ORDERING CATACONDENSED HEXAGONAL SYSTEMS WITH RESPECT TO VDB TOPOLOGICAL INDICES

ORDENACIÓN DE LOS SISTEMAS HEXAGONALES CATACONDENSADOS CON RESPECTO A LOS ÍNDICES TOPOLÓGICOS VDB

JUAN RADA*

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*Instituto de Matemáticas, Universidad de Antioquia, Medellín, Colombia. E-Mail: pablo.rada@udea.edu.co
Abstract

In this paper we give a complete description of the ordering relations in the set of catacondensed hexagonal systems, with respect to a vertex-degree-based topological index. As a consequence, extremal values of vertex-degree-based topological indices in special subsets of the set of catacondensed hexagonal systems are computed.

Keywords: VDB topological indices; catacondensed hexagonal systems; ordering; extremal values.

1 Introduction

A vertex-degree-based topological index (VDB for short) is denoted by $TI$ and defined from a set of real numbers \{$\varphi_{ij}$\}, for $1 \leq i \leq j \leq n - 1$, as

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

where $G$ is a graph (i.e. undirected graph) with $n$ vertices and $m_{ij} = m_{ij}(G)$ the number of $ij$-edges, i.e. the number of edges in $G$ with end vertices of degree $i$ and $j$ ([1],[10],[18]). When $\varphi_{ij} = \frac{1}{\sqrt{ij}}$ we obtain the Randić index ([20]), one of the most widely used in applications to physical and chemical properties ([3],[12],[13],[21]). For a recent survey on the mathematical properties of the Randić index we refer to ([14],[15]). Due to the success of the Randić index many other topological indices appeared in the mathematical-chemistry literature, which are particular cases of the formula given in (1), as we can see in Table 1.

We will study VDB topological indices over hexagonal systems, natural graph representations of benzenoid hydrocarbons which are of great importance.
in chemistry. For further results on VDB topological indices over hexagonal systems we refer to ([1], [2], [17], [19]). Recall that a hexagonal system is a finite connected plane graph without cut vertices, in which all interior regions are mutually congruent regular hexagons. The inner dual of an hexagonal system $G$, denoted by $ID (G)$, is the graph whose vertices are the hexagons of $G$ and two vertices are adjacent in $ID (G)$, if the correspondent hexagons are adjacent in $G$. A catacondensed hexagonal system (resp. hexagonal chain) is an hexagonal system whose inner dual graph is a tree (resp. a path). The hexagons in a catacondensed system are classified as linear ($L_1$ and $L_2$) or angular ($A_2$ and $A_3$), according to the number and position of edges shared with the adjacent hexagons (See Figure 1). More details on this class of graphs can be found in [9].

### Table 1: Some well-known VDB topological indices.

<table>
<thead>
<tr>
<th>Index</th>
<th>Notation</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Zagreb [7]</td>
<td>$FZ$</td>
<td>$i + j$</td>
</tr>
<tr>
<td>Second Zagreb [7]</td>
<td>$SZ$</td>
<td>$ij$</td>
</tr>
<tr>
<td>Randić [20]</td>
<td>$\chi$</td>
<td>$\frac{1}{\sqrt{ij}}$</td>
</tr>
<tr>
<td>Harmonic [24]</td>
<td>$\mathcal{H}$</td>
<td>$\frac{2}{i+j}$</td>
</tr>
<tr>
<td>Geometric-Arithmetic [22]</td>
<td>$GA$</td>
<td>$\frac{2\sqrt{ij}}{i+j}$</td>
</tr>
<tr>
<td>Sum-Connectivity [23]</td>
<td>$SC$</td>
<td>$\frac{1}{\sqrt{i+j}}$</td>
</tr>
<tr>
<td>Atom-Bond-Connectivity [4]</td>
<td>$ABC$</td>
<td>$\sqrt{i+j-2}$</td>
</tr>
<tr>
<td>Augmented Zagreb [5]</td>
<td>$AZ$</td>
<td>$\left(\frac{ij}{i+j-2}\right)^3$</td>
</tr>
</tbody>
</table>

In this paper we give a complete description of the order relation in the set of catacondensed hexagonal systems with respect to a VDB topological index $TI$. As a consequence, extremal values of $TI$ in special subsets of the set of of catacondensed hexagonal systems with a fixed number of hexagons are computed.
2 Ordering catacondensed hexagonal systems induced by VDB topological indices

We denote by \( CH_h \) the set of catacondensed hexagonal systems with \( h \) hexagons. Since every \( W \in CH_h \) has only vertices of degree 2 and 3, a topological index \( TI \) defined from the numbers \( \{ \varphi_{ij} \} \) as in (1) can be expressed as

\[
TI(W) = m_{22}\varphi_{22} + m_{23}\varphi_{23} + m_{33}\varphi_{33}.
\]

(2)

From now on we denote by \( a_2(W), a_3(W), l_1(W) \) and \( l_2(W) \) the number of \( A_2, A_3, L_1 \) and \( L_2 \) hexagons \( W \) has, respectively. If it is clear from the context we just write \( a_2, a_3, l_1 \) and \( l_2 \).

Lemma 2.1 Let \( W \in CH_h \). Then

\[
\begin{align*}
    m_{22} &= a_2 + 3a_3 + 6 \\
    m_{23} &= 4(h - 1) - 2a_2 - 6a_3 \\
    m_{33} &= h - 1 + 3a_3 + a_2.
\end{align*}
\]

Proof. The following relations are well-known [8]

\[
\begin{align*}
    m_{22} &= a_2 + 3a_3 + 6 \\
    m_{23} &= 4l_1 + 4l_2 + 2a_2 - 2a_3 - 4 \\
    m_{33} &= l_1 + l_2 + 2a_2 + 4a_3 - 1.
\end{align*}
\]

(3)

Since

\[
\begin{align*}
    l_1 &= a_3 + 2 \\
    h &= l_1 + l_2 + a_2 + a_3
\end{align*}
\]

(4)

we deduce

\[
\begin{align*}
    l_2 &= h - l_1 - a_2 - a_3 \\
    &= h - (a_3 + 2) - a_2 - a_3 \\
    &= h - 2a_3 - a_2 - 2.
\end{align*}
\]

Now substituting the expressions

\[
\begin{align*}
    l_1 &= a_3 + 2 \\
    l_2 &= h - 2a_3 - a_2 - 2
\end{align*}
\]

in (3) gives the result. ■

The following result was shown in [17] using linearizing and unbranching operations over catacondensed hexagonal systems. Now we simplify the proof based on the combinatorial arguments given in Lemma 2.1.
Proposition 2.2 Let $TI$ be a VDB topological index induced by the numbers $\{\varphi_{ij}\}$ and $W \in \mathcal{CH}_h$. Then

$$TI(W) = (\varphi_{22} - 2\varphi_{23} + \varphi_{33})(a_2 + 3a_3) + (4\varphi_{23} + \varphi_{33})h$$
$$+ (6\varphi_{22} - 4\varphi_{23} - \varphi_{33}).$$

Proof. From the expression given in (2) and Lemma 2.1,

$$TI(W) = m_{22}\varphi_{22} + m_{23}\varphi_{23} + m_{33}\varphi_{33}$$
$$= (a_2 + 3a_3 + 6)\varphi_{22} + (4(h - 1) - 2a_2 - 6a_3)\varphi_{23}$$
$$+ (h - 1 + 3a_3 + a_2)\varphi_{33}$$
$$= (\varphi_{22} - 2\varphi_{23} + \varphi_{33})(a_2 + 3a_3) + (4\varphi_{23} + \varphi_{33})h$$
$$+ (6\varphi_{22} - 4\varphi_{23} - \varphi_{33}).$$

Consider the subset of $\mathcal{CH}_h$ denoted by $\mathcal{CH}_{h,p}$ and defined by

$$\mathcal{CH}_{h,p} = \{W \in \mathcal{CH}_h : a_3(W) = p\}.$$

**Figure 1:** Catacondensed hexagonal system and its inner dual graph.

**Example 2.3** The hexagonal system $W$ in Figure 1 belongs to $\mathcal{CH}_{8,2}$. Note that $\mathcal{CH}_{h,0}$ consists of all hexagonal chains with $h$ hexagons. In particular, the linear hexagonal chain $L_h$ and the zig-zag chain $Z_h$ belong to $\mathcal{CH}_{h,0}$ (see Figure 2). The hexagonal system $E_h$ belongs to $\mathcal{CH}_{h,\left\lfloor \frac{1}{2}(h-2) \right\rfloor}$ (see Figure 3).
Lemma 2.4 Let $h \geq 3$ and $W \in CH_h$. Then

$$0 \leq a_3(W) \leq \left\lfloor \frac{1}{2} (h - 2) \right\rfloor.$$  

Moreover, equality on the left is attained in hexagonal chains and the equality on the right is attained in $E_h$ (see Figure 3).

Proof. From the relations given in (4) we deduce

$$a_3 = \frac{1}{2} (h - (a_2 + l_2 + 2)).$$

(5)

If $h$ is even then it follows from (5)

$$a_3 \leq \frac{1}{2} (h - 2)$$

since $a_2 + l_2 \geq 0$. If $h$ is odd then again by (5) $a_2 + l_2 \geq 1$, since $a_2 + l_2 = 0$ implies that $a_3$ is not an integer, a contradiction. Hence

$$a_3 \leq \frac{1}{2} (h - 3).$$
The equality on the left is clear for hexagonal chains. On the other hand, note that
\[ a_2 (E_h) = 0 = l_2 (E_h) \] if \( h \) is even, \( a_2 (E_h) = 1 \) and \( l_2 (E_h) = 0 \) if \( h \) is odd. It follows from (5) that
\[
a_3 (E_h) = \begin{cases} 
\frac{1}{2} (h - 2) & \text{if } h \text{ is even} \\
\frac{1}{2} (h - 3) & \text{if } h \text{ is odd.}
\end{cases}
\]

Lemma 2.5 Let \( h \geq 3 \) and \( 0 \leq p \leq \left\lfloor \frac{1}{2} (h - 2) \right\rfloor \). If \( W \in CH_{h,p} \) then
\[
0 \leq a_2 (W) \leq h - 2(p + 1).
\]

Proof. From relations (4) and the fact that \( l_2 \geq 0 \) we deduce
\[
a_2 = h - 2p - l_2 - 2 \leq h - 2(p + 1). \]

Let us denote by \( CH_{h,p,q} \) the subset of \( CH_{h,p} \) defined as
\[
CH_{h,p,q} = \{ W \in CH_{h,p} : a_2 (W) = q \}
\]
Clearly if \( TI \) is a VDB topological index induced by the numbers \( \{ \varphi_{ij} \} \) then by Proposition 2.2 \( TI \) is constant over \( CH_{h,p,q} \). We will use the notation
\[
TI (CH_{h,p,q}) \leq TI (CH_{h,p',q'})
\]
to indicate that \( TI (U) \leq TI (V) \) for all \( U \in CH_{h,p,q} \) and \( V \in CH_{h,p',q'} \). The following result gives a complete description of the order relations in the set of catacondensed hexagonal systems with respect to a VDB topological index.

Theorem 2.6 Let \( TI \) be a VDB topological index induced by the numbers \( \{ \varphi_{ij} \} \). Let \( h \geq 3 \) and \( 0 \leq p \leq \left\lfloor \frac{1}{2} (h - 2) \right\rfloor \). Assume that \( \varphi_{22} - 2 \varphi_{23} + \varphi_{33} > 0 \). Then
\[
1. TI (CH_{h,p,i}) < TI (CH_{h,p,i+1}) \text{ for all } i = 0, \ldots, h - 2p - 3.
2. TI (CH_{h,p,q}) < TI (CH_{h,p+1,q'}) \text{ if and only if } q' > q - 3.
3. TI (CH_{h,p,q}) = TI (CH_{h,p+1,q'}) \text{ if and only if } q' = q - 3.
\]
Proof. 1. Let $U \in CH_{h,p,i}$ and $V \in CH_{h,p,i+1}$. Then by Proposition 2.2

$$TI(U) = (\varphi_{22} - 2\varphi_{23} + \varphi_{33})(i + 3p) + (4\varphi_{23} + \varphi_{33})h$$
$$+ (6\varphi_{22} - 4\varphi_{23} - \varphi_{33})$$

$$TI(V) = (\varphi_{22} - 2\varphi_{23} + \varphi_{33})(i + 1 + 3p) + (4\varphi_{23} + \varphi_{33})h$$
$$+ (6\varphi_{22} - 4\varphi_{23} - \varphi_{33}).$$

Consequently

$$TI(U) - TI(V) = (\varphi_{22} - 2\varphi_{23} + \varphi_{33})(-1) < 0.$$

2. Let $X \in CH_{h,p,q}$ and $Y \in CH_{h,p+1,q'}$. Then by Proposition 2.2

$$TI(X) = (\varphi_{22} - 2\varphi_{23} + \varphi_{33})(q + 3p) + (4\varphi_{23} + \varphi_{33})h$$
$$+ (6\varphi_{22} - 4\varphi_{23} - \varphi_{33})$$

$$TI(Y) = (\varphi_{22} - 2\varphi_{23} + \varphi_{33})(q' + 3(p + 1)) + (4\varphi_{23} + \varphi_{33})h$$
$$+ (6\varphi_{22} - 4\varphi_{23} - \varphi_{33}).$$

Hence

$$TI(X) - TI(Y) = (\varphi_{22} - 2\varphi_{23} + \varphi_{33})(q - q' - 3) < 0 \quad (6)$$

if and only if $q' > q - 3$.

3. It follows from relation (6). □

Dually we have the following result.
Theorem 2.7 Let $TI$ be a VDB topological index induced by the numbers $\{\varphi_{ij}\}$. Let $h \geq 3$ and $0 \leq p \leq \left\lfloor \frac{1}{2} (h - 2) \right\rfloor$. Assume that $\varphi_{22} - 2\varphi_{23} + \varphi_{33} < 0$. Then

1. $TI(CH_{h,p,i}) > TI(CH_{h,p,i+1})$ for all $i = 0, \ldots, h - 2p - 3$.
2. $TI(CH_{h,p,q}) > TI(CH_{h,p+1,q'})$ if and only if $q' > q - 3$.
3. $TI(CH_{h,p,q}) = TI(CH_{h,p+1,q'})$ if and only if $q' = q - 3$.

Proof. The proof is similar to the proof of Theorem 2.6.

Theorems 2.6 and 2.7 can be nicely illustrated organizing the information in a table. First it is important to notice that a consequence of Lemmas 2.4 and 2.5 is the fact that it is possible to partition the set $CH_h$ of all catacondensed hexagonal systems as a disjoint union

$$CH_h = \bigcup CH_{h,p,q}$$  \hspace{1cm} (7)

where $(p, q)$ runs through the set

$$\{(p, q) \in \mathbb{N} \times \mathbb{N} : 0 \leq p \leq \left\lfloor \frac{1}{2} (h - 2) \right\rfloor \text{ and } 0 \leq q \leq h - 2(p + 1)\}.$$

Example 2.8 We first consider an example when $h$ is even. Assume that $h = 8$. Then by Lemmas 2.4 and 2.5 $0 \leq p \leq 3$ and $0 \leq q \leq 8 - 2(p + 1)$. The partition of $CH_8$ is displayed in the following table:

| CH_{8,0,0} | CH_{8,0,1} | CH_{8,0,2} | CH_{8,0,3} | CH_{8,0,4} | CH_{8,0,5} | CH_{8,0,6} | CH_{8,0,7} | CH_{8,1,0} | CH_{8,1,1} | CH_{8,1,2} | CH_{8,1,3} | CH_{8,1,4} | CH_{8,1,5} | CH_{8,1,6} | CH_{8,1,7} | CH_{8,2,0} | CH_{8,2,1} | CH_{8,2,2} | CH_{8,2,3} | CH_{8,2,4} | CH_{8,2,5} | CH_{8,2,6} | CH_{8,2,7} | CH_{8,3,0} |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|

Theorem 2.6 should be read as follows: if $\varphi_{22} - 2\varphi_{23} + \varphi_{33} > 0$ then moving to the right in any row the value of the topological index $TI$ strictly increases. Moving in the same column the value of $TI$ is constant. Consequently,

1. The minimal value of $TI$ over $CH_8$ is attained in the linear chain $L_8$ since $L_8 \in CH_{8,0,0}$. The maximal value of $TI$ over $CH_8$ is attained in the system $E_8$ since $E_8 \in CH_{8,3,0}$.

2. More generally, there are exactly 10 different values of $TI$ over $CH_8$, being the $i^{th}$-maximal value of $TI$ any hexagonal system which belongs to the $i^{th}$ column of the table above.
3. For each $0 \leq p \leq 3$, the minimal value of $TI$ over the set

$$\bigcup_{0 \leq q \leq 8-2(p+1)} \mathcal{CH}_{8,p,q}$$

is attained in a system belonging to $\mathcal{CH}_{8,p,0}$ and the maximal value in a system belonging to $\mathcal{CH}_{8,p,8-2(p+1)}$. In particular, when $p = 0$ then

$$\bigcup_{0 \leq q \leq 8-2(p+1)} \mathcal{CH}_{8,p,q} = \bigcup_{0 \leq q \leq 6} \mathcal{CH}_{8,0,q}$$

is the set of hexagonal chains with 8 hexagons. So among all hexagonal chains with 8 hexagons, the minimal value of $TI$ is attained in $L_8 \in \mathcal{CH}_{8,0,0}$ and the maximal value in the zig-zag chain $Z_8 \in \mathcal{CH}_{8,0,6}$.

4. Two hexagonal systems $U \in \mathcal{CH}_{8,p,q}$ and $V \in \mathcal{CH}_{8,p',q'}$ in $\mathcal{CH}_8$ have equal $TI$ if and only if $p - p' = 3(q - q')$.

Example 2.9 Assume that $h = 9$. Then by Lemmas 2.4 and 2.5, $0 \leq p \leq 3$ and $0 \leq q \leq 7 - 2p$. The partition of $\mathcal{CH}_9$ is displayed in the following table:

<table>
<thead>
<tr>
<th>$\mathcal{CH}_{9,0,0}$</th>
<th>$\mathcal{CH}_{9,0,1}$</th>
<th>$\mathcal{CH}_{9,0,2}$</th>
<th>$\mathcal{CH}_{9,0,3}$</th>
<th>$\mathcal{CH}_{9,0,4}$</th>
<th>$\mathcal{CH}_{9,0,5}$</th>
<th>$\mathcal{CH}_{9,0,6}$</th>
<th>$\mathcal{CH}_{9,0,7}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathcal{CH}_{9,1,0}$</td>
<td>$\mathcal{CH}_{9,1,1}$</td>
<td>$\mathcal{CH}_{9,1,2}$</td>
<td>$\mathcal{CH}_{9,1,3}$</td>
<td>$\mathcal{CH}_{9,1,4}$</td>
<td>$\mathcal{CH}_{9,1,5}$</td>
<td>$\mathcal{CH}_{9,1,6}$</td>
<td>$\mathcal{CH}_{9,1,7}$</td>
</tr>
<tr>
<td>$\mathcal{CH}_{9,2,0}$</td>
<td>$\mathcal{CH}_{9,2,1}$</td>
<td>$\mathcal{CH}_{9,2,2}$</td>
<td>$\mathcal{CH}_{9,2,3}$</td>
<td>$\mathcal{CH}_{9,2,4}$</td>
<td>$\mathcal{CH}_{9,2,5}$</td>
<td>$\mathcal{CH}_{9,2,6}$</td>
<td>$\mathcal{CH}_{9,2,7}$</td>
</tr>
<tr>
<td>$\mathcal{CH}_{9,3,0}$</td>
<td>$\mathcal{CH}_{9,3,1}$</td>
<td>$\mathcal{CH}_{9,3,2}$</td>
<td>$\mathcal{CH}_{9,3,3}$</td>
<td>$\mathcal{CH}_{9,3,4}$</td>
<td>$\mathcal{CH}_{9,3,5}$</td>
<td>$\mathcal{CH}_{9,3,6}$</td>
<td>$\mathcal{CH}_{9,3,7}$</td>
</tr>
</tbody>
</table>

Theorem 2.7 should be read as follows: if $\varphi_{22} - 2\varphi_{23} + \varphi_{33} < 0$ then moving to the right in any row the value of the topological index $TI$ strictly decreases. Moving in the same column the value of $TI$ is constant. Consequently, a dual statement to the one given in Example 2.8 holds.

In conclusion, for every $h \geq 3$ the information of a VDB topological index $TI$ over $\mathcal{CH}_h$ is completely determined from a table constructed as in Examples 2.8 and 2.9 based on the partition (7) and Theorems 2.6 and 2.7.
Corollary 2.10 Let TI be a VDB topological index induced by the numbers \(\{\varphi_{ij}\}\). If \(\varphi_{22} - 2\varphi_{23} + \varphi_{33} > 0\) (resp. \(\varphi_{22} - 2\varphi_{23} + \varphi_{33} < 0\)) then

1. The minimal value of TI over \(CH_h\) is attained in \(L_h\) (resp. \(E_h\)) and the maximal value in \(E_h\) (resp. \(L_h\)) (17).

2. There are exactly \(h - 1 + \left\lfloor \frac{1}{2} (h - 2) \right\rfloor\) different values of TI over \(CH_h\). The \((i)\)th-maximal (resp. \((i)\)th-minimal) value of TI over \(CH_h\) is attained in a hexagonal system belonging to

\[
\begin{align*}
CH_{h,0,i-1} & \quad \text{if } 1 \leq i \leq h - 1 \\
CH_{h,i-h+1,3h-2i-4} & \quad \text{if } h \leq i \leq h - 1 + \left\lfloor \frac{1}{2} (h - 2) \right\rfloor.
\end{align*}
\]

3. For each \(0 \leq p \leq \left\lfloor \frac{1}{2} (h - 2) \right\rfloor\), the minimal (resp. maximal) value of TI over the set

\[
\bigcup_{0 \leq q \leq h - 2(p+1)} CH_{h,p,q}
\]

is attained in a system belonging to \(CH_{h,p,0}\) and the maximal (resp. minimal) value in a system belonging to \(CH_{h,p,h-2(p+1)}\). In particular, when \(p = 0\) then

\[
\bigcup_{0 \leq q \leq h - 2(p+1)} CH_{h,p,q} = \bigcup_{0 \leq q \leq h - 2} CH_{h,0,q}
\]

is the set of hexagonal chains with \(h\) hexagons. So among all hexagonal chains with \(h\) hexagons, the minimal (resp. maximal) value of TI is attained in \(L_h \in CH_{h,0,0}\) and the maximal (resp. minimal) value in the zig-zag chain \(Z_h \in CH_{h,0,h-2}\).

4. Two hexagonal systems \(U \in CH_{h,p,q}\) and \(V \in CH_{h,p',q'}\) in \(CH_h\) have equal TI if and only if \(p - p' = 3(q - q')\).

Note that in order to apply Corollary 2.10 to a specific VDB topological index TI induced by the numbers \(\{\varphi_{ij}\}\), we first must determine the sign of \(\varphi = \varphi_{22} - 2\varphi_{23} + \varphi_{33}\). Clearly by Proposition 2.2 if \(\varphi = 0\) then TI is constant over \(CH_h\). In the following table we compute the values of \(\varphi\) for the main VDB topological indices:

<table>
<thead>
<tr>
<th></th>
<th>(FZ)</th>
<th>(SZ)</th>
<th>(\chi)</th>
<th>(\mathcal{H})</th>
<th>(\mathcal{G}A)</th>
<th>(SC)</th>
<th>(ABC)</th>
<th>(AZ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\varphi)</td>
<td>0</td>
<td>1</td>
<td>.0168</td>
<td>.0333</td>
<td>.0404</td>
<td>.0138</td>
<td>-.0404</td>
<td>3.3906</td>
</tr>
</tbody>
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References


