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Research Paper

VDB-Hosoya Index of Hexagonal Chains

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Abstract

Our main interest in this paper is the study of the Hosoya index $Z(G;\varphi)$ of weighted graphs $(G;\varphi)$, when G is a hexagonal chain with weight function induced by a vertex-degree-based topological index φ. Recall that a hexagonal chain is a special type of hexagonal systems, natural graph representations of benzenoid hydrocarbons. On the other hand, vertex-degree based topological indices are (molecular) graph descriptors which play a significant role in chemical graph theory.

Concretely, if G is a hexagonal chain and φ is a vertex-degree-based topological index, we give a method to compute $Z(G;\varphi)$ in terms of products of namely four types of 4×4 matrices associated to φ. As a consequence, under certain conditions on φ, we show that the φ-weighted linear hexagonal chain attains the minimal value of the Hosoya index, among all φ-weighted hexagonal chains.

1 Introduction and preliminaries

Let $(G;\omega)$ be a weighted graph, where $G=(V,E)$ is a graph with vertex set $V=V(G)$ and edge set $E=E(G)$, and $\omega : E \to \mathbb{R}^+$ is a (weight) function. We begin by recalling the concept of k-matching number and Hosoya index of $(G;\omega)$, which was recently introduced in [1]. Given a non-negative integer k, the number of k-matchings of $(G;\omega)$ is denoted by $m((G;\omega),k)$ and it is defined as

$$m((G;\omega),0)=1,$$

and for $k\geq 1$,

$$m\left(\left(G;\omega\right),k\right)=\sum_{U\in\{k\text{-matchings of } G\}}\left[\prod_{u\in U}\omega\left(u\right)\right].$$

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Moreover, the Hosoya index of $(G;\omega)$, denoted as $Z(G;\omega)$, is

$$Z(G;\omega) = \sum_{k\geq 0} m\left((G;\omega), k\right).$$

Clearly, if $\omega(e) = 1$ for all $e \in E(G)$, then we recover the usual concepts of k-matchings and Hosoya index of the underlying graph G [2].

Let $(G;\omega)$ be a weighted graph and H a subgraph of G. We denote by $(H;\omega)$ the weighted graph $\left(H;\omega|_{E(H)}\right)$, where $\omega|_{E(H)}$ is the restriction of ω to $E(H)$. Given an edge uv of G, we denote by $G - uv$ (respectively $G - u$) the graph obtained from G by deleting the edge uv (respectively the vertex u and edges adjacent to it). The following properties of the Hosoya index of a weighted graph hold [1]:

1. If $(G_1;\omega), \ldots, (G_r;\omega)$ are the weighted connected components of the weighted graph $(G;\omega)$, then
$$Z(G;\omega) = \prod_{i=1}^{r} Z(G_i;\omega). \tag{1}$$
2. Let $e = uv$ be an edge of G. Then
$$Z(G;\omega) = Z(G - uv;\omega) + \omega(e)\, Z(G - u - v;\omega). \tag{2}$$
3. If u is an isolated vertex of G then
$$Z(G;\omega) = Z(G - u;\omega). \tag{3}$$

We generalize the Hosoya vector of a graph introduced in [3] to the case of a weighted graph. The Hosoya vector of the weighted graph $(G;\omega)$ at the edge $uv \in E(G)$ is defined as the column vector

$$Z_{uv}(G;\omega) = (Z(G;\omega), Z(G-u;\omega), Z(G-v;\omega), Z(G-u-v;\omega))^{\intercal}.$$

Note that

$$Z_{uv}(G;\omega) = P Z_{vu}(G;\omega),$$

where P is the permutation matrix

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

In case that the weighted graph $(G;\omega)$ is simply an edge st with weight ω_{st}, then the Hosoya vector of $(G;\omega)$ will be denoted by $X_0(\omega)$, and it is clearly given by

$$X_0(\omega) = (1 + \omega_{st}, 1, 1, 1)^{\intercal}.$$

The interest of this study are the weighted graphs $(G;\varphi)$, where G is a hexagonal chain with weight induced by a vertex-degree-based topological index φ. Recall that a hexagonal system is a finite connected planar graph without cut vertices, in which all interior regions are mutually congruent regular hexagons. For more details we refer to [4], and for mathematical properties of degree-based topological indices over hexagonal systems see [5]. A hexagonal chain is a hexagonal system where any hexagon is adjacent to at most two hexagons, in other words, it only has an initial hexagon, linear hexagons, angular hexagons, and a final hexagon. The set of hexagonal chains with h hexagons will be denoted by $\mathcal{C}_h$.

Let $H \in \mathcal{C}_h$ be a hexagonal chain with h hexagons $H_1, H_2, \ldots, H_h$. Consider the sequence of vertices $u, u_1, u_2, \ldots, u_{h-1}, u_h, v_h, v_{h-1} \ldots, v_2, v_1, v$ in H constructed as follow. Let u and v be two adjacent vertices of degree 2 in the initial hexagon, both with no neighbors of degree 3. If one goes along the perimeter of H starting from u and finishing in v, then $u_1, u_2, \ldots, u_{h-1}$ are the vertices of degree 3 belonging to hexagons $H_1, \ldots, H_h$, respectively. The vertices u_h and v_h are of degree 2 in H_h, located at distance 2 and 3 from u_{h-1}, respectively. Furthermore, the vertices $v_{h-1} \ldots, v_2, v_1$ are the vertices of degree 3 belonging to hexagons $H_{h-1}, \ldots, H_1$, respectively.

Note that $u_i v_i \in E(H)$ for $i = 1, \ldots, h$. Moreover, for $i = 2, \ldots, h-1$, H_i is a linear hexagon if $d(u_{i-1}, u_i) = 2$ or an angular hexagon if $d(u_{i-1}, u_i) \in \{1, 3\}$. In Figure 1, a hexagonal chain in $\mathcal{C}_7$ and its sequence of vertices $u_1, \ldots, u_7, v_7, \ldots, v_1$ are depicted. In this hexagonal chain, H_1 is the initial hexagon, H_2 is a linear hexagon, H_3, H_4, H_5 and H_6 are angular hexagons, and H_7 is the final hexagon.

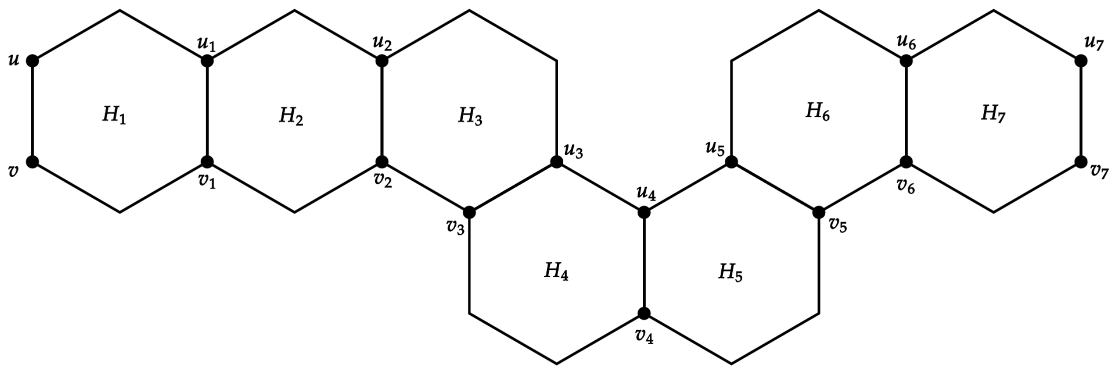

Figure 1: Hexagonal chain in $\mathcal{C}_7$.

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On the other hand, a VDB topological index φ is defined for a graph G as

$$\varphi = \varphi(G) = \sum_{uv \in E} \varphi_{d_G(u), d_G(v)},$$

where $d_G(u)$ denotes the degree of the vertex $u \in G$, and $\varphi_{i,j}$ is a bivariate symmetric function (i.e. $\varphi_{i,j} = \varphi_{j,i}$).

Topological indices are numerical values associated with molecular graphs that correlate chemical structure with physical properties, chemical reactivity, or biological activity, particularly in QSPR/QSAR studies [6, 7]. The best-known VDB topological indices are the following:

1. The First Zagreb index [8], denoted by $\mathcal{FZ}$ and defined as $\varphi_{ij} = i + j$,
2. The Second Zagreb index [8], denoted by $\mathcal{SZ}$ and defined as $\varphi_{ij} = ij$,
3. The Randić index [9], denoted by $\mathcal{R}$ and defined as $\varphi_{ij} = \frac{1}{\sqrt{ij}}$,
4. The Harmonic index [10], denoted by $\mathcal{H}$ and defined as $\varphi_{ij} = \frac{2}{i+j}$,
5. The Geometric-Arithmetic index [11], denoted by $\mathcal{GA}$ and defined as $\varphi_{ij} = \frac{2\sqrt{ij}}{i+j}$,

6. The Sum-Connectivity index [12], denoted by $\mathcal{SC}$ and defined as $\varphi_{ij} = \frac{1}{\sqrt{i+j}}$,
7. The Atom-Bond-Connectivity index [13], denoted by $\mathcal{ABC}$ and defined as $\varphi_{ij} = \sqrt{\frac{i+j-2}{ij}}$,
8. The Augmented Zagreb index [14], denoted by $\mathcal{AZ}$ and defined as $\varphi_{ij} = \left(\frac{ij}{i+j-2}\right)^3$.

The Hosoya index is also a well-known topological invariant with extensive use in chemical graph theory as a molecular descriptor in several QSPR studies [15, 16]. The computation of the Hosoya index of several relevant families of graphs, especially of different classes of benzenoid systems, has recently appeared in the Mathematical Chemistry literature [15, 17–20]. The main subject of our work is the Hosoya index of graphs weighted with a VDB topological index, which can be used as a molecular descriptor resulting from a combination of two important topological indices: the Hosoya index and a vertex-degree-based topological index.

In this paper we give a method to compute the Hosoya index of the weighted graph $(G;\varphi)$, when G is a hexagonal chain with weight induced by a vertex-degree-based topological index φ. Namely, we show that the Hosoya index of $(G;\varphi)$ can be computed in terms of a product of 4×4 matrices associated to the VDB topological index φ, evaluated at a fixed vector X_0 also associated to φ. As a consequence, we solve the extremal value problem of hexagonal chains with minimal VDB-Hosoya index.

2 Hosoya index of weighted hexagonal chains

Our main interest in this section is to study the Hosoya index of weighted hexagonal chains. In order to accomplish this, we show reduction procedures to compute the Hosoya vector of a hexagonal chain.

Proposition 2.1. *Let $(G;\omega)$ be a weighted graph depicted in Figure 2. Then*

$$Z_{uv}(G;\omega) = Q(\omega) Z_{st}(H;\omega),$$

where

$$Q(\omega) = \begin{pmatrix} (1+\omega_{ux})(1+\omega_{vy})+\omega_{uv} & \omega_{xs}(1+\omega_{ux}+\omega_{uv}) & \omega_{yt}(1+\omega_{ux}+\omega_{uv}) & \omega_{yt}\omega_{xs}(1+\omega_{uv}) \\ 1+\omega_{vy} & \omega_{xs}(1+\omega_{vy}) & \omega_{yt} & \omega_{yt}\omega_{xs} \\ 1+\omega_{ux} & \omega_{xs} & \omega_{yt}(1+\omega_{ux}) & \omega_{yt}\omega_{xs} \\ 1 & \omega_{xs} & \omega_{yt} & \omega_{yt}\omega_{xs} \end{pmatrix}.$$

Proof. Deleting the independent edges xs and yt from G (see Figure 2) and using relations (1), (2) and (3) we deduce

$$\begin{aligned} Z(G;\omega) &= Z(G-yt-xs;\omega) + \omega_{xs} Z(G-yt-x-s;\omega) \\ &\quad + \omega_{yt} Z(G-y-t-xs;\omega) + \omega_{yt}\omega_{xs} Z(G-y-t-x-s;\omega) \\ &= [(1+\omega_{ux})(1+\omega_{vy})+\omega_{uv}] Z(H;\omega) + \omega_{xs}(1+\omega_{ux}+\omega_{uv}) Z(H-s;\omega) \\ &\quad + \omega_{yt}(1+\omega_{ux}+\omega_{uv}) Z(H-t;\omega) + \omega_{yt}\omega_{xs}(1+\omega_{uv}) Z(H-s-t;\omega) \\ &= \begin{pmatrix} 1+\omega_{ux}+\omega_{uv}+\omega_{vy}+\omega_{ux}\omega_{vy} \\ \omega_{xs}(1+\omega_{ux}+\omega_{uv}) \\ \omega_{yt}(1+\omega_{ux}+\omega_{uv}) \\ \omega_{yt}\omega_{xs}(1+\omega_{uv}) \end{pmatrix}^{\mathsf{T}} \cdot Z_{st}(H;\omega), \end{aligned}$$

$$
\begin{aligned}
Z(G-u;\omega) &= Z(G-u-yt-xs;\omega)+\omega_{xs}Z(G-u-yt-x-s;\omega)\\
&\quad+\omega_{yt}Z(G-u-y-t-xs;\omega)+\omega_{yt}\omega_{xs}Z(G-u-y-t-x-s;\omega)\\
&=(1+\omega_{vy})Z(H;\omega)+\omega_{xs}(1+\omega_{vy})Z(H-s;\omega)\\
&\quad+\omega_{yt}Z(H-t,\omega)+\omega_{yt}\omega_{xs}Z(H-s-t;\omega)\\
&=(1+\omega_{vy},\omega_{xs}(1+\omega_{vy}),\omega_{yt},\omega_{yt}\omega_{xs})\cdot Z_{st}(H;\omega),
\end{aligned}
$$

$$
\begin{aligned}
Z(G-v;\omega) &= Z(G-v-yt-xs;\omega)+\omega_{xs}Z(G-v-yt-x-s;\omega)\\
&\quad+\omega_{yt}Z(G-v-y-t-xs;\omega)+\omega_{yt}\omega_{xs}Z(G-v-y-t-x-s;\omega)\\
&=(1+\omega_{ux})Z(H;\omega)+\omega_{xs}Z(H-s;\omega)\\
&\quad+\omega_{yt}(1+\omega_{ux})Z(H-t,\omega)+\omega_{yt}\omega_{xs}Z(H-s-t;\omega)\\
&=(1+\omega_{ux},\omega_{xs},\omega_{yt}(1+\omega_{ux}),\omega_{yt}\omega_{xs})\cdot Z_{st}(H;\omega),
\end{aligned}
$$

$$
\begin{aligned}
Z(G-u-v;\omega) &= Z(G-u-v-yt-xs;\omega)+\omega_{xs}Z(G-u-v-yt-x-s;\omega)\\
&\quad+\omega_{yt}Z(G-u-v-y-t-xs;\omega)\\
&\quad+\omega_{yt}\omega_{xs}Z(G-u-v-y-t-x-s;\omega)\\
&=Z(H;\omega)+\omega_{xs}Z(H-s;\omega)+\omega_{yt}Z(H-t;\omega)\\
&\quad+\omega_{yt}\omega_{xs}Z(H-s-t;\omega)\\
&=(1,\omega_{xs},\omega_{yt},\omega_{yt}\omega_{xs})\cdot Z_{st}(H;\omega).
\end{aligned}
$$

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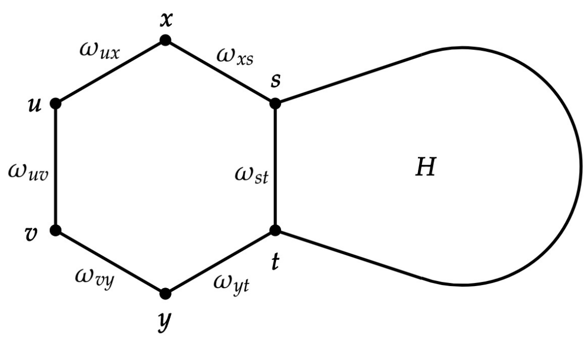

Figure 2: Graph used in Propositions 2.1 and 2.2.

Proposition 2.2. *Let $(G;\omega)$ be the weighted graph depicted in Figure 2. Then*

$$Z_{vy}(G;\omega)=S(\omega)Z_{st}(H;\omega),$$

where

$$
S(\omega)=\begin{pmatrix}
(1+\omega_{vy})(1+\omega_{ux})+\omega_{uv} & \omega_{xs}(1+\omega_{vy}+\omega_{uv}) & \omega_{yt}(1+\omega_{ux}+\omega_{uv}) & \omega_{yt}\omega_{xs}(1+\omega_{uv})\\
1+\omega_{ux} & \omega_{xs} & \omega_{yt}(1+\omega_{ux}) & \omega_{yt}\omega_{xs}\\
1+\omega_{ux}+\omega_{uv} & \omega_{xs}+\omega_{xs}\omega_{uv} & 0 & 0\\
1+\omega_{ux} & \omega_{xs} & 0 & 0
\end{pmatrix}.
$$

Proof. Deleting the independent edges uv, xs and yt from G (see Figure 2) and using relations (1), (2) and (3) we deduce

$$\begin{aligned}
Z(G) &= Z(G-yt-xs-uv;\omega)+\omega_{uv}Z(G-yt-xs-u-v;\omega)\\
&\quad+\omega_{xs}Z(G-yt-uv-x-s;\omega)+\omega_{xs}\omega_{uv}Z(G-yt-x-s-u-v;\omega)\\
&\quad+\omega_{yt}Z(G-xs-uv-y-t;\omega)+\omega_{yt}\omega_{uv}Z(G-xs-y-t-u-v;\omega)\\
&\quad+\omega_{yt}\omega_{xs}Z(G-uv-y-t-x-s;\omega)\\
&\quad+\omega_{yt}\omega_{xs}\omega_{uv}Z(G-y-t-x-s-u-v;\omega)\\
&=[(1+\omega_{vy})(1+\omega_{ux})+\omega_{uv}]Z(H;\omega)+[\omega_{xs}(1+\omega_{vy})+\omega_{xs}\omega_{uv}]Z(H-s;\omega)\\
&\quad+[\omega_{yt}(1+\omega_{ux})+\omega_{yt}\omega_{uv}]Z(H-t;\omega)\\
&\quad+[\omega_{yt}\omega_{xs}+\omega_{yt}\omega_{xs}\omega_{uv}]Z(H-s-t;\omega),
\end{aligned}$$

$$\begin{aligned}
Z(G-v;\omega) &= Z(G-v-yt-xs;\omega)+\omega_{xs}Z(G-v-yt-x-s;\omega)\\
&\quad+\omega_{yt}Z(G-v-xs-y-t;\omega)+\omega_{yt}\omega_{xs}Z(G-v-y-t-x-s;\omega)\\
&=(1+\omega_{ux})Z(H;\omega)+\omega_{xs}Z(H-s;\omega)+\omega_{yt}(1+\omega_{ux})Z(H-t;\omega)\\
&\quad+\omega_{yt}\omega_{xs}Z(H-s-t;\omega),
\end{aligned}$$

$$\begin{aligned}
Z(G-y;\omega) &= Z(G-y-xs-uv;\omega)+\omega_{uv}Z(G-y-xs-u-v;\omega)\\
&\quad+\omega_{xs}Z(G-y-uv-x-s;\omega)+\omega_{xs}\omega_{uv}Z(G-y-x-s-u-v;\omega)\\
&=[(1+\omega_{ux})+\omega_{uv}]Z(H;\omega)+[\omega_{xs}+\omega_{xs}\omega_{uv}]Z(H-s;\omega),
\end{aligned}$$

$$\begin{aligned}
Z(G-v-y;\omega) &= Z(G-v-y-xs;\omega)+\omega_{xs}Z(G-v-y-x-s;\omega)\\
&=(1+\omega_{ux})Z(H;\omega)+\omega_{xs}Z(H-s;\omega).
\end{aligned}$$

∎

From now on we will simply write $Q=Q(\omega), S=S(\omega)$ and $X_0=X_0(\omega)$ if the weight of each edge is clear from the context. Propositions 2.1 and 2.2 can be used to compute the Hosoya index of any weighted hexagonal chain as we illustrate in our next example.

Example 2.3. Let us compute the Hosoya index of the weighted hexagonal chain $(H;\omega)$ shown in Figure 3. For each $j=2,\ldots,6$, we denote by $(H^{(j)};\omega)$ the weighted hexagonal subchain of $(H;\omega)$ which initiates in edge $u_{j-1}v_{j-1}$ and ends in edge u_7v_7. A repeated application of Propositions 2.1 and 2.2 gives

$$\begin{aligned}
Z_{uv}(H;\omega) &= Q_{H_1}Z_{u_1v_1}\left(H^{(2)};\omega\right)=Q_{H_1}Q_{H_2}Z_{u_2v_2}\left(H^{(3)};\omega\right)\\
&= Q_{H_1}Q_{H_2}S_{H_3}Z_{u_3v_3}\left(H^{(4)};\omega\right)=Q_{H_1}Q_{H_2}S_{H_3}PZ_{v_3u_3}\left(H^{(4)};\omega\right)\\
&= Q_{H_1}Q_{H_2}S_{H_3}PS_{H_4}Z_{v_4u_4}\left(H^{(5)};\omega\right)\\
&= Q_{H_1}Q_{H_2}S_{H_3}PS_{H_4}S_{H_5}Z_{v_5u_5}\left(H^{(6)};\omega\right)\\
&= Q_{H_1}Q_{H_2}S_{H_3}PS_{H_4}S_{H_5}PZ_{u_5v_5}\left(H^{(6)};\omega\right)\\
&= Q_{H_1}Q_{H_2}S_{H_3}PS_{H_4}S_{H_5}PS_{H_6}Z_{u_6v_6}\left(H^{(7)};\omega\right)\\
&= Q_{H_1}Q_{H_2}S_{H_3}PS_{H_4}S_{H_5}PS_{H_6}Q_{H_7}X_0,
\end{aligned}$$

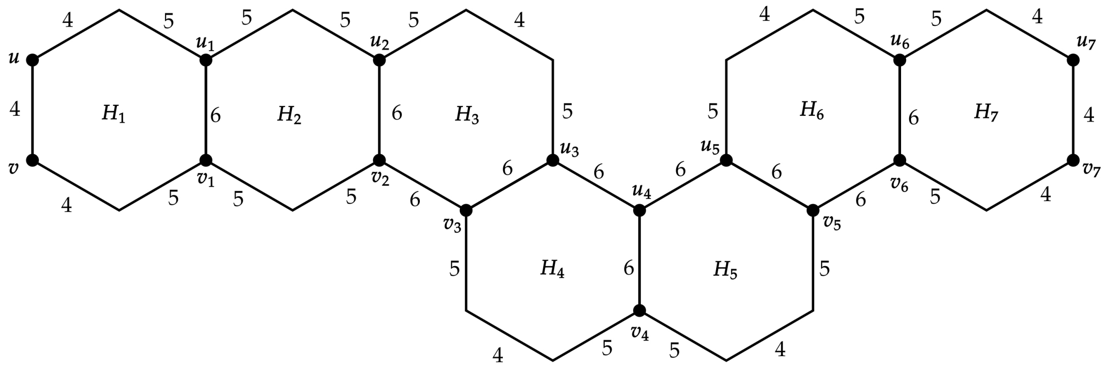

Figure 3: Weighted graph used in Example 2.3.

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where

$$Q_{H_1} = \begin{pmatrix} 29 & 45 & 45 & 125 \\ 5 & 25 & 5 & 25 \\ 5 & 5 & 25 & 25 \\ 1 & 5 & 5 & 25 \end{pmatrix}, Q_{H_2} = \begin{pmatrix} 42 & 60 & 60 & 175 \\ 6 & 30 & 5 & 25 \\ 6 & 5 & 30 & 25 \\ 1 & 5 & 5 & 25 \end{pmatrix}, Q_{H_7} = \begin{pmatrix} 42 & 48 & 48 & 112 \\ 6 & 24 & 4 & 16 \\ 6 & 4 & 24 & 16 \\ 1 & 4 & 4 & 16 \end{pmatrix},$$

$$S_{H_3} = S_{H_4} = S_{H_5} = S_{H_6} = \begin{pmatrix} 40 & 60 & 60 & 180 \\ 5 & 5 & 30 & 30 \\ 10 & 30 & 0 & 0 \\ 5 & 5 & 0 & 0 \end{pmatrix}, X_0 = \begin{pmatrix} 5 \\ 1 \\ 1 \\ 1 \end{pmatrix}.$$

Hence,

$$Z_{u_1v_1}(H;\omega) = (60088205420000, 13540312100000, 13729597100000, 4955396980000)^{\intercal}.$$

In particular, $Z(H;\omega) = 60088205420000$.

3 VDB-Hosoya index of hexagonal chains

We are particularly interested in weighted graphs with a weight function induced by a vertex-degree-based (VDB, for short) topological index. Recall that a VDB topological index φ is defined for a graph G as

$$\varphi = \varphi(G) = \sum_{uv\in E} \varphi_{d_G(u),d_G(v)}\,,$$

where $d_G(u)$ denotes the degree of the vertex $u \in G$, and $\varphi_{i,j}$ is a bivariate symmetric function (i.e. $\varphi_{i,j} = \varphi_{j,i}$). Then we consider the weighted graph $(G;\varphi)$ with weight function $\varphi : E \to \mathbb{R}$ defined as

$$\varphi(uv) = \varphi_{d_G(u),d_G(v)}\,,$$

for all $uv \in E(G)$.

Example 3.1. The weighted hexagonal chain in Figure 3 is an example of a VDB-weighted graph when the VDB topological index φ is the First Zagreb index.

Our main result in this section is to show that if H is a hexagonal chain, then the Hosoya vector of the VDB-weighted graph $(H;\varphi)$ is the evaluation at

$$X_0 = (1+\varphi_{2,2}, 1, 1, 1)^{\intercal},$$

of a product of the following 4×4 matrices:

$$Q_1 = \begin{pmatrix} (1+\varphi_{2,2})^2+\varphi_{2,2} & \varphi_{2,3}(1+2\varphi_{2,2}) & \varphi_{2,3}(1+2\varphi_{2,2}) & \varphi_{2,3}^2(1+\varphi_{2,2}) \\ 1+\varphi_{2,2} & \varphi_{2,3}(1+\varphi_{2,2}) & \varphi_{2,3} & \varphi_{2,3}^2 \\ 1+\varphi_{2,2} & \varphi_{2,3} & \varphi_{2,3}(1+\varphi_{2,2}) & \varphi_{2,3}^2 \\ 1 & \varphi_{2,3} & \varphi_{2,3} & \varphi_{2,3}^2 \end{pmatrix},$$

$$Q_2 = \begin{pmatrix} (1+\varphi_{2,3})^2+\varphi_{3,3} & \varphi_{2,3}(1+\varphi_{2,3}+\varphi_{3,3}) & \varphi_{2,3}(1+\varphi_{2,3}+\varphi_{3,3}) & \varphi_{2,3}^2(1+\varphi_{3,3}) \\ 1+\varphi_{2,3} & \varphi_{2,3}(1+\varphi_{2,3}) & \varphi_{2,3} & \varphi_{2,3}^2 \\ 1+\varphi_{2,3} & \varphi_{2,3} & \varphi_{2,3}(1+\varphi_{2,3}) & \varphi_{2,3}^2 \\ 1 & \varphi_{2,3} & \varphi_{2,3} & \varphi_{2,3}^2 \end{pmatrix},$$

$$Q_3 = \begin{pmatrix} (1+\varphi_{2,3})^2+\varphi_{3,3} & \varphi_{2,2}(1+\varphi_{2,3}+\varphi_{3,3}) & \varphi_{2,2}(1+\varphi_{2,3}+\varphi_{3,3}) & \varphi_{2,2}^2(1+\varphi_{3,3}) \\ 1+\varphi_{2,3} & \varphi_{2,2}(1+\varphi_{2,3}) & \varphi_{2,2} & \varphi_{2,2}^2 \\ 1+\varphi_{2,3} & \varphi_{2,2} & \varphi_{2,2}(1+\varphi_{2,3}) & \varphi_{2,2}^2 \\ 1 & \varphi_{2,2} & \varphi_{2,2} & \varphi_{2,2}^2 \end{pmatrix},$$

and

$$S = \begin{pmatrix} (1+\varphi_{3,3})(1+\varphi_{2,2})+\varphi_{2,3} & \varphi_{2,3}(1+\varphi_{3,3}+\varphi_{2,3}) & \varphi_{3,3}(1+\varphi_{2,2}+\varphi_{2,3}) & \varphi_{3,3}\varphi_{2,3}(1+\varphi_{2,3}) \\ 1+\varphi_{2,2} & \varphi_{2,3} & \varphi_{3,3}(1+\varphi_{2,2}) & \varphi_{3,3}\varphi_{2,3} \\ 1+\varphi_{2,2}+\varphi_{2,3} & \varphi_{2,3}+\varphi_{2,3}^2 & 0 & 0 \\ 1+\varphi_{2,2} & \varphi_{2,3} & 0 & 0 \end{pmatrix}.$$

Theorem 3.2. *Let $H \in \mathcal{C}_r$ and $u, u_1, \dots, u_r, v_r, \dots, v_1, v$ the sequence of vertices of H as described in Section 1. Then,*

$$Z_{uv}(H;\varphi) = Q_1 M_2 \cdots M_{r-1} Q_3 X_0,$$

where

$$M_j = \begin{cases} PSP, & \text{if } \; d(u_{j-1}, u_j) = 1, \\ Q_2, & \text{if } \; d(u_{j-1}, u_j) = 2, \\ S, & \text{if } \; d(u_{j-1}, u_j) = 3, \end{cases}$$

for $j = 2, \dots, r-1$.

Proof. Let $1 \le j \le r$ and $(H^{(j)};\varphi)$ be the weighted subchain of $(H;\varphi)$ starting in the hexagon H_j and finishing in the hexagon H_r. Note that $(H^{(1)};\varphi) = (H;\varphi)$. From Proposition 2.1

$$Z_{uv}(H;\varphi) = Q_1 Z_{u_1 v_1}(H^{(2)};\varphi).$$

If $2 \le j \le r-1$, from Propositions 2.1 and 2.2, we have to consider three cases:

1. If $d(u_{j-1}, u_j) = 1$,

$$Z_{u_{j-1}v_{j-1}}(H^{(j)};\varphi) = PZ_{v_{j-1}u_{j-1}}(H^{(j)};\varphi) = PSZ_{v_j,u_j}(H^{(j+1)};\varphi) = PSPZ_{u_j v_j}(H^{(j+1)};\varphi).$$

2. If $d(u_{j-1}, u_j) = 2$,

$$Z_{u_{j-1}v_{j-1}}(H^{(j)};\varphi) = Q_2 Z_{u_j v_j}(H^{(j+1)};\varphi).$$

3. If $d(u_{j-1}, u_j) = 3$,
$$Z_{u_{j-1}v_{j-1}}(H^{(j)}; \varphi) = SZ_{u_j v_j}(H^{(j+1)}; \varphi).$$

Finally, from Proposition 2.1 we have

$$Z_{u_{r-1}v_{r-1}}(H^{(r)}; \varphi) = Q_3 X_0.$$

Hence,

$$Z_{uv}(H; \varphi) = Q_1 M_2 \cdots M_{r-1} Q_3 X_0,$$

where

$$M_j = \begin{cases} PSP, & \text{if} \quad d(u_{j-1}, u_j) = 1, \\ Q_2, & \text{if} \quad d(u_{j-1}, u_j) = 2, \\ S, & \text{if} \quad d(u_{j-1}, u_j) = 3, \end{cases}$$

for $j = 2, \ldots, r-1$. ■

Example 3.3. Consider the hexagonal chain shown in Figure 1 weighted by a VDB topological index φ. Then, by Theorem 3.2,

$$Z_{uv}(H; \varphi) = Q_1 Q_2 SPSPPSPSQ_3 X_0 = Q_1 Q_2 SPSSPSQ_3 X_0,$$

since P^2 is the identity matrix.

Example 3.4. Consider the zig-zag chain with h hexagons Z_h weighted by a VDB topological index φ (see Figure 4 if h is even and Figure 5 if h is odd). Then, by Theorem 3.2,

$$Z_{uv}(Z_h; \varphi) = \begin{cases} Q_1 (PSPS)^{\frac{h-2}{2}} Q_3 X_0, & \text{if h is even,} \\ \\ Q_1 (PSPS)^{\frac{h-3}{2}} PSPQ_3 X_0, & \text{if h is odd.} \end{cases}$$

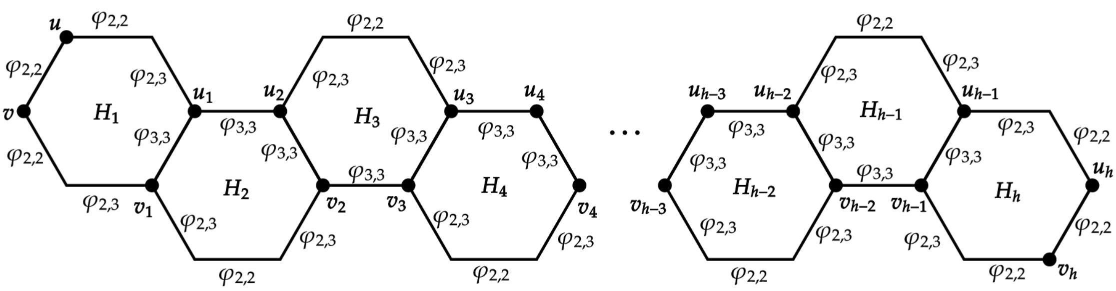

Figure 4: Zig-zag hexagonal chain weighted by a VDB topological index φ for even h.

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Example 3.5. Consider the linear hexagonal chain with h hexagons L_h weighted by a VDB topological index φ (see Figure 6). Then, by Theorem 3.2,

$$Z_{uv}(L_h; \varphi) = Q_1 Q_2^{h-2} Q_3 X_0.$$

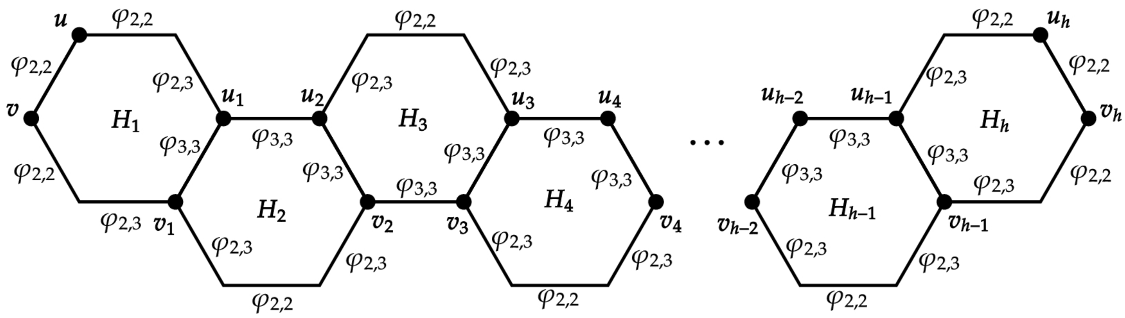

Figure 5: Zig-zag hexagonal chain weighted by a VDB topological index φ for odd h.

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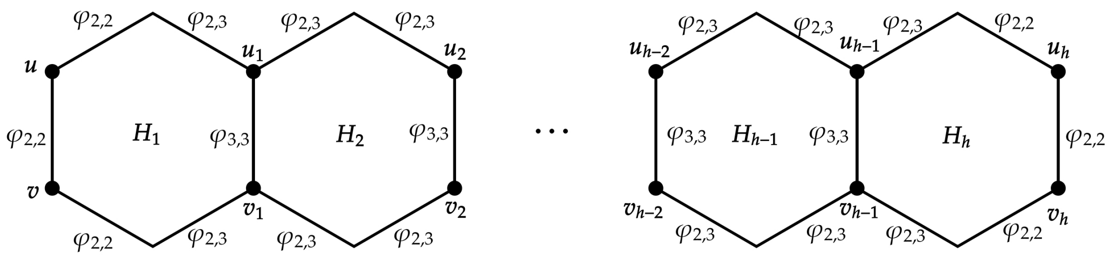

Figure 6: Linear hexagonal chain weighted by a VDB topological index φ.

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4 Minimal value of VDB-Hosoya index among hexagonal chains

It is well known that among hexagonal chains, the linear chain has the minimal Hosoya index [15]. In this section, we show that under certain conditions on the VDB topological index, it remains true for the VDB-Hosoya index. If A is an $m \times n$ matrix with all entries non-negative real numbers, we write $A \geq 0$.

Proposition 4.1. *Let φ be a VDB topological index such that $x_k = (S - Q_2)Q_2^{k-2}Q_3X_0 \geq 0$ for all $k \geq 2$. Consider the hexagonal chains $H_{k,1}$, $H_{k,2}$ and $H_{k,3}$ depicted in Figure 7. Then*

$$\begin{aligned} Z(H_{k,1};\varphi) &\leq Z(H_{k,2};\varphi), \\ Z(H_{k,1};\varphi) &\leq Z(H_{k,3};\varphi), \end{aligned}$$

for all $k \geq 2$.

Proof. By virtue of Theorem 3.2,

$$\begin{aligned} Z_{uv}(H_{k,1};\varphi) &= Q_1MQ_2^{k-1}Q_3X_0, \\ Z_{uv}(H_{k,2};\varphi) &= Q_1MSQ_2^{k-2}Q_3X_0, \\ Z_{uv}(H_{k,3};\varphi) &= Q_1MPSPQ_2^{k-2}Q_3X_0, \end{aligned}$$

where M is a product of matrices associated to the VDB topological index φ. Hence,

$$\begin{aligned} Z(H_{k,1};\varphi) &= e_1^\intercal Q_1 M Q_2^{k-1} Q_3 X_0 = y^\intercal Q_2^{k-1} Q_3 X_0, \\ Z(H_{k,2};\varphi) &= e_1^\intercal Q_1 M S Q_2^{k-2} Q_3 X_0 = y^\intercal S Q_2^{k-2} Q_3 X_0, \\ Z(H_{k,3};\varphi) &= e_1^\intercal Q_1 M PSP Q_2^{k-2} Q_3 X_0 = y^\intercal PSP Q_2^{k-2} Q_3 X_0, \end{aligned}$$

where $y^\intercal = e_1^\intercal Q_1 M$ with $e_1^\intercal = (1,0,0,0)^\intercal$. Note that

$$\begin{aligned} Z(H_{k,2};\varphi) - Z(H_{k,1};\varphi) &= y^\intercal (S - Q_2) Q_2^{k-2} Q_3 X_0 = y^\intercal x_k, \\ Z(H_{k,3};\varphi) - Z(H_{k,1};\varphi) &= y^\intercal (PSP - Q_2) Q_2^{k-2} Q_3 X_0 = y^\intercal (PSP - PQ_2P) Q_2^{k-2} Q_3 X_0 \\ &= y^\intercal P (S - Q_2) P Q_2^{k-2} Q_3 X_0 = y^\intercal P (S - Q_2) Q_2^{k-2} Q_3 P X_0 \\ &= y^\intercal P (S - Q_2) Q_2^{k-2} Q_3 X_0 = y^\intercal P x_k, \end{aligned}$$

since $PQ_2 = Q_2P$, $PQ_3 = Q_3P$ and $PX_0 = X_0$. Consequently, since $x_k \geq 0$ for all $k \geq 2$ and $y^\intercal \geq 0$, we conclude that $Z(H_{k,2};\varphi) \geq Z(H_{k,1};\varphi)$ and $Z(H_{k,3};\varphi) \geq Z(H_{k,1};\varphi)$. ■

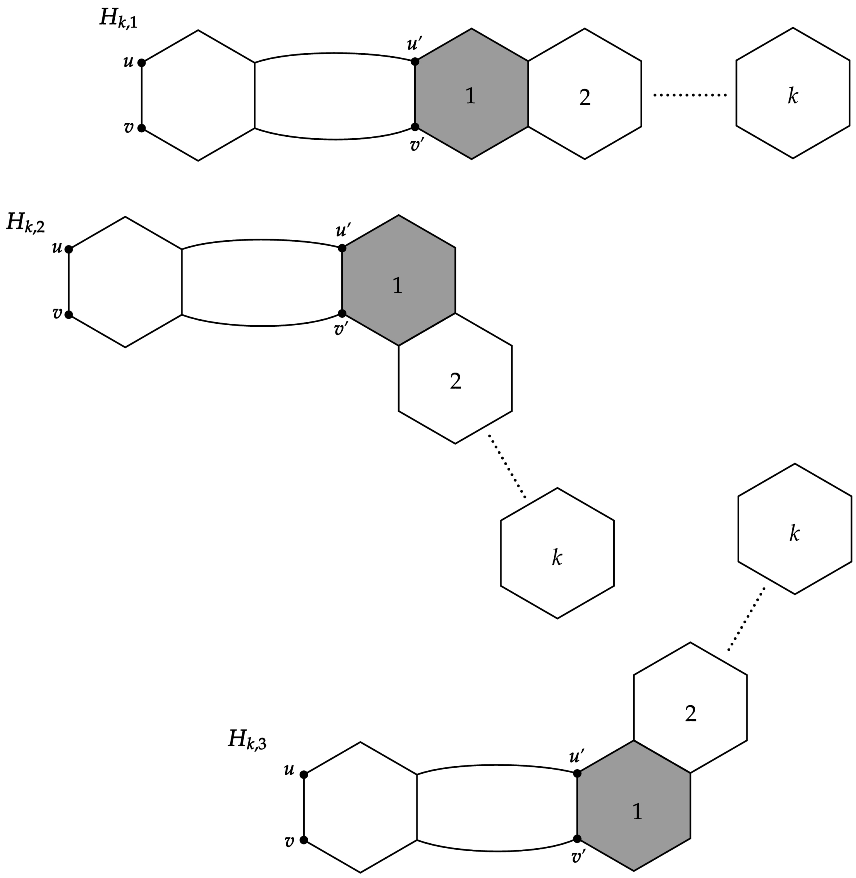

Figure 7: Graphs used in Proposition 4.1.

Example 4.2. By Proposition 4.1 we can see that the sequence of hexagonal chains in Figure 8 satisfies

$$Z(C_1;\varphi) \geq Z(C_2;\varphi) \geq Z(C_3;\varphi) \geq Z(C_4;\varphi) \geq Z(C_5;\varphi),$$

when $(S-Q_2)Q_2^{k-2}Q_3X_0 \geq 0$ for all $k \geq 2$.

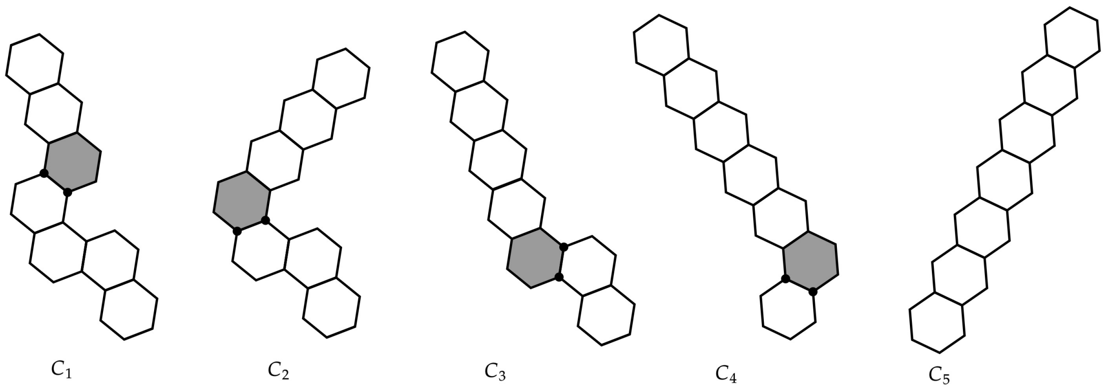

Figure 8: $Z(C_1;\varphi) \geq Z(C_2;\varphi) \geq Z(C_3;\varphi) \geq Z(C_4;\varphi) \geq Z(C_5;\varphi)$.

As a consequence of Proposition 4.1, we have a condition that guarantees the minimality of the linear chain with respect to the VDB-Hosoya index, among hexagonal chains.

Theorem 4.3. *Let φ be a VDB topological index such that $x_k = (S-Q_2)Q_2^{k-2}Q_3X_0 \geq 0$ for all $k \geq 2$. If $h \geq 3$, then*

$$Z(L_h;\varphi) \leq Z(H;\varphi),$$

for all $H \in \mathcal{C}_h$.

Proof. The proof is by induction on number of angular hexagons. If $H = L_h$, then the number of angular hexagon is zero and we are done. Assume the result is valid for any hexagonal chain in $\mathcal{C}_h$ with $r \geq 0$ angular hexagons and let H be a hexagonal chain with $r+1$ angular hexagons. Then, H is of the form $H_{k,2}$ or $H_{k,3}$ as depicted in Figure 7. Applying Proposition 4.1 we obtain a hexagonal chain $H' \in \mathcal{C}_h$ with r angular hexagons and by the induction hypothesis

$$Z(H;\varphi) \geq Z(H';\varphi) \geq Z(L_h;\varphi).$$

■

Corollary 4.4. *Let $h \geq 3$ and $\varphi \in \{\mathcal{R}, \mathcal{H}, \mathcal{GA}, \mathcal{SC}, \mathcal{AZ}\}$. Then*

$$Z(L_h;\varphi) \leq Z(H;\varphi),$$

for all $H \in \mathcal{C}_h$.

Proof. Using Theorem 4.3, we prove that for each of the indices $\mathcal{R}, \mathcal{H}, \mathcal{GA}, \mathcal{SC}, \mathcal{AZ}$ that $x_k \geq 0$ for all $k \geq 2$. Let $A = (S-Q_2)Q_2$

1. For the Randić index $\mathcal{R}$

$$AQ_2 = \begin{pmatrix} 0.2248 & 0.0722 & 0.0701 & 0.0228 \\ 0.2248 & 0.0676 & 0.0748 & 0.0228 \\ 1.2249 & 0.3981 & 0.3775 & 0.1241 \\ 1.2249 & 0.3935 & 0.3821 & 0.1241 \end{pmatrix}, \quad x_3 = \begin{pmatrix} 0.5456 \\ 0.5456 \\ 2.9733 \\ 2.9733 \end{pmatrix}, \quad x_2 = \begin{pmatrix} 0.1579 \\ 0.1579 \\ 0.8605 \\ 0.8605 \end{pmatrix}.$$

2. For the Geometric-Arithmetic index $\mathcal{GA}$

$$AQ_2 = \begin{pmatrix} 3.454 & 2.2577 & 2.3132 & 1.5637 \\ 1.9467 & 0.3822 & 2.2072 & 0.8879 \\ 12.1669 & 8.8918 & 6.2193 & 4.987 \\ 12.1669 & 8.007 & 7.1041 & 4.987 \end{pmatrix}, \; x_3 = \begin{pmatrix} 13.2019 \\ 7.4611 \\ 44.9513 \\ 44.9513 \end{pmatrix}, \; x_2 = \begin{pmatrix} 1.6485 \\ 0.9366 \\ 5.2198 \\ 5.2198 \end{pmatrix}.$$

3. For the Sum-Connectivity index $\mathcal{SC}$

$$AQ_2 = \begin{pmatrix} 0.2512 & 0.0874 & 0.086 & 0.0303 \\ 0.2143 & 0.0665 & 0.0811 & 0.0258 \\ 1.2564 & 0.4457 & 0.4118 & 0.1484 \\ 1.2564 & 0.4377 & 0.4198 & 0.1484 \end{pmatrix}, \; x_3 = \begin{pmatrix} 0.6084 \\ 0.5187 \\ 3.0289 \\ 3.0289 \end{pmatrix}, \; x_2 = \begin{pmatrix} 0.1644 \\ 0.1398 \\ 0.8009 \\ 0.8009 \end{pmatrix}.$$

4. For the Harmonic index $\mathcal{H}$

$$A = \begin{pmatrix} 0.134 & 0.0393 & 0.0297 & 0.0089 \\ 0.1187 & 0.0091 & 0.0507 & 0.0075 \\ 0.4267 & 0.1483 & 0.0331 & 0.0171 \\ 0.4267 & 0.1227 & 0.0587 & 0.0171 \end{pmatrix}, \; x_2 = \begin{pmatrix} 0.301 \\ 0.2643 \\ 0.8933 \\ 0.8933 \end{pmatrix}.$$

5. For the Augmented Zagreb index $\mathcal{AZ}$

$$AQ_2Q_2 = \begin{pmatrix} 60950346.835 & 186649648.1159 & 194649136.1159 & 747590606.5364 \\ 9454391.4735 & 9369109.3975 & 50923029.3975 & 112557185.0549 \\ 9447251.4514 & 45796083.4866 & 10144499.4866 & 113126370.8926 \\ 9447251.4514 & 29018867.4866 & 26921715.4866 & 113126370.8926 \end{pmatrix},$$

$$x_4 = \begin{pmatrix} 1677442512.2835 \\ 257938847.1115 \\ 254092216.9287 \\ 254092216.9287 \end{pmatrix}, \; x_3 = \begin{pmatrix} 10358277.2649 \\ 1563926.2581 \\ 1543909.5176 \\ 1543909.5176 \end{pmatrix}, \; x_2 = \begin{pmatrix} 62194.6582 \\ 9280.1406 \\ 8110.125 \\ 8110.125 \end{pmatrix}.$$

Hence, in virtue of Theorem 4.3, for all $\varphi \in \{\mathcal{R}, \mathcal{H}, \mathcal{GA}, \mathcal{SC}, \mathcal{AZ}\}$,

$$Z(L_h; \varphi) \leq Z(H; \varphi),$$

for all $H \in \mathcal{C}_h$. In other words, the linear chain is the hexagonal chain with minimal value of the VDB-Hosoya index. ■

The VDB topological indices $\varphi \in \{\mathcal{FZ}, \mathcal{SZ}, \mathcal{ABC}\}$ do not satisfy the condition in Theorem 4.3. However, it is possible to obtain a similar result to Theorem 4.3 over the subfamily $\mathcal{C}_h^*$ of hexagonal chains with no adjacent angular hexagons.

Proposition 4.5. *Let φ be a VDB topological index such that $x'_k = Q_2(S - Q_2)Q_2^{k-2}Q_3X_0 \geq 0$ for all $k \geq 2$. Assume that the hexagonal chains $H_{k,1}$, $H_{k,2}$ and $H_{k,3}$ in Figure 7 belong to $\mathcal{C}_h^*$. Then*

$$\begin{aligned} Z(H_{k,1}; \varphi) &\leq Z(H_{k,2}; \varphi), \\ Z(H_{k,1}; \varphi) &\leq Z(H_{k,3}; \varphi), \end{aligned}$$

for all $k \geq 2$.

Proof. The proof is similar to the proof of Proposition 4.1. By Theorem 3.2,

$$\begin{aligned} Z(H_{k,1};\varphi) &= e_1^\intercal Q_1 M Q_2 Q_2^{k-1} Q_3 X_0 = y^\intercal Q_2 Q_2^{k-1} Q_3 X_0, \\ Z(H_{k,2};\varphi) &= e_1^\intercal Q_1 M Q_2 S Q_2^{k-2} Q_3 X_0 = y^\intercal Q_2 S Q_2^{k-2} Q_3 X_0, \\ Z(H_{k,3};\varphi) &= e_1^\intercal Q_1 M Q_2 PSP Q_2^{k-2} Q_3 X_0 = y^\intercal Q_2 PSP Q_2^{k-2} Q_3 X_0, \end{aligned}$$

where M is a product of matrices associated to the VDB topological index φ and $y^\intercal = e_1^\intercal Q_1 M$ with $e_1^\intercal = (1,0,0,0)^\intercal$. Then

$$\begin{aligned} Z(H_{k,2};\varphi) - Z(H_{k,1};\varphi) &= y^\intercal Q_2 (S - Q_2) Q_2^{k-2} Q_3 X_0 = y^\intercal x_k' \geq 0, \\ Z(H_{k,3};\varphi) - Z(H_{k,1};\varphi) &= y^\intercal Q_2 (PSP - Q_2) Q_2^{k-2} Q_3 X_0 \\ &= y^\intercal Q_2 (PSP - PQ_2P) Q_2^{k-2} Q_3 X_0 \\ &= y^\intercal P Q_2 (S - Q_2) Q_2^{k-2} Q_3 X_0 = y^\intercal P x_k' \geq 0. \end{aligned}$$

We conclude that $Z(H_{k,2};\varphi) \geq Z(H_{k,1};\varphi)$ and $Z(H_{k,3};\varphi) \geq Z(H_{k,1};\varphi)$. ■

Theorem 4.6. *Let φ be a VDB topological index such that $x_k' = Q_2(S - Q_2)Q_2^{k-2}Q_3X_0 \geq 0$ for all $k \geq 2$. If $h \geq 4$, then*

$$Z(L_h;\varphi) \leq Z(H;\varphi),$$

for all $H \in \mathcal{C}_h^*$.

Proof. The proof is similar to the proof of Theorem 4.3 using Proposition 4.5 instead of Proposition 4.1. ■

Corollary 4.7. *Let $\varphi \in \{\mathcal{FZ}, \mathcal{SZ}, \mathcal{ABC}\}$ and $h \geq 4$. Then*

$$Z(L_h;\varphi) \leq Z(H;\varphi),$$

for all $H \in \mathcal{C}_h^*$.

Proof. Using Theorem 4.6, we prove that for each of the indices $\mathcal{FZ}, \mathcal{SZ}, \mathcal{ABC}$ that $x_k' \geq 0$ for all $k \geq 2$. Let $A = Q_2(S - Q_2)Q_2Q_2$

1. For the First Zagreb index $\mathcal{FZ}$

$$AQ_2Q_2 = \begin{pmatrix} 3810385661 & 8615526480 & 8156542105 & 21834212650 \\ 243292398 & 314988515 & 744676015 & 1388121450 \\ 1077622398 & 2674466640 & 2078763515 & 6180902700 \\ 620276958 & 1398299940 & 1339706190 & 3559218575 \end{pmatrix},$$

$$x_5' = \begin{pmatrix} 46443479269 \\ 2952591342 \\ 13146473842 \\ 7569689582 \end{pmatrix},\ x_4' = \begin{pmatrix} 621036222 \\ 39459246 \\ 175822371 \\ 101247991 \end{pmatrix},\ x_3' = \begin{pmatrix} 8138436 \\ 511098 \\ 2309848 \\ 1331533 \end{pmatrix},\ x_2' = \begin{pmatrix} 90193 \\ 4974 \\ 26224 \\ 15254 \end{pmatrix}.$$

2. For the Second Zagreb index $\mathcal{SZ}$

$$AQ_2Q_2 = \begin{pmatrix} 30488306320 & 81288914496 & 77469467712 & 250374385728 \\ 1407771400 & 1576663584 & 5753868576 & 11560822560 \\ 5751751720 & 17512289952 & 12438170016 & 47234217888 \\ 3097097080 & 8257581024 & 7869589728 & 25433809632 \end{pmatrix},$$

$$x_5' = \begin{pmatrix} 369557957840 \\ 17064021800 \\ 69718717640 \\ 37540847960 \end{pmatrix},\ x_4' = \begin{pmatrix} 3589757624 \\ 165753980 \\ 677223404 \\ 364658756 \end{pmatrix},\ x_3' = \begin{pmatrix} 34454132 \\ 1590890 \\ 6499922 \\ 3499958 \end{pmatrix},\ x_2' = \begin{pmatrix} 291830 \\ 13475 \\ 55055 \\ 29645 \end{pmatrix}.$$

3. For the Atom-Bond-Connectivity index $\mathcal{ABC}$

$$A = \begin{pmatrix} 2.1774 & 1.125 & 0.5902 & 0.3579 \\ 0.7184 & 0.313 & 0.1743 & 0.084 \\ 2.8894 & 1.5378 & 1.0694 & 0.6188 \\ 2.158 & 1.1013 & 0.8585 & 0.4676 \end{pmatrix}, \; x_3' = \begin{pmatrix} 5.7901 \\ 1.7977 \\ 8.1585 \\ 6.1113 \end{pmatrix}, \; x_2' = \begin{pmatrix} 0.7537 \\ 0.1839 \\ 1.2732 \\ 0.9613 \end{pmatrix}.$$

Hence, in virtue of Theorem 4.6, if $\varphi \in \{\mathcal{FZ}, \mathcal{SZ}, \mathcal{ABC}\}$, then

$$Z(L_h, \varphi) \leq Z(H, \varphi),$$

for all $H \in \mathcal{C}_h^*, h \geq 4$. In other words, the linear chain attains the minimal VDB-Hosoya index over the family $\mathcal{C}_h^*$ of hexagonal chains with no adjacent angular hexagons. ■

5 Concluding remarks

In this paper, we compute the Hosoya index of the weighted hexagonal chain $(H; \varphi)$, where the weight is induced by a vertex-degree-based topological index φ. In our main result (see Theorem 3.2, we give an expression to compute the Hosoya index of $(H; \varphi)$ in terms of a product of 4×4 matrices associated to the VDB topological index φ.

We also give conditions on φ to assure that the VDB weighted linear hexagonal chain is the minimal weighted hexagonal chain with h hexagons with respect to the Hosoya index. As a consequence, we proved that the mentioned result is true for the Randić, Harmonic, Geometric-Arithmetic, Sum-Connectivity and Augmented Zagreb indices.

Although the First Zagreb, Second Zagreb and Bond-Connectivity do not satisfy the mentioned conditions, we obtained a similar result over the subfamily of hexagonal chains with no adjacent angular hexagons.

As a future work we propose to solve the following problem.

Problem 5.1. Prove that the VDB weighted linear hexagonal chain is the minimal weighted hexagonal chain with h hexagons with respect to the Hosoya index for the First Zagreb, Second Zagreb and Atom-Bond-Connectivity indices.

It is known that the zig-zag hexagonal chain is maximal with respect to the Hosoya index over the set of hexagonal chains with h hexagons [15]. This fact motivates us to pose another problem.

Problem 5.2. Find the maximal VDB weighted hexagonal chain with respect to the Hosoya index for known VDB topological indices.

Author Contributions: Roberto Cruz, Mateo Lopez and Juan Rada conceived of the presented idea. Roberto Cruz, Mateo Lopez and Juan Rada developed the theory and performed the computations. Roberto Cruz, Mateo Lopez and Juan Rada verified the analytical methods. All authors discussed the results and contributed to the final manuscript.

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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