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Computing the Hosoya Index of Catacondensed Hexagonal Systems

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Abstract

The Hosoya index of a graph G is defined as $Z(G) = \sum_{k \geq 0} m(G,k)$, where $m(G,k)$ the number of ways in which k mutually independent edges can be selected in G. In this article we introduce the Hosoya vector of a graph at a given edge. Based on this concept and the recurrence relations known for Z, we give reduction formulas to compute the Hosoya index of any catacondensed hexagonal system via a product of 4×4 matrices with entries in $\mathbb{N}$. As a consequence, we discuss the extremal value problem of the Hosoya index over certain subsets of the set of cataconsed hexagonal systems.

1 Introduction

Let G be a graph. We denote by $m(G,k)$ the number of ways in which k mutually independent edges can be selected in G. By definition $m(G,0) = 1$ and clearly $m(G,1)$ is the number of edges of G. The Hosoya index of G [4] is denoted by $Z(G)$ and defined as

$$Z(G) = \sum_{k \geq 0} m(G,k)$$

The Hosoya index is a graph invariant used in mathematical chemistry for quantifying certain structural features of organic molecules. We refer the reader to the survey [12] for further details.

The following recurrence relations are fundamental and can be found in [12]:

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a) If $G_1, \ldots, G_r$ are the connected components of the graph G, then

$$Z(G) = \prod_{i=1}^{r} Z(G_i) \tag{1}$$

b) Let $e = vw$ be an edge of G. Then

$$Z(G) = Z(G - uv) + Z(G - v - w) \tag{2}$$

Our interest is the Hosoya index over hexagonal systems, natural representations of benzenoid hydrocarbons, which play an important role in mathematical chemistry. For the definition and basic properties of hexagonal systems we refer to ([1], [2]), and for recent results on the study of the Hosoya index over hexagonal systems see ([3], [8]- [15]). An important class of hexagonal systems are the catacondensed hexagonal systems, whose hexagons are terminal, linear, angular or branched as we can see in Figure 1.

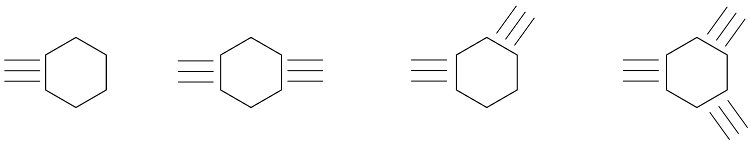

Figure 1. Types of hexagons in catacondensed hexagonal systems

In this article we introduce the Hosoya vector of a graph at a given edge. Based on this concept and the recurrence relations given above, we give reduction formulas to compute the Hosoya index of any catacondensed hexagonal system via a product of 4×4 matrices with entries in $\mathbb{N}$. As a consequence, we discuss the extremal value problem of the Hosoya index over certain subsets of the set of cataconsed hexagonal systems.

2 Computing the Hosoya index of catacondensed hexagonal systems

We begin introducing the Hosoya vector of a graph at an edge.

Definition 2.1 *Let uv be an edge of a graph G. We define the Hosoya vector of G at uv, denoted by $Z_{uv}(G)$, as the column vector*

$$Z_{uv}(G) = (Z(G), Z(G-u), Z(G-v), Z(G-u-v))^{\top}$$

Note that

$$Z_{uv}(G) = PZ_{vu}(G) \tag{3}$$

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 $G = L_j$, the linear hexagonal chain with j hexagons (see Figure 2), we will write

$$Z_{uv}(L_j) = (\lambda_j, \xi_j, \xi_j, \eta_j)^\top$$

In other words,

$$\lambda_j = Z(L_j), \quad \xi_j = Z(L_j - u) = Z(L_j - v), \quad \eta_j = Z(L_j - u - v). \tag{4}$$

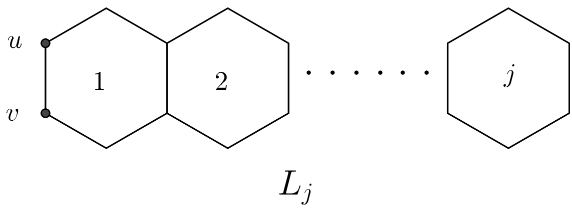

Figure 2. Linear hexagonal chain L_j

Proposition 2.2 *Let G be the graph obtained from the edge-coalescence of the graph H and a hexagon at st (see Figure 3). Then*

$$Z_{uv}(G) = QZ_{st}(H)$$

where $Q = \begin{pmatrix} 5 & 3 & 3 & 2 \\ 2 & 2 & 1 & 1 \\ 2 & 1 & 2 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$.

Proof. We delete the independent edges xs and yt from G (see Figure 3) using relations (1) and (2):

$$\begin{aligned} Z(G) &= Z(G-yt-xs)+Z(G-yt-x-s) \\ &\quad +Z(G-y-t-xs)+Z(G-y-t-x-s) \\ &= Z(P_4)\,Z(H)+Z(P_3)\,Z(H-s)+Z(P_3)\,Z(H-t)+ \\ &\quad +Z(P_2)\,Z(H-s-t) \\ &= 5Z(H)+3Z(H-s)+3Z(H-t)+2Z(H-s-t) \\ &= (5,3,3,2)\cdot Z_{uv}(H), \end{aligned}$$

$$\begin{aligned} Z(G-u) &= Z(G-u-yt-xs)+Z(G-u-yt-x-s)+ \\ &\quad +Z(G-u-y-t-xs)+Z(G-u-y-t-x-s) \\ &= Z(P_1)\,Z(P_2)\,Z(H)+Z(P_2)\,Z(H-s)+Z(P_1)\,Z(P_1)\,Z(H-t)+ \\ &\quad +Z(P_1)\,Z(H-s-t) \\ &= 2Z(H)+2Z(H-s)+Z(H-t)+Z(H-s-t) \\ &= (2,2,1,1)\cdot Z_{uv}(H), \end{aligned}$$

$$\begin{aligned} Z(G-v) &= Z(G-v-yt-xs)+Z(G-v-yt-x-s)+ \\ &\quad +(G-v-y-t-xs)+Z(G-v-y-t-x-s) \\ &= Z(P_1)\,Z(P_2)\,Z(H)+Z(P_1)\,Z(P_1)\,Z(H-s)+Z(P_2)\,Z(H-t)+ \\ &\quad +Z(P_1)\,Z(H-s-t) \\ &= 2Z(H)+Z(H-s)+2Z(H-t)+Z(H-s-t) \\ &= (2,1,2,1)\cdot Z_{uv}(H), \end{aligned}$$

$$\begin{aligned} Z(G-u-v) &= Z(G-u-v-yt-xs)+Z(G-u-v-yt-x-s)+ \\ &\quad +Z(G-u-v-y-t-xs)+Z(G-u-v-y-t-x-s) \\ &= Z(P_1)\,Z(P_1)\,Z(H)+Z(P_1)\,Z(H-s)+Z(P_1)\,Z(H-t)+ \\ &\quad +Z(H-s-t) \\ &= Z(H)+Z(H-s)+Z(H-t)+Z(H-s-t) \\ &= (1,1,1,1)\cdot Z_{uv}(H), \end{aligned}$$

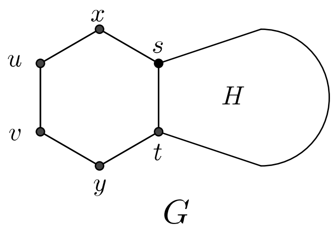

Figure 3. Graph used in Proposition 2.2

where P_k denotes the path on k vertices. ■

A direct consequence of Proposition 2.2 is

$$(\lambda_j, \xi_j, \xi_j, \eta_j)^\top = Q\,(\lambda_{j-1}, \xi_{j-1}, \xi_{j-1}, \eta_{j-1})^\top \tag{5}$$

Corollary 2.3 *Let G be the graph obtained from the coalescence of the graph H and the linear chain L_j at an edge st (see Figure 4). Then*

$$Z_{uv}(G) = Q^j Z_{st}(H)$$

In particular, $Z_{uv}(L_j) := (\lambda_j, \xi_j, \xi_j, \eta_j)^\top = Q^j X_0$, where $X_0 = (2,1,1,1)^\top$ is the Hosoya vector of K_2.

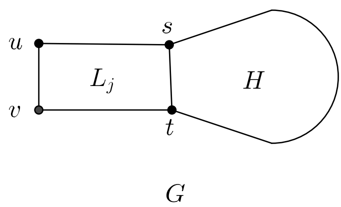

Figure 4. Graph used in Corollary 2.3

Proof. This is a consequence of Proposition 2.2 and induction. Note that $Z_{uv}(K_2) = (2,1,1,1)^\top = X_0$. ■

If uv is an edge of the graph H we will denote by $Z^*_{st}(H)$ the (4×4)-matrix

$$Z^*_{st}(H) = (E_k Z_{st}(H))_k \tag{6}$$

whose 4 columns are given by $E_1 Z_{st}(H), E_2 Z_{st}(H), E_3 Z_{st}(H)$ and $E_4 Z_{st}(H)$, where

$$E_1 = \begin{pmatrix} 2 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, E_2 = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

and

$$E_3 = \begin{pmatrix} 0 & 0 & 2 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, E_4 = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Proposition 2.4 *Let G be the graph obtained from the edge-coalescence of the graphs H and K to a hexagon at the edges st and xy, respectively (see Figure 5). Then*

$$Z_{uv}(G) = Z^*_{st}(H)\, Z_{xy}(K)$$

Proof. We delete the independent edges us, vx and yt from G (see Figure 5) using relations (1) and (2):

$$\begin{aligned}
Z(G) &= Z(G - yt - xv - us) + Z(G - yt - xv - u - s) \\
&\quad + Z(G - yt - us - x - v) + Z(G - yt - x - v - u - s) + \\
&\quad + Z(G - xv - us - y - t) + Z(G - xv - y - t - u - s) + \\
&\quad + Z(G - us - y - t - x - v) + Z(G - y - t - x - v - u - s) \\
&= [2Z(H) + Z(H - s)]\, Z(K) + [Z(H) + Z(H - s)]\, Z(K - x) + \\
&\quad + [2Z(H - t) + Z(H - s - t)]\, Z(K - y) + \\
&\quad + [Z(H - t) + Z(H - s - t)]\, Z(K - x - y) \\
&= [(2,1,0,0) \cdot Zst(H)]\, Z(K) + [(1,1,0,0) \cdot Zst(H)]\, Z(K - x) + \\
&\quad + [(0,0,2,1) \cdot Zst(H)]\, Z(K - y) + [(0,0,1,1) \cdot Zst(H)]\, Z(K - x - y)
\end{aligned}$$

$$\begin{aligned}
Z(G - u) &= Z(G - u - yt - xv) + Z(G - u - yt - x - v) + \\
&\quad + Z(G - u - xv - y - t) + Z(G - u - y - t - x - v) \\
&= Z(H)\, Z(K) + Z(H)\, Z(K - x) + \\
&\quad + Z(H - t)\, Z(K - y) + Z(H - t)\, Z(K - x - y) \\
&= [(1,0,0,0) \cdot Zst(H)]\, Z(K) + [(1,0,0,0) \cdot Zst(H)]\, Z(K - x) + \\
&\quad + [(0,0,1,0) \cdot Zst(H)]\, Z(K - y) + [(0,0,1,0) \cdot Zst(H)]\, Z(K - x - y)
\end{aligned}$$

$$\begin{aligned} Z(G-v) &= Z(G-u-yt-us)+Z(G-v-yt-u-s)+ \\ &\quad +Z(G-v-us-y-t)+Z(G-v-y-t-u-s) \\ &= [Z(H)+Z(H-s)Z(K)]+ \\ &\quad +[Z(H-t)+Z(H-t-s)]Z(K-y) \\ &= [(1,1,0,0)\cdot Zst(H)]Z(K)+[(0,0,0,0)\cdot Zst(H)]Z(K-x)+ \\ &\quad +[(0,0,1,1)\cdot Zst(H)]Z(K-y)+[(0,0,0,0)\cdot Zst(H)]Z(K-x-y) \end{aligned}$$

$$\begin{aligned} Z(G-u-v) &= Z(G-u-v-yt)+Z(G-u-v-y-t) \\ &= Z(H)Z(K)+Z(H-t)Z(K-y) \\ &= [(1,0,0,0)\cdot Zst(H)]Z(K)+[(0,0,0,0)\cdot Zst(H)]Z(K-x)+ \\ &+ [(0,0,1,0)\cdot Zst(H)]Z(K-y)+[(0,0,0,0)\cdot Zst(H)]Z(K-x-y) \end{aligned}$$

■

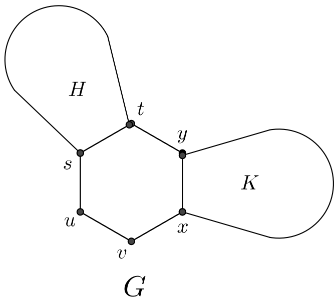

Figure 5. Graph used in Proposition 2.4

Let us define for every integer $j \geq 0$ the 4×4-matrix associated to the linear hexagonal chain L_j

$$S_j = Z^{*}_{uv}(L_j)$$

Note that by Corollary 2.3

$$S_j = \left(E_k Q^j X_0\right)_k \tag{7}$$

In particular,

$$S_0 = (E_k X_0)_k = \begin{pmatrix} 5 & 3 & 3 & 2 \\ 2 & 2 & 1 & 1 \\ 3 & 0 & 2 & 0 \\ 2 & 0 & 1 & 0 \end{pmatrix}$$

Corollary 2.5 *Let G be a graph as in the hypothesis of Proposition 2.4, where $H = L_i$ and $K = L_j$. Then*

$$Z_{uv}(G) = S_i Q^j X_0 = (\lambda_j E_1 + \xi_j (E_2 + E_3) + \eta_j E_4) Q^i X_0$$

Proof. By Proposition 2.4 and (4)

$$\begin{aligned} Z_{uv}(G) &= Z^*_{st}(L_i) Z_{xy}(L_j) = S_i Q^j X_0 = S_i (\lambda_j, \xi_j, \xi_j, \eta_j)^\top \\ &= \lambda_j E_1 Q^i X_0 + \xi_j (E_2 + E_3) Q^i X_0 + \eta_j E_4 Q^i X_0 \\ &= (\lambda_j E_1 + \xi_j (E_2 + E_3) + \eta_j E_4) Q^i X_0 \end{aligned}$$

■

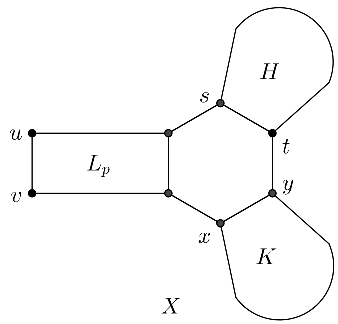

Figure 6. General form of catacondensed hexagonal systems

Note that Proposition 2.2, Corollary 2.3 and Proposition 2.4 gives a reduction formula to find the Hosoya index of any catacondensed hexagonal system. In fact, if X is any catacondensed hexagonal system then X has the form depicted in Figure 6 (H or K can be isomorphic to K_2). Hence

$$Z_{uv}(X) = Q^p \{E_k Z_{st}(H)\}_k Z_{xy}(K).$$

After a finite number of steps, which ends when there are no more branched or angular hexagons, we have expressed the vector $Z_{uv}(X)$ as a product of matrices evaluated in X_0.

Example 2.6 *Consider the hexagonal system $S(i,j,k)$ (see Figure 7). Then by Proposition 2.2 and Corollary 2.5*

$$Z_{uv}(S(i,j,k)) = Q^k S_i Q^j X_0 = Q^k (\lambda_j E_1 + \xi_j (E_2 + E_3) + \eta_j E_4) Q^i X_0 \tag{8}$$

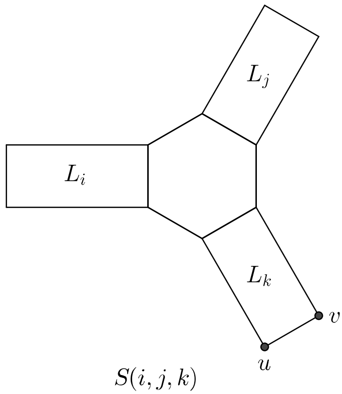

Figure 7. Catacondensed hexagonal system $S(i,j,k)$.

More generally, let H be any hexagonal chain with angular hexagons

$$H_1, \ldots, H_r$$

Assume that H_0 is the first hexagon and H_{r+1} is the last hexagon of the chain. For $i = 0, \ldots, r$ let $p_i \geq 0$ be the number of (linear) hexagons between H_i and H_{i+1}. We construct a catacondensed hexagonal system $\widehat{H}$ from H by attaching to each 22-edge of H_i $(i = 1, \ldots, r)$ a linear hexagonal chain L_{q_i} (see Figure 8). We construct a sequence of vertices $x_1, y_1, x_2, y_2, \ldots, x_r, y_r$ in H as follows: Let x_1 be the closest vertex to u belonging to H_1, and y_1 the closest vertex to x_1 in the hexagon adjacent to H_1. Then choose x_2 the closest vertex to y_1 in H_2 and y_2 the closest vertex to x_2 in the next hexagon adjacent to H_2, and so on .... (see Figure 8).

Theorem 2.7 *Let $\widehat{H}$ be the catacondensed hexagonal system described above with sequence of vertices $x_1, y_1, x_2, y_2, \ldots, x_r, y_r$ in H. Then*

$$Z_{uv}\left(\widehat{H}\right) = Q^{p_0+1}\mathcal{H}_1 Q^{p_1}\mathcal{H}_2 Q^{p_2}\cdots\mathcal{H}_{r-1}Q^{p_{r-1}}\mathcal{H}_r Q^{p_r+1}X_0$$

where $\mathcal{H}_i = PS_i$ if $d(x_i, y_i) = 1$ and $\mathcal{H}_i = S_i$ if $d(x_i, y_i) = 2$.

Proof. The proof will be using induction on the number $N\left(\widehat{H}\right)$ of non-linear hexagons of the catacondensed hexagonal system $\widehat{H}$ (equivalently, the sum of the numbers of angular hexagons and branching hexagons of $\widehat{H}$). If $N\left(\widehat{H}\right) = 0$ then clearly $\widehat{H} = L_{p_0+1}$ and $Z_{uv} = Q^{p_0+1}X_0$ by Corollary 2.3. Now assume that the results holds for hexagonal systems $\widehat{X}$ such that $N\left(\widehat{X}\right) = h$. Let $\widehat{Y} = \widehat{H}$ (see Figure 8) such that $N\left(\widehat{Y}\right) = h+1$. By Corollary 2.3 and Proposition 2.4

$$Z_{uv}\left(\widehat{Y}\right) = Q^{p_0+1}\mathcal{H}_1 Z_{y_1w_1}\left(\widehat{K}\right)$$

where $\widehat{K}$ is obtained from $\widehat{H}$ by deleting the (sub)hexagonal system in bold of $\widehat{H}$ (see Figure 8) and

$$\mathcal{H}_1 = \begin{cases} PS_1 & d(x_1, y_1) = 1 \\ S_1 & d(x_1, y_1) = 2. \end{cases}$$

Hence, by induction

$$Z_{y_1w_1}\left(\widehat{K}\right) = Q^{p_1}\mathcal{H}_1 Q^{p_2}\cdots$$

and we are done. ■

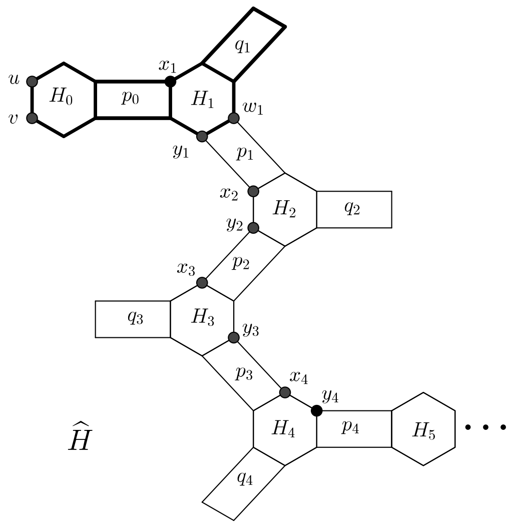

Figure 8. Sequence of vertices associated to a catacondensed hexagonal system.

Note that all catacondensed hexagonal systems with at most three branched hexagons are of the type $\widehat{H}$ described in Theorem 2.7.

Example 2.8 *Consider the catacondensed hexagonal system Y shown in Figure 9. Then*

$$Z_{uv}(Y) = Q^2 S_1 Q S_1 Q^3 X_0$$

$$\text{where } S_1 = (E_k Q X_0)_k = \begin{pmatrix} 44 & 26 & 21 & 13 \\ 18 & 18 & 8 & 8 \\ 26 & 0 & 13 & 0 \\ 18 & 0 & 8 & 0 \end{pmatrix}, \ Q = \begin{pmatrix} 5 & 3 & 3 & 2 \\ 2 & 2 & 1 & 1 \\ 2 & 1 & 2 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \text{ and } X_0 = \begin{pmatrix} 2 \\ 1 \\ 1 \\ 1 \end{pmatrix}.$$

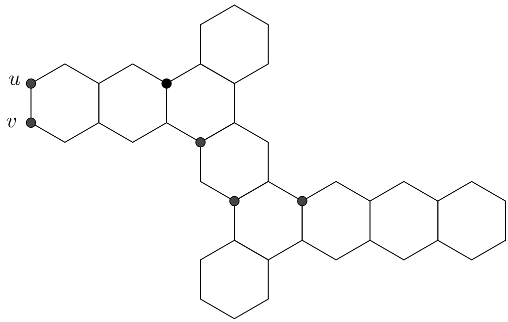

Figure 9. Catacondensed hexagonal system used in Example 2.8

When no linear hexagonal chains are attached to the 22-edge of H_i $(i = 1, \ldots, r)$ then $\widehat{H} = H$ is a hexagonal chain. In this case $\mathcal{H}_i = PS_0$ if $d(x_i, y_i) = 1$ and $\mathcal{H}_i = S_0$ if $d(x_i, y_i) = 2$, for all $i = 1, \ldots, r$. In other words, we have a formula for the Hosoya vector of any hexagonal chain.

Corollary 2.9 *Let H be a hexagonal chain with angular hexagons $H_1, \ldots, H_r$ and sequence $x_1, y_1, \ldots, x_r, y_r$ as above. Then*

$$Z_{uv}\left(\widehat{H}\right) = Q^{p_0+1}\mathcal{H}_1 Q^{p_1}\mathcal{H}_2 Q^{p_2} \cdots \mathcal{H}_{r-1} Q^{p_{r-1}}\mathcal{H}_r Q^{p_r+1} X_0$$

$$\text{where } \mathcal{H}_i = \begin{pmatrix} 5 & 3 & 3 & 2 \\ 3 & 0 & 2 & 0 \\ 2 & 2 & 1 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \text{ if } d(x_i, y_i) = 1 \text{ and } \mathcal{H}_i = \begin{pmatrix} 5 & 3 & 3 & 2 \\ 2 & 2 & 1 & 1 \\ 3 & 0 & 2 & 0 \\ 2 & 0 & 1 & 0 \end{pmatrix} \text{ if } d(x_i, y_i) = 2.$$

We next discuss the extremal value problem of the Hosoya index over certain subsets of the set of cataconsed hexagonal systems. Let $S(i, j, k)$ be the catacondensed hexagonal system introduced in Example 2.6. We take the difference between Hosoya vectors of catacondensed hexagonal systems $S(i, j, k)$ and $S(i-1, j+1, k)$ (see Figure 10). Then by (8)

$$\begin{aligned} Z_{uv}(S(i,j,k)) &= Q^k S_i Q^j X_0 \\ &= Q^k \left(\lambda_j E_1 + \xi_j (E_2 + E_3) + \eta_j E_4\right) (\lambda_i, \xi_i, \xi_i, \eta_i)^\top \end{aligned}$$

and

$$\begin{aligned}
& Z_{vu}\left(S\left(i-1,j+1,k\right)\right) \\
= \; & Q^k S_{j+1} Q^{i-1} X_0 \\
= \; & Q^k \left(\lambda_{i-1}E_1 + \xi_{i-1}\left(E_2+E_3\right) + \eta_{i-1}E_4\right)\left(\lambda_{j+1},\xi_{j+1},\xi_{j+1},\eta_{j+1}\right)^\top
\end{aligned}$$

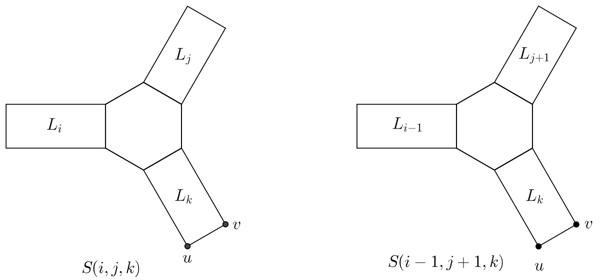

Figure 10. Catacondensed hexagonal systems $S(i,j,k)$ and $S(i-1,j+1,k)$.

It follows from (5)

$$\begin{aligned}
& Z_{uv}\left(S\left(i,j,k\right)\right) - Z_{vu}\left(S\left(i-1,j+1,k\right)\right) \\
= \; & Q^k \begin{pmatrix} 3\left(\lambda_j\xi_{i-1}-\xi_j\lambda_{i-1}\right)+2\left(\lambda_j\eta_{i-1}-\eta_j\lambda_{i-1}\right)+\left(\xi_j\eta_{i-1}-\eta_j\xi_{i-1}\right) \\ -\left(\lambda_j\xi_{i-1}-\xi_j\lambda_{i-1}\right) \\ 6\left(\lambda_j\xi_{i-1}-\xi_j\lambda_{i-1}\right)+3\left(\lambda_j\eta_{i-1}-\eta_j\lambda_{i-1}\right)+2\left(\xi_j\eta_{i-1}-\eta_j\xi_{i-1}\right) \\ 4\left(\lambda_j\xi_{i-1}-\xi_j\lambda_{i-1}\right)+2\left(\lambda_j\eta_{i-1}-\eta_j\lambda_{i-1}\right)+\left(\xi_j\eta_{i-1}-\eta_j\xi_{i-1}\right) \end{pmatrix}
\end{aligned}$$

Let $\left(q_{11}^{(k)},q_{12}^{(k)},q_{13}^{(k)},q_{14}^{(k)}\right)$ be the first row of the matrix Q^k. Since $q_{11}^{(k)},q_{12}^{(k)},q_{13}^{(k)},q_{14}^{(k)}$ are all positive, $q_{12}^{(k)}=q_{13}^{(k)}$ and $\frac{\xi_k}{\lambda_k},\frac{\eta_k}{\lambda_k},\frac{\eta_k}{\xi_k}$ are strict decrease functions on k [15], it follows that

$$\begin{aligned}
& Z\left(S\left(i,j,k\right)\right) - Z\left(S\left(i-1,j+1,k\right)\right) \\
= \; & q_{11}^{(k)}\left(3\left(\lambda_j\xi_{i-1}-\xi_j\lambda_{i-1}\right)+2\left(\lambda_j\eta_{i-1}-\eta_j\lambda_{i-1}\right)+\left(\xi_j\eta_{i-1}-\eta_j\xi_{i-1}\right)\right) \\
& +q_{12}^{(k)}\left(5\left(\lambda_j\xi_{i-1}-\xi_j\lambda_{i-1}\right)+3\left(\lambda_j\eta_{i-1}-\eta_j\lambda_{i-1}\right)+2\left(\xi_j\eta_{i-1}-\eta_j\xi_{i-1}\right)\right) \\
& +q_{14}^{(k)}\left(4\left(\lambda_j\xi_{i-1}-\xi_j\lambda_{i-1}\right)+2\left(\lambda_j\eta_{i-1}-\eta_j\lambda_{i-1}\right)+\left(\xi_j\eta_{i-1}-\eta_j\xi_{i-1}\right)\right) \\
> \; & 0 \qquad (9)
\end{aligned}$$

This fact can be used to find extremal values of the Hosoya index over significant classes of catacondensed hexagonal systems. Let $\mathcal{CH}_h$ be the set of catacondensed hexagonal systems and $\mathcal{CH}_{h,p,q}$ is formed by those $X \in \mathcal{CH}_h$ such that X has p branched hexagons and q angular hexagons. It was shown in [7] that $\mathcal{CH}_h$ can be partitioned as a disjoint union

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

where (p,q) runs through the set

$$\left\{(p,q) \in \mathbb{N} \times \mathbb{N} : 0 \leq p \leq \left\lfloor \frac{1}{2}(h-2) \right\rfloor, 0 \leq q \leq h - 2(p+1)\right\} \tag{10}$$

So a natural question is: find the extremal values of the Hosoya index over $\mathcal{CH}_{h,p,q}$, for each p,q as in (10). This problem is far from being solved. However, we can use relation (9) to deduce the extremal values of the Hosoya index over $\mathcal{CH}_{h,0,1}$ and $\mathcal{CH}_{h,1,0}$.

Theorem 2.10 *The minimal value of the Hosoya index over* $\mathcal{CH}_{h,0,1}$ *is attained* $S(1,h-2,0)$ *the minimal; the maximal in* $S\left(\left\lfloor \frac{h-1}{2} \right\rfloor, h - \left\lfloor \frac{h-1}{2} \right\rfloor - 1, 0\right)$.

Proof. Every catacondensed hexagonal system in $\mathcal{CH}_{h,0,1}$ is of the form $S(i,j,0)$. The result follows from (9). ■

Theorem 2.11 *The minimal value of the Hosoya index over* $\mathcal{CH}_{h,1,0}$ *is attained in* $S(1,1,h-3)$. *The maximal value in*

$$\begin{cases} S\left(\frac{h}{3}, \frac{h}{3}, \frac{h}{3} - 1\right) & h \equiv 0 mod(3) \\ S\left(\frac{h-1}{3}, \frac{h-1}{3}, \frac{h-1}{3}\right) & h \equiv 1 mod(3) \\ S\left(\frac{h-2}{3}, \frac{h-2}{3}, \frac{h+11}{3}\right) & h \equiv 2 mod(3) \end{cases}$$

Proof. From (9) it is clear that the minimal occurs in $S(1,1,h-3)$ and the maximal when the differences of the lengths of the branches are at most one. ■

Using the algorithm given in Theorem 2.7, we found the extremal values of the Hosoya index over $\mathcal{CH}_{h,2,0}$, $\mathcal{CH}_{h,1,1}$ and $\mathcal{CH}_{h,0,2}$ for $8 \leq h \leq 40$. These extremal catacondensed systems are depicted in Figures 11, 12 and 13 respectively.

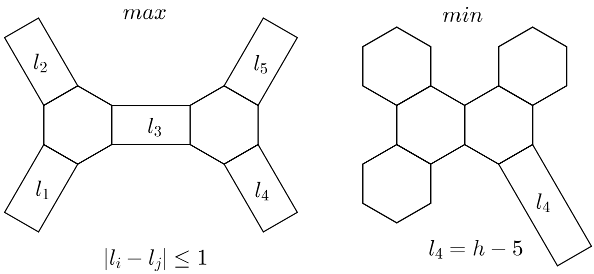

Figure 11. Catacondensed hexagonal systems in $\mathcal{CH}_{h,2,0}$ with the extremal values of the Hosoya index for $8 \leq h \leq 40$.

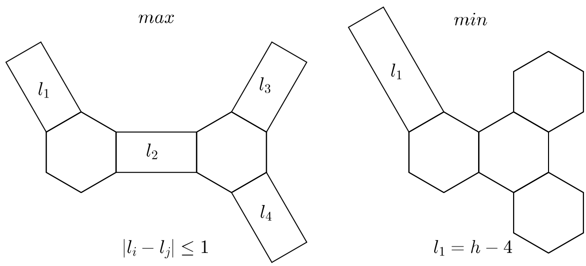

Figure 12. Catacondensed hexagonal systems in $\mathcal{CH}_{h,1,1}$ with the extremal values of the Hosoya index for $8 \leq h \leq 40$.

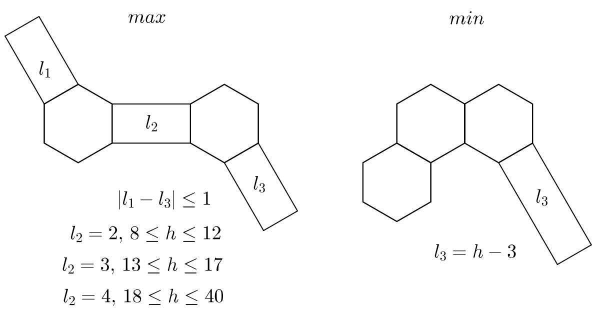

Figure 13. Catacondensed hexagonal systems in $\mathcal{CH}_{h,0,2}$ with the extremal values of the Hosoya index for $8 \leq h \leq 40$.

A problem we propose is the following:

Problem 2.12 *Find the extremal values of the Hosoya index over the set $\mathcal{CH}_{h,p,q}$ for other values of p, q.*

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