{33} + 2\varphi_{34} + \varphi_{3d(u)} + \varphi_{3d(v)}\right] \\ &\quad - \left[\varphi_{23} + 2\varphi_{24} + \varphi_{34} + \varphi_{44} + \varphi_{3d(u)} + \varphi_{4d(v)}\right] \\ &= 2\varphi_{33} + \varphi_{34} + \varphi_{3d(v)} - 2\varphi_{24} - \varphi_{44} - \varphi_{4d(v)} \\ &= \begin{cases} l_5 & \text{if} \quad d(v) = 3 \\ z_1 & \text{if} \quad d(v) = 4 \end{cases} \\ &\leq 0 \end{aligned}$$

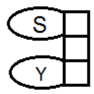
Consequently $T(U) \leq T(V)$. ■

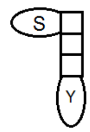
Lemma 3.3 *Let T be a VDB topological index induced by the numbers $\{\varphi_{ij}\}$ such that $l_3 \geq 0$, $z_2 \leq 0$ and $z_3 \leq 0$. Then for each each $P \in \mathcal{P}_n$ of the form $P =$* 

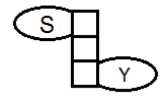
with $|X| \neq 2$, there exists $U \in \mathcal{P}_n$ of the form $U =$ 

such that $T(P) \geq T(U)$.

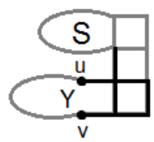
Proof. Note that P is of the form

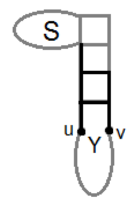
$U =$ 

or $V =$ 

or $W =$ 

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

$U =$ 

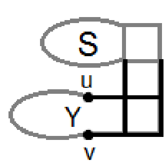
and $V =$ 

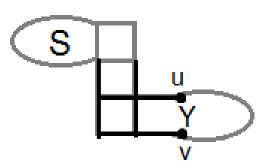
As in the our previous theorem, looking at the edges in bold in U and V, we conclude that

$$\begin{aligned} T(U) - T(V) &= \left[\varphi_{44} + 2\varphi_{34} + 2\varphi_{23} + \varphi_{4d(u)} + \varphi_{3d(v)}\right] \\ &\quad - \left[\varphi_{34} + 4\varphi_{33} + \varphi_{3d(u)} + \varphi_{3d(v)}\right] \\ &= \varphi_{44} + 2\varphi_{23} + \varphi_{34} + \varphi_{4d(u)} - 4\varphi_{33} - \varphi_{3d(u)} \\ &= \begin{cases} -l_3 & \text{if } \; d(u) = 3 \\ z_2 & \text{if } \; d(u) = 4 \end{cases} \end{aligned}$$

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

On the other hand, comparing

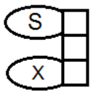
$U =$ 

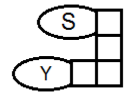
and $W =$ 

we deduce

$$\begin{aligned} T(U) - T(W) &= \left[\varphi_{44} + 2\varphi_{34} + 2\varphi_{23} + \varphi_{33} + \varphi_{4d(u)} + \varphi_{3d(v)}\right] \\ &\quad - \left[4\varphi_{34} + 2\varphi_{23} + \varphi_{4d(u)} + \varphi_{3d(v)}\right] \\ &= z_3 \leq 0 \end{aligned}$$

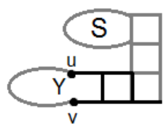
Hence $T(U) \leq T(W)$. ■

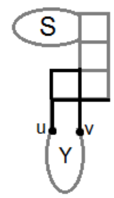
Lemma 3.4 *Let T be a VDB topological index induced by the numbers $\{\varphi_{ij}\}$ such that $l_5 \leq 0$ and $z_1 \leq 0$. Then for each each $P \in \mathcal{P}_n$ of the form $P =$* 

with $|X| \neq 2$, there exists $U \in \mathcal{P}_n$ of the form $U =$ 

such that $T(P) \geq T(U)$.

Proof. We can write P as

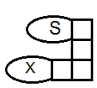
$U =$ 

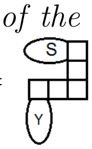
or $V =$ 

Then

$$\begin{aligned} T(U) - T(V) &= \left[\varphi_{23} + 2\varphi_{33} + 2\varphi_{34} + \varphi_{3d(u)} + \varphi_{3d(v)}\right] \\ &\quad - \left[\varphi_{23} + 2\varphi_{24} + \varphi_{34} + \varphi_{44} + \varphi_{3d(u)} + \varphi_{4d(v)}\right] \\ &= 2\varphi_{33} + \varphi_{34} + \varphi_{3d(v)} - \varphi_{44} - 2\varphi_{24} - \varphi_{4d(v)} \\ &= \begin{cases} l_5 & \text{if } d(v) = 3 \\ z_1 & \text{if } d(v) = 4 \end{cases} \\ &\leq 0 \end{aligned}$$

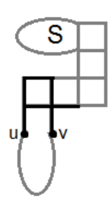
Consequently $T(U) \leq T(V)$. ■

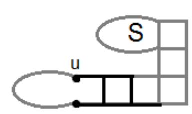
Lemma 3.5 *Let T be a VDB topological index induced by the numbers $\{\varphi_{ij}\}$ such that $l_3 \geq 0$ and $z_4 \leq 0$. Then for each each $P \in \mathcal{P}_n$ of the form $P =$* 

with $|X| \neq 2$, there exists $U \in \mathcal{P}_n$ of the form $U =$ 

such that $T(P) \geq T(U)$.

Proof. We can write P as

$U =$ 

or $V =$ 

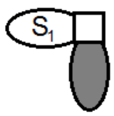
Then

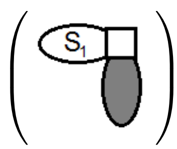
$$\begin{aligned} T(U) - T(V) &= \left[3\varphi_{34} + 2\varphi_{23} + \varphi_{3d(u)} + \varphi_{4d(v)}\right] \\ &\quad - \left[5\varphi_{33} + \varphi_{3d(u)} + \varphi_{3d(v)}\right] \\ &= 2\varphi_{23} + 3\varphi_{34} + \varphi_{4d(v)} - 5\varphi_{33} - \varphi_{3d(v)} \\ &= \begin{cases} z_4 & \text{if } d(v) = 3 \\ -l_3 & \text{if } d(v) = 4 \end{cases} \\ &\leq 0 \end{aligned}$$

and so $T(U) \leq T(V)$. ■

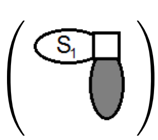
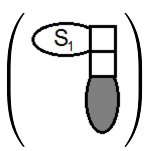
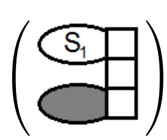
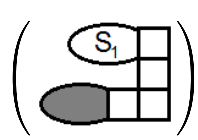
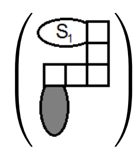
We can now state and prove the main result of this paper.

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_n^3 of segments of length 3 has minimal value among all polyomino chains in $\mathcal{P}_n$.*

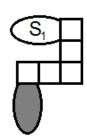
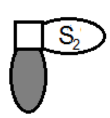
Proof. Let $P \in \mathcal{P}_n$. By Lemma 3.1 there exists a polyomino chain of the form  such that

$T(P) \geq T$  .

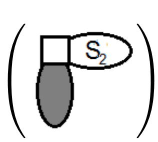
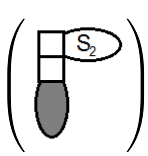
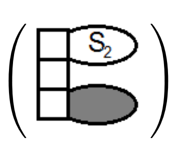
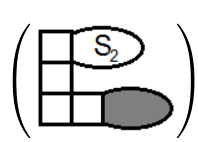
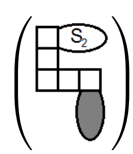
Now we apply Lemmas 3.2 - 3.5 to find polyomino chains in $\mathcal{P}_n$ such that

$T(P) \geq T$  $\geq T$  $\geq T$  $\geq T$  $\geq T$ 

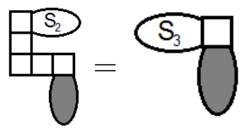
Note that the last polyomino chain in the previous sequence of inequalities is of the form

 $=$ 

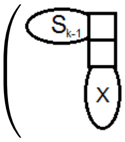
Applying Lemmas 3.2 - 3.5 again we find polyomino chains in $\mathcal{P}_n$ such that

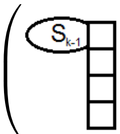
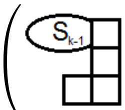
T  $\geq T$  $\geq T$  $\geq T$  $\geq T$ 

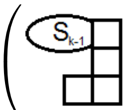
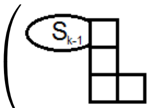
Note now that the last polyomino chain in the previous sequence of inequalities is of the form

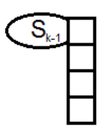


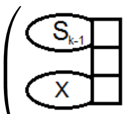
Continuing this way and bearing in mind that S_k is a polyomino chain with $4k-2$ squares, we clearly arrive at one of the following four cases:

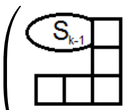
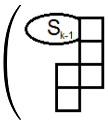
If $n = 4k-2$ then $T(P) \geq T$ () where $|X| = 2$. It is easy to see that

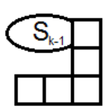
T () $- T$ () $= l_4 \leq 0$

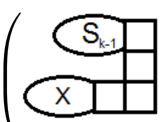
T () $- T$ () $= z_3 \leq 0$

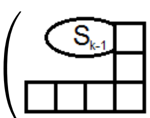
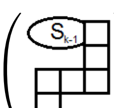
Since  $= Z_n^3$ we obtain $T(P) \geq T(Z_n^3)$.

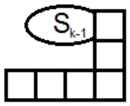
If $n = 4k-1$ then $T(P) \geq T$ () where $|X| = 2$. It is easy to see that

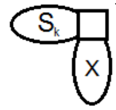
T () $- T$ () $= l_6 \leq 0$

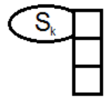
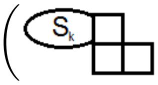
Since  $= Z_n^3$ we obtain $T(P) \geq T(Z_n^3)$.

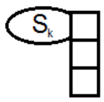
If $n = 4k$ then $T(P) \geq T$ () where $|X| = 2$. It is easy to see that

T () $- T$ () $= l_2 \leq 0$

Since  $= Z_n^3$ we obtain $T\,(P) \geq T\,(Z_n^3)$.

If $n = 4k+1$ then $T(P) \geq T$ () where $|X| = 2$. It is easy to see that

T () $- T$ () $= l_6 \leq 0$

Since  $= Z_n^3$ 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 $\mathcal{P}_n$.*

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.*

	l_1	l_2	l_3	l_4	l_5	l_6	z_1	z_2	z_3	z_4
ABC	$+$	$-$	$+$	$-$	$-$	$-$	$-$	$-$	$-$	$-$

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 $\mathcal{P}_n$.

Next we determine the values of α where Z_n^3 has extremal value of the generalized Randić index R_α over $\mathcal{P}_n$. 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_α:
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_α value among all polyomino chains in $\mathcal{P}_n$ for any $\alpha \in (r_4, -1)$.*

α	z_1	z_2	z_3	z_4
$(-\infty, \xi_1)$	$-$	$+$	$+$	$+$
$(\xi_1, -1)$	$+$	$+$	$+$	$+$
$(-1, \xi_2)$	$+$	$+$	$+$	$-$
$(\xi_2, 0)$	$+$	$-$	$+$	$-$
$(0, +\infty)$	$-$	$+$	$+$	$+$

Table 8: Signs of the numbers $z_1 - z_4$ corresponding to R_α

As we mentioned in our previous section, an interesting problem is to determine the extremal value of R_α over $\mathcal{P}_n$ for those α that do not satisfy the hypothesis of our results.

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