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ORDERING CATACONDENSED HEXAGONAL SYSTEMS WITH RESPECT TO VDB TOPOLOGICAL INDICES

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

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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.

Resumen

En este artículo presentamos una descripción completa de la relación de orden en el conjunto de sistemas hexagonales catacondensados, con respecto a un índice topológico basado en los grados de los vértices. Como consecuencia, se determinan los valores extremos de un índice topológico basados en los grados de los vértices en subconjuntos especiales del conjunto de sistemas hexagonales catacondensados.

Palabras clave: índices topológicos VDB; sistemas hexagonales catacondensados; orden; valores extremos.

Mathematics Subject Classification: 05C12, 05C05.

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

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

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 ([11],[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.

Index	**Notation**	φ_{ij}
First Zagreb [7]	$\mathcal{FZ}$	$i+j$
Second Zagreb [7]	$\mathcal{SZ}$	ij
Randić [20]	χ	$\frac{1}{\sqrt{ij}}$
Harmonic [24]	$\mathcal{H}$	$\frac{2}{i+j}$
Geometric-Arithmetic [22]	$\mathcal{GA}$	$\frac{2\sqrt{ij}}{i+j}$
Sum-Connectivity [23]	$\mathcal{SC}$	$\frac{1}{\sqrt{i+j}}$
Atom-Bond-Connectivity [4]	$\mathcal{ABC}$	$\sqrt{\frac{i+j-2}{ij}}$
Augmented Zagreb [5]	$\mathcal{AZ}$	$\left(\frac{ij}{i+j-2}\right)^3$

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 $\mathcal{CH}_h$ the set of catacondensed hexagonal systems with h hexagons. Since every $W \in \mathcal{CH}_h$ 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

$$TI\left(W\right) = m_{22}\varphi_{22} + m_{23}\varphi_{23} + m_{33}\varphi_{33}. \tag{2}$$

From now on we denote by $a_2\left(W\right), a_3\left(W\right), l_1\left(W\right)$ and $l_2\left(W\right)$ 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 $W \in \mathcal{CH}_h$. Then*

$$\begin{aligned} m_{22} &= a_2 + 3a_3 + 6 \\ m_{23} &= 4\left(h-1\right) - 2a_2 - 6a_3 \\ m_{33} &= h - 1 + 3a_3 + a_2. \end{aligned}$$

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

$$\begin{aligned} m_{22} &= a_2 + 3a_3 + 6 \\ m_{23} &= 4l_1 + 4l_2 + 2a_2 - 2a_3 - 4 \\ m_{33} &= l_1 + l_2 + 2a_2 + 4a_3 - 1. \end{aligned} \tag{3}$$

Since

$$\begin{gathered} l_1 = a_3 + 2 \\ h = l_1 + l_2 + a_2 + a_3 \end{gathered} \tag{4}$$

we deduce

$$\begin{aligned} l_2 &= h - l_1 - a_2 - a_3 \\ &= h - \left(a_3 + 2\right) - a_2 - a_3 \\ &= h - 2a_3 - a_2 - 2. \end{aligned}$$

Now substituting the expressions

$$\begin{aligned} l_1 &= a_3 + 2 \\ l_2 &= h - 2a_3 - a_2 - 2 \end{aligned}$$

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,

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

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

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

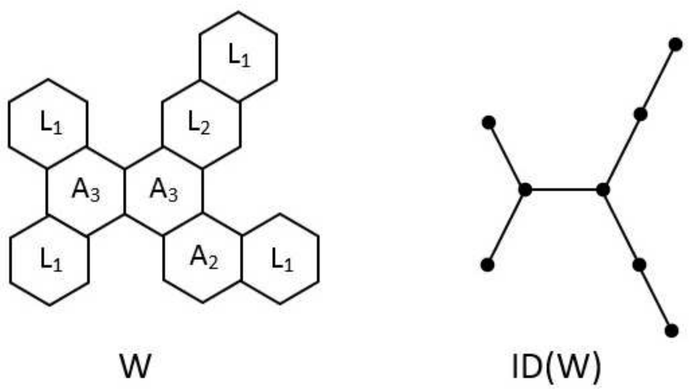

Figure 1: Catacondensed hexagonal system and its inner dual graph.

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 $\mathcal{CH}_{h,\lfloor \frac{1}{2}(h-2) \rfloor}$ (see Figure 3).*

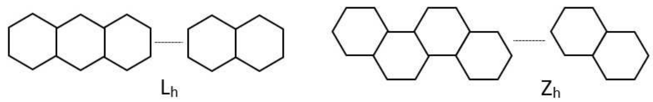

Figure 2: The linear chain L_h and the zig-zag chain Z_h.

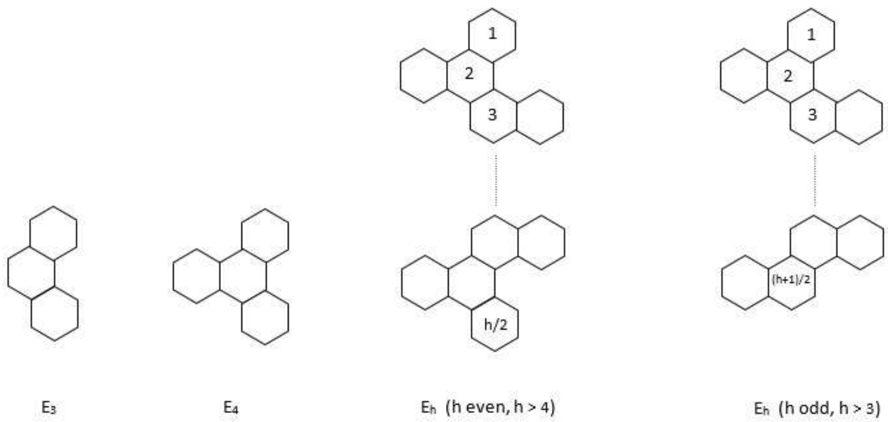

Figure 3: The hexagonal system E_h.

Lemma 2.4 *Let $h \geq 3$ and $W \in \mathcal{CH}_h$. 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

$$a_3 = \frac{1}{2}(h - (a_2 + l_2 + 2)) . \tag{5}$$

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 $W \in \mathcal{CH}_{h,p}$ 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

$$a_2 = h - 2p - l_2 - 2 \leq h - 2(p+1). \blacksquare$$

Let us denote by $\mathcal{CH}_{h,p,q}$ the subset of $\mathcal{CH}_{h,p}$ defined as

$$\mathcal{CH}_{h,p,q} = \{W \in \mathcal{CH}_{h,p} : a_2(W) = q\}$$

Clearly if TI is a VDB topological index induced by the numbers $\{\varphi_{ij}\}$ then by Proposition 2.2, TI is constant over $\mathcal{CH}_{h,p,q}$. We will use the notation

$$TI(\mathcal{CH}_{h,p,q}) \leq TI\left(\mathcal{CH}_{h,p',q'}\right)$$

to indicate that $TI(U) \leq TI(V)$ for all $U \in \mathcal{CH}_{h,p,q}$ and $V \in \mathcal{CH}_{h,p',q'}$. 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. $TI(\mathcal{CH}_{h,p,i}) < TI(\mathcal{CH}_{h,p,i+1})$ *for all* $i = 0, \ldots, h-2p-3$.

2. $TI(\mathcal{CH}_{h,p,q}) < TI\left(\mathcal{CH}_{h,p+1,q'}\right)$ *if and only if* $q' > q-3$.

3. $TI(\mathcal{CH}_{h,p,q}) = TI\left(\mathcal{CH}_{h,p+1,q'}\right)$ *if and only if* $q' = q-3$.

Proof. 1. Let $U \in \mathcal{CH}_{h,p,i}$ and $V \in \mathcal{CH}_{h,p,i+1}$. Then by Proposition 2.2

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

Consequently

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

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

$$\begin{aligned} TI(X) &= (\varphi_{22} - 2\varphi_{23} + \varphi_{33})(q + 3p) + (4\varphi_{23} + \varphi_{33})h \\ &\quad + (6\varphi_{22} - 4\varphi_{23} - \varphi_{33}) \\ TI(Y) &= (\varphi_{22} - 2\varphi_{23} + \varphi_{33})\big(q' + 3(p+1)\big) + (4\varphi_{23} + \varphi_{33})h \\ &\quad + (6\varphi_{22} - 4\varphi_{23} - \varphi_{33}). \end{aligned}$$

Hence

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

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. *$TI(\mathcal{CH}_{h,p,i}) > TI(\mathcal{CH}_{h,p,i+1})$ for all $i = 0, \ldots, h-2p-3$.*
2. *$TI(\mathcal{CH}_{h,p,q}) > TI\left(\mathcal{CH}_{h,p+1,q'}\right)$ if and only if $q' > q-3$.*
3. *$TI(\mathcal{CH}_{h,p,q}) = TI\left(\mathcal{CH}_{h,p+1,q'}\right)$ 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 $\mathcal{CH}_h$ of all catacondensed hexagonal systems as a disjoint union

$$\mathcal{CH}_h = \bigcup \mathcal{CH}_{h,p,q} \tag{7}$$

where (p,q) runs through the set

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

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 $\mathcal{CH}_8$ is displayed in the following table:*

$\mathcal{CH}_{8,0,0}$	$\mathcal{CH}_{8,0,1}$	$\mathcal{CH}_{8,0,2}$	$\mathcal{CH}_{8,0,3}$	$\mathcal{CH}_{8,0,4}$	$\mathcal{CH}_{8,0,5}$	$\mathcal{CH}_{8,0,6}$			
			$\mathcal{CH}_{8,1,0}$	$\mathcal{CH}_{8,1,1}$	$\mathcal{CH}_{8,1,2}$	$\mathcal{CH}_{8,1,3}$	$\mathcal{CH}_{8,1,4}$		
						$\mathcal{CH}_{8,2,0}$	$\mathcal{CH}_{8,2,1}$	$\mathcal{CH}_{8,2,2}$	
									$\mathcal{CH}_{8,3,0}$

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 $\mathcal{CH}_8$ is attained in the linear chain L_8 since $L_8 \in \mathcal{CH}_{8,0,0}$. The maximal value of TI over $\mathcal{CH}_8$ is attained in the system E_8 since $E_8 \in \mathcal{CH}_{8,3,0}$.*
2. *More generally, there are exactly 10 different values of TI over $\mathcal{CH}_8$, 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:*

$\mathcal{CH}_{9,0,0}$	$\mathcal{CH}_{9,0,1}$	$\mathcal{CH}_{9,0,2}$	$\mathcal{CH}_{9,0,3}$	$\mathcal{CH}_{9,0,4}$	$\mathcal{CH}_{9,0,5}$	$\mathcal{CH}_{9,0,6}$	$\mathcal{CH}_{9,0,7}$			
			$\mathcal{CH}_{9,1,0}$	$\mathcal{CH}_{9,1,1}$	$\mathcal{CH}_{9,1,2}$	$\mathcal{CH}_{9,1,3}$	$\mathcal{CH}_{9,1,4}$	$\mathcal{CH}_{9,1,5}$		
						$\mathcal{CH}_{9,2,0}$	$\mathcal{CH}_{9,2,1}$	$\mathcal{CH}_{9,2,2}$	$\mathcal{CH}_{9,2,3}$	
									$\mathcal{CH}_{9,3,0}$	$\mathcal{CH}_{9,3,1}$

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 $\mathcal{CH}_h$ 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 $\mathcal{CH}_h$. The $(i)^{th}$-maximal (resp. $(i)^{th}$-minimal) value of TI over $\mathcal{CH}_h$ is attained in a hexagonal system belonging to*

$$\begin{array}{cc} \mathcal{CH}_{h,0,i-1} & \text{if } 1 \leq i \leq h-1 \\ \mathcal{CH}_{h,i-h+1,3h-2i-4} & \text{if } h \leq i \leq h-1+\left\lfloor \frac{1}{2}(h-2) \right\rfloor. \end{array}$$

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*

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

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

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

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 $L_h \in \mathcal{CH}_{h,0,0}$ and the maximal (resp. minimal) value in the zig-zag chain $Z_h \in \mathcal{CH}_{h,0,h-2}$.

4. *Two hexagonal systems $U \in \mathcal{CH}_{h,p,q}$ and $V \in \mathcal{CH}_{h,p',q'}$ in $\mathcal{CH}_h$ 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 $\mathcal{CH}_h$. In the following table we compute the values of φ for the main VDB topological indices:

	$\mathcal{FZ}$	$\mathcal{SZ}$	χ	$\mathcal{H}$	$\mathcal{GA}$	$\mathcal{SC}$	$\mathcal{ABC}$	$\mathcal{AZ}$
φ	0	1	$.0168$	$.0333$	$.0404$	$.0138$	$-.0404$	3.3906

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