

# Extreme hollow hexagons with respect to the Mostar index

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## Abstract

The Mostar index of a connected graph is a well-known distance-based topological index. Hollow hexagons are coronoid systems that represent coronoid hydrocarbons belonging to the class of cycloarenes. They are formed by a single chain in a macro-cyclic arrangement consisting of linearly and angularly annelated hexagons, with exactly six angular hexagons. In this paper, we compute the Mostar index of hollow hexagons and find maximal and minimal values of the Mostar index over the set of hollow hexagons with a fixed number of hexagons.

*Keywords:* Mostar index, hollow hexagons, cut method, extremal values.

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## 1 Introduction

A topological index is a graph theoretical invariant that describes some structural properties of the graph. They are widely used to establish quantitative structure-activity or structure-property relationships that correlate some properties of a chemical compound with its chemical structure represented by a molecular graph [1, 10, 20, 27, 28].

The Wiener index, one of the oldest topological indices, provided a good correlation between the boiling points of paraffins and their molecular structures [31]. Let  $G$  be a connected graph with vertex set  $V(G)$ . For  $u, v \in V(G)$ , the distance between  $u$  and  $v$ ,

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denoted by  $d_G(u, v) = d(u, v)$ , is the length of the shortest path connecting vertices  $u$  and  $v$ . The Wiener index of  $G$  is defined as the sum of the distances between all pairs of vertices in  $G$  [18]. The expression, originally used to compute the Wiener index of a tree, motivated a new topological index based on the same formula but used for any connected graph, not necessarily acyclic. This topological index, introduced by Gutman in [16], was called the Szeged index and is defined as

$$\text{Sz}(G) = \sum_{e=uv \in E(G)} n_u(e|G) n_v(e|G), \quad (1.1)$$

where  $E(G)$  is the edge set of  $G$  and  $n_u(e|G)$  is the cardinality of the set  $N_u(e|G) = \{x \in V(G) : d(x, u) < d(x, v)\}$ .

The Mostar index is a Szeged-like topological index defined as

$$\text{Mo}(G) = \sum_{e=uv \in E(G)} |n_u(e|G) - n_v(e|G)|. \quad (1.2)$$

This index provides a global measure of the peripherality of a given graph and was introduced in [13].

The distance between a vertex  $u \in V(G)$  and an edge  $f = xy \in E(G)$  is defined as  $d_G(u, f) = d(u, f) = \min\{d(u, x), d(u, y)\}$ . Based on this notion, Arockiaraj et al. introduced in [3] two variations of the Mostar index: the edge-Mostar index, defined as

$$\text{Mo}_e(G) = \sum_{e=uv \in E(G)} |m_u(e|G) - m_v(e|G)|,$$

and the total Mostar index, defined as

$$\text{Mo}_t(G) = \sum_{e=uv \in E(G)} |t_u(e|G) - t_v(e|G)|,$$

where  $m_u(e|G)$  is the cardinality of the set  $M_u(e|G) = \{f \in E(G) : d(u, f) < d(v, f)\}$ , and  $t_u(e|G) = n_u(e|G) + m_u(e|G)$ . Recent research on the Mostar index and its variations can be found in [4, 6, 11, 15, 19, 21, 26, 29, 30].

Coronoid hydrocarbons are represented by simple graphs called coronoid systems. Let  $C'$  and  $C''$  be two cycles in the plane hexagonal lattice, where  $C''$  is contained in the interior of  $C'$ . A coronoid system is the graph obtained by considering all vertices and edges in the inner perimeter  $C''$ , in the interior of  $C'$  but outside  $C''$ , and in  $C'$  [17]. In [8, 7] it is possible to find more information about the structure of coronoid systems. A primitive coronoid system is a coronoid system consisting of a single chain in a macrocyclic arrangement of linearly and angularly annelated hexagons. An angularly annelated hexagon, also called a corner, is protruding or intruding if its unique edge with terminal vertices of degree two belongs to the outer or inner perimeter. A primitive coronoid with six protruding corners is called a hollow hexagon (see Figure 1(a)). For a more detailed description of hollow hexagons and their enumeration, we refer the reader to [9].

Known synthesized coronoid hydrocarbons belong to the class of cycloarenes [24]. The first synthesized cycloarene was the  $C_{48}H_{24}$  molecule cyclo  $[d.e.d.e.d.e.d.e.d.e.d.e]$  dodekakisbenzene, also called kekulene [12]. The cycloarene  $C_{40}H_{20}$  cyclo  $[d.e.d.e.d.e.d.e.d.e]$  dekakisbenzene was synthesized in 1986 [14] while the attempt to synthesize  $C_{36}H_{18}$  cyclo  $[d.e.d.e.d.e.d.e.d.e]$  nonakisbenzene was reported in [25], however, as of the time of

writing, there has been no report on the synthesis of this molecule. The above-mentioned cycloarenes are all hollow hexagons.

In this paper, we compute the Mostar index of a hollow hexagon. In general, the structure of coronoid systems makes the problem of computing distance-based topological indices challenging. The calculation of certain distance-based topological indices for coronoid systems—primarily for circumscribed donut-like benzenoid systems—has been the subject of several recent investigations [2, 3, 5, 6]. To obtain the Mostar index of a hollow hexagon, we apply the cut method following the approach used in [22] for the Szeged index. Moreover, we find maximal and minimal values of the Mostar index over the set of hollow hexagons with a fixed number of hexagons.

This paper is organized as follows: In Section 2, the concepts of strength-weighted graph and  $c$ -partition are presented, and the cut method is described. The  $c$ -partition of a hollow hexagon, obtained in [22], is outlined in Section 3, and the expression for computing the Mostar index of a hollow hexagon is obtained in Section 4 (Theorem 4.6). The extremal values of the index over the set of hollow hexagons with a fixed number of hexagons are obtained in Section 5. We draw some conclusions and propose further work in Section 6.

## 2 Cut method, $c$ -partitions, and strength-weighted graphs

Let  $G$  be a connected graph and  $E_1, \dots, E_l$  be a partition of the edge set  $E(G)$  of  $G$ , such that each subgraph  $G - E_i$  is disconnected for  $i \in \{1, \dots, l\}$ . The cut method uses the properties of components of  $G - E_i$  to obtain a specific property of  $G$ .

We say that two edges  $e = xy$  and  $f = uv$  of  $G$  are in the Djoković-Winkler relation  $\Theta$  if  $d(x, u) + d(y, v) \neq d(x, v) + d(y, u)$  [23, 32]. For example, if  $e$  and  $f$  lie in an even induced cycle with  $d(x, u) = d(y, v)$ , then these edges are in  $\Theta$  relation. The relation  $\Theta$  is reflexive and symmetric on  $E(G)$ , but in general, it is not transitive. By  $\Theta^*$  we denote the transitive closure of  $\Theta$ . Let  $\mathcal{Q} = \{Q_1, \dots, Q_r\}$  be a  $\Theta^*$  partition on  $E(G)$ . A  $c$ -partition of  $E(G)$  is a partition  $\mathcal{P} = \{E_1, \dots, E_l\}$  where each  $E_i$  is the union of one or more subsets of  $\mathcal{Q}$ . A  $c$ -partition of a hollow hexagon with  $h$  hexagons was introduced in [22] and it is described in Section 3.

In [2], Arockiaraj et al. introduced the concept of the strength-weighted graph  $G_{sw} = (G, SW_V, SW_E)$  of a simple connected graph  $G$ . It is defined by pairs of strength-weighted functions  $SW_V = (w_v, s_v)$  and  $SW_E = (w_e, s_e)$ , where  $w_v, s_v: V(G) \rightarrow [0, +\infty)$  and  $w_e, s_e: E(G) \rightarrow [0, +\infty)$ . The strength-weighted graph  $G_{sw}$  is normally strength-weighted, if  $w_e(f) \equiv 1$ ,  $s_e(f) \equiv 1$ ,  $w_v(x) \equiv 1$ , and  $s_v(x) \equiv 0$  for any edge  $f \in E(G_{sw})$  and any vertex  $x \in V(G_{sw})$ . If  $e = uv \in E(G_{sw})$ , then

$$n_u(e|G_{sw}) = \sum_{x \in N_u(e|G_{sw})} w_v(x).$$

For a connected, normally strength-weighted graph  $G_{sw}$ , the Mostar index of  $G$  can be expressed as

$$\text{Mo}(G) = \text{Mo}(G_{sw}) = \sum_{\substack{e=uv, \\ e \in E(G_{sw})}} w_e(e|G_{sw}) |n_u(e|G_{sw}) - n_v(e|G_{sw})|. \quad (2.1)$$

Given a graph  $G$  and a subset of edges  $E' \subseteq E(G)$ , by  $G/E'$  we denote the graph with vertex set consisting of connected components of  $G - E'$  and edge subset formed by pairs

of connected components  $X, Y$  such that there is an edge  $uv \in E(G)$  with  $u \in V(X)$  and  $v \in V(Y)$ . This graph is called the quotient graph of  $G$  with respect to  $E'$ .

If  $G_{sw}$  is a normally strength-weighted graph of a connected graph  $G$ ,  $\mathcal{P} = \{E_1, \dots, E_l\}$  a  $c$ -partition of  $E(G)$ , and for  $i \in \{1, \dots, l\}$ ,  $G_{sw}/E_i = (G/E_i, SW_V^i, SW_E^i)$  is the  $i$ th strength-weighted quotient graph, then for  $X \in V(G_{sw}/E_i)$ , the weight  $w_v^i(X)$  is the number of vertices and the strength  $s_v^i(X)$  is the number of edges in the connected component  $X$  of  $G/E_i$ . Moreover, if  $E = XY \in E(G_{sw}/E_i)$  and  $E_{XY}$  is the set of edges between connected components  $X$  and  $Y$  of  $G - E_i$ , then  $s_e^i(E) = |E_{XY}|$  and  $w_e^i(E) = s_e^i(E)$ .

The main result in [6], adapted to the Mostar index, is the following:

**Theorem 2.1.** *Let  $G_{sw}$  be a connected, normally strength-weighted graph of  $G$ . If the set  $\{E_1, \dots, E_l\}$  is a  $c$ -partition of  $E(G) = E(G_{sw})$  then*

$$\begin{aligned} \text{Mo}(G) &= \text{Mo}(G_{sw}) = \sum_{i=1}^l \text{Mo}(G_{sw}/E_i) \\ &= \sum_{i=1}^l \sum_{\substack{e=uv, \\ e \in E(G_{sw}/E_i)}} w_e(e|G_{sw}/E_i) |n_u(e|G_{sw}/E_i) - n_v(e|G_{sw}/E_i)|. \end{aligned}$$

In Section 4, we use the  $c$ -partition described in Section 3 and Theorem 2.1 to compute the Mostar index of a hollow hexagon with  $h$  hexagons. From the expression 2.1, it follows that it is not necessary to compute the vertex strengths in the quotient graphs we use.

### 3 A $c$ -partition of a hollow hexagon

Recall that a hollow hexagon is a primitive coronoid system with exactly six corners and can be described with six positive integer parameters  $a_1, a_2, a_3, a_4, a_5, a_6$ . For each  $i \in \{1, \dots, 6\}$ , the value of  $a_i - 1$  is the number of hexagons between two consecutive corners (see Figure 1(a)). These parameters are related by the following equalities:

$$a_5 = a_1 + a_2 - a_4, \tag{3.1}$$

$$a_6 = a_3 + a_4 - a_1. \tag{3.2}$$

We used the notation introduced in [22] for hollow hexagons. The set of hollow hexagons with  $h$  hexagons is denoted by  $\mathcal{HH}_h$  and each hollow hexagon in  $\mathcal{HH}_h$  is denoted using its four independent parameters as  $a_1, a_2, a_3, a_4$  as  $H(a_1, a_2, a_3, a_4)$ , where

$$h = a_1 + a_2 + a_3 + a_4 + a_5 + a_6 = a_1 + 2(a_2 + a_3) + a_4. \tag{3.3}$$

As an example, the above-mentioned cycloarenes  $C_{48}H_{24}$ ,  $C_{40}H_{20}$ , and  $C_{36}H_{18}$  are represented by  $H(2, 2, 2, 2) \in \mathcal{HH}_{12}$ ,  $H(2, 1, 2, 2) \in \mathcal{HH}_{10}$ , and  $H(2, 1, 2, 1) \in \mathcal{HH}_9$ , respectively.

In order to obtain a  $c$ -partition of the hollow hexagon  $H = H(a_1, a_2, a_3, a_4) \in \mathcal{HH}_h$ , we first describe the set of edges of  $H$ . For  $i \in \{1, \dots, 6\}$ , we denote by  $A_i$  the angular hexagon corresponding to the parameter  $a_i$  and by  $E_i$  the set of edges orthogonal to the straight line intersecting the centers of angular hexagons  $A_i$  and  $A_{i+1}$ . All subscripts are of the form  $j + 1$  where  $j$  is an integer modulo 6 (see Figure 1(b)).

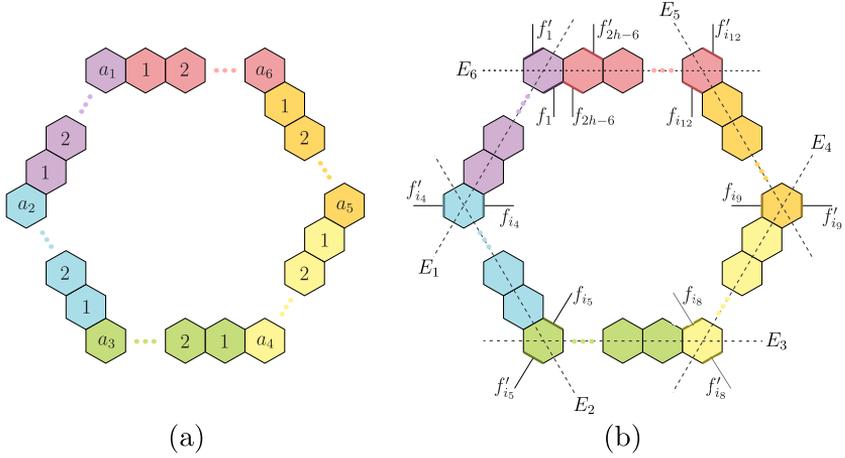


Figure 1: A hollow hexagon with its parameters and different types of edges.

We denote by  $f_1, \dots, f_{2h-6}$  the edges lying in the inner perimeter, indexed counter-clockwise, where  $f_1$  is the edge of the angular hexagon  $A_1$ . For each  $i \in \{1, \dots, 2h-6\}$ , by  $f'_i$  we denote the edge lying in the outer perimeter that is parallel to the edge  $f_i$  in the inner perimeter and belongs to the hexagon that contains  $f_i$  (see Figure 1(b)).

**Remark 3.1.** Two edges  $f_i = uv$  and  $f_j = xy$  in the inner perimeter are diametrically opposite if  $d(u, x) = d(v, y) = h-4$  or equivalently, if  $|i-j| = h-3$ . In this case,  $f_i, f'_i, f_j, f'_j$  can be included in the same subset of a  $c$ -partition of  $E(H)$ . Also, if  $f_{j+1} = yz$  lies in the same linear hexagon of  $f_j$  and  $f'_{j+1} = y'z'$ , then  $d(u, y') = h-3 = d(v, z')$ . In this case,  $f_i, f'_i, f_{j+1}, f'_{j+1}$  can be included in the same subset of a  $c$ -partition of  $E(H)$ .

In what follows, we consider  $a_1 \geq a_4$ . By relation (3.3),  $h$  and  $a_1 - a_4$  have the same parity. Note that when  $h$  is even and  $a_1 = a_4$ , the edges in the inner perimeter belonging to angular hexagons  $A_i$  and  $A_{i+3}$  are diametrically opposite to each other for  $i \in \{1, 2, 3\}$ .

As in [22], for each  $k \in \{1, 2, 3\}$ ,  $i_{4k-3}$  denotes the index of the edge  $f_{i_{4k-3}}$  in the angular hexagon  $A_{2k-1}$  and  $i_{4k}$  denotes the index of the edge  $f_{i_{4k}}$  in the angular hexagon  $A_{2k}$ . Similarly,  $i_{4k+3}$  and  $i_{4k+6}$  denote the indices of edges diametrically opposite to  $f_{i_{4k-3}}$  and  $f_{i_{4k}}$ , respectively. All subscripts are of the form  $j+1$  where  $j$  is an integer modulo 12. The values of these indices were computed in [22] and are presented in Table 1.

	indices of edges in angular hexagons	indices of diametrically opposite edges
$A_1$	$i_1 = 1$	$i_7 = i_8 - (a_1 - a_4)$
$A_2$	$i_4 = 2a_1$	$i_{10} = i_9 + (a_1 - a_4)$
$A_3$	$i_5 = 2a_1 + 2a_2 - 1$	$i_{11} = i_{12} - (a_1 - a_4)$
$A_4$	$i_8 = 2a_1 + 2a_2 + 2a_3 - 2$	$i_2 = i_1 + (a_1 - a_4)$
$A_5$	$i_9 = 2a_1 + 2a_2 + 2a_3 + 2a_4 - 3$	$i_3 = i_4 - (a_1 - a_4)$
$A_6$	$i_{12} = 2a_1 + 2a_2 + 2a_3 + 2a_4 + 2a_5 - 4$	$i_6 = i_5 + (a_1 - a_4)$

Table 1: Indices of diametrically opposite edges  $f_{i_k}$  and  $f_{i_k+6}$ , where  $f_{i_k}$  belongs to an angular hexagon.

For each  $i \in \{1, \dots, 6\}$ , the edges in  $E_i$  are in  $\Theta$  relation, then  $E_1, \dots, E_6$  are subsets of a  $c$ -partition of  $E(H)$  and are illustrated in Figure 1(b).

Let  $h$  be even, and

$$\begin{aligned} E_7 &= f_1, \dots, f_{i_2}, f_{i_7}, \dots, f_{i_8}, f'_1, \dots, f'_{i_2}, f'_{i_7}, \dots, f'_{i_8}, \\ E_8 &= f_{i_3}, \dots, f_{i_4}, f_{i_9}, \dots, f_{i_{10}}, f'_{i_3}, \dots, f'_{i_4}, f'_{i_9}, \dots, f'_{i_{10}}, \\ E_9 &= f_{i_5}, \dots, f_{i_6}, f_{i_{11}}, \dots, f_{i_{12}}, f'_{i_5}, \dots, f'_{i_6}, f'_{i_{11}}, \dots, f'_{i_{12}}. \end{aligned}$$

$E_7$  contains consecutive edges in the inner perimeter, from the edge  $f_1$  of  $A_1$  to the edge  $f_{i_2}$  which is diametrically opposite to the edge  $f_{i_8}$  of  $A_4$ . It also contains consecutive edges from  $f_{i_7}$ , which is diametrically opposite to the edge  $f_1$ , to the edge  $f_{i_8}$ . The set  $E_7$  is completed with the corresponding edges in the outer perimeter (see Figure 2(a)).  $E_8$  is similar to  $E_7$  but contains edges from the angular hexagons  $A_5$  and  $A_2$ .  $E_9$  is also similar to  $E_7$ , but contains edges from the angular hexagons  $A_3$  and  $A_6$ . By Remark 3.1,  $E_7, E_8$ , and  $E_9$  are subsets of a  $c$ -partition of  $E(H)$ .

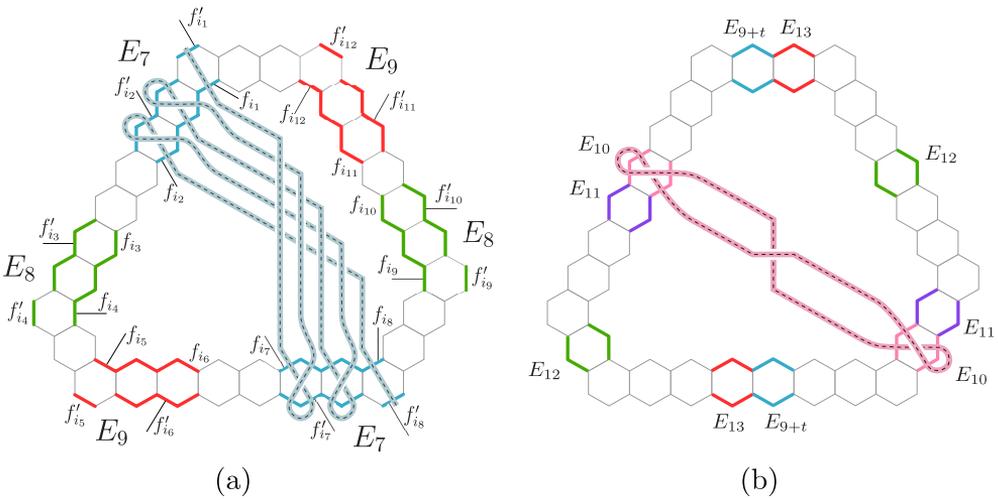


Figure 2: Subsets  $E_7, \dots, E_{9+t}$  that complete the  $c$ -partition of  $H(a_1, a_2, a_3, a_4) \in \mathcal{HH}_h$  when  $h$  is even.

Each of the classes  $E_7, E_8$ , and  $E_9$  contains  $4(a_1 - a_4 + 1)$  edges. If  $a_1 = a_4$ , each class  $E_7, E_8$ , and  $E_9$  contains only 4 edges belonging to the corresponding angular hexagons. Consequently, the edge subsets  $E_7, E_8$ , and  $E_9$ , contain all edges in the inner perimeter belonging to six angular hexagons and  $3(a_1 - a_4)$  linear hexagons. It means that there are  $2t = h - 6 - 3(a_1 - a_4)$  linear hexagons whose edges are not included in  $\cup_{i=1}^9 E_i$ . We denote by  $E_{10}, \dots, E_{9+t}$ , the subsets of edges such that each contains 8 edges: two edges lying in the inner perimeter and belonging to the same linear hexagon, their respective diametrically opposite edges in the inner perimeter, both belonging to one linear hexagon, and the corresponding four edges in the outer perimeter (see Figure 2(b)). For each  $i \in \{10, \dots, 9 + t\}$ , by Remark 3.1,  $E_i$  is a subset of a  $c$ -partition of  $E(H)$ .

It follows that, for  $h$  even,

$$E_1, \dots, E_6, E_7, \dots, E_9, E_{10}, \dots, E_{9+t} \tag{3.4}$$

form a  $c$ -partition of  $E(H)$ , where  $t = \frac{h-6-3(a_1-a_4)}{2}$ .

Let  $h$  be odd, then  $a_1 - a_4$  is also odd. Let

$$\begin{aligned} E'_7 &= f_{i_{12}}, \dots, f_{2h-6}, f_1, f_{i_6}, \dots, f_{i_7}, f'_{i_{12}}, \dots, f'_{2h-6}, f'_1, f'_{i_6}, \dots, f'_{i_7}, \\ E'_8 &= f_{i_4}, \dots, f_{i_5}, f_{i_{10}}, \dots, f_{i_{11}}, f'_{i_4}, \dots, f'_{i_5}, f'_{i_{10}}, \dots, f'_{i_{11}}, \\ E'_9 &= f_{i_8}, \dots, f_{i_9}, f_{i_2}, \dots, f_{i_3}, f'_{i_8}, \dots, f'_{i_9}, f'_{i_2}, \dots, f'_{i_3}. \end{aligned}$$

$E'_7$  contains consecutive edges in the inner perimeter from the edge  $f_{i_{12}}$  of  $A_6$  to the edge  $f_1$  of  $A_1$ , the edges in the inner perimeter diametrically opposite to the mentioned edges, and the corresponding edges in the outer perimeter.  $E'_8$  is similar to  $E'_7$  but containing edges from the angular hexagons  $A_2$  and  $A_3$ . Finally,  $E'_9$  is also similar to  $E'_7$  but containing edges of angular hexagons  $A_4$  and  $A_5$  (see Figure 3(a)). By Remark 3.1,  $E'_7, E'_8$ , and  $E'_9$  are subsets a  $c$ -partiton of  $E(H)$ .

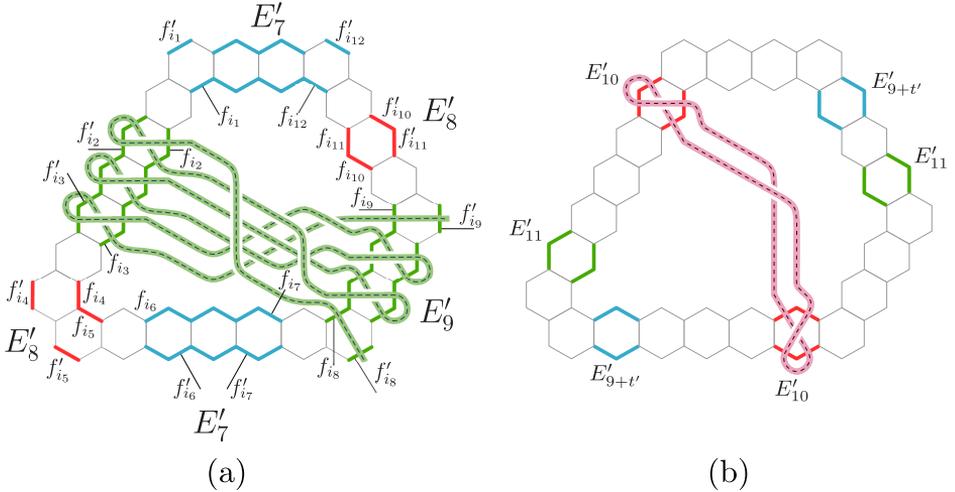


Figure 3: Subsets  $E'_7, \dots, E'_{9+t'}$  that complete the  $c$ -partition of  $H(a_1, a_2, a_3, a_4) \in \mathcal{HH}_h$  when  $h$  is odd.

The edge subset  $E'_7$  contains  $4a_6$  edges lying in  $2a_6 + 1$  hexagons,  $E'_8$  contains  $4a_2$  edges lying in  $2a_2 + 1$  hexagons, and  $E'_9$  contains  $4a_4$  edges lying in  $2a_4 + 1$  hexagons. Then  $E'_7, E'_8$ , and  $E'_9$ , contain all edges in the inner perimeter belonging to  $2(a_2 + a_4 + a_6) + 3$  hexagons, including all the six angular hexagons. Since  $2(a_2 + a_4 + a_6) = h - 3(a_1 - a_4)$ , there are  $2t' = 3(a_1 - a_4 - 1)$  linear hexagons whose edges are not included in  $(\cup_{i=1}^6 E_i) \cup (\cup_{i=7}^9 E'_i)$ . We denote by  $E'_{10}, \dots, E'_{9+t'}$  the subsets of edges such that each contains 8 edges, two edges lying in the inner perimeter and belonging to the same linear hexagon, their diametrically opposite edges in inner perimeter, both belonging to one linear hexagon, and the corresponding 4 edges in the outer perimeter (see Figure 3(b)). For each  $i \in \{10, \dots, 9 + t'\}$ , by Remark 3.1,  $E'_i$  is a subset of a  $c$ -partition of  $E(H)$ .

Consequently, for  $h$  odd,

$$E_1, \dots, E_6, E'_7, \dots, E'_9, E'_{10}, \dots, E'_{9+t'} \tag{3.5}$$

form a  $c$ -partition of  $E(H)$ , where  $t' = \frac{3(a_1 - a_4 - 1)}{2}$ .

### 4 Mostar index of a hollow hexagon

Let  $H = H(a_1, a_2, a_3, a_4) \in \mathcal{HH}_h$  and  $H_{sw}$  its strength-weighted graph. Now we describe the quotient graphs corresponding to each subset in the  $c$ -partition of  $E(H)$ . These quotient graphs were obtained in [22].

For  $i \in \{1, \dots, 6\}$ , let  $H_i = (H_{sw}/E_i, (w_v^i, s_v^i), (w_e^i, s_e^i))$  be the strength-weighted quotient graph of  $H_{sw}$  corresponding to edge subset  $E_i$ . The quotient graph  $H_i$  depends on the parameter  $a_i$  and it is depicted in Figure 4(a). The subsets  $E_1, \dots, E_6$  are shown in Figure 1(b).

If  $h$  is even, for  $i \in \{7, \dots, 9 + t\}$ , let  $H_i = (H_{sw}/E_i, (w_v^i, s_v^i), (w_e^i, s_e^i))$  be the strength-weighted quotient graph of  $H_{sw}$  corresponding to edge subset  $E_i$ , where  $2t = h - 6 - 3(a_1 - a_4)$ . The subsets  $E_7, E_8$ , and  $E_9$  are depicted in Figure 2(a) while the subsets  $E_{10}, \dots, E_{9+t}$  are depicted in Figure 2(b). The quotient graphs  $H_7, H_8$ , and  $H_9$  are isomorphic, so we depict only  $H_7$  in Figure 4(b) if  $a_1 > a_4$  and in Figure 4(c) if  $a_1 = a_4$ . Similarly, the quotient graphs  $H_{10}, \dots, H_{9+t}$  are isomorphic, so we show only  $H_{10}$  in Figure 4(d). Using Theorem 2.1, for  $h$  even we obtain

$$\text{Mo}(H) = \sum_{i=1}^6 \text{Mo}(H_i) + 3 \text{Mo}(H_7) + t \text{Mo}(H_{10}). \tag{4.1}$$

If  $h$  is odd, for  $i \in \{7, \dots, 9 + t'\}$ , let  $H'_i = (H_{sw}/E'_i, (w_v^i, s_v^i), (w_e^i, s_e^i))$  be the strength-weighted quotient graph of  $H_{sw}$  corresponding to edge subset  $E'_i$ , where  $2t' = 3(a_1 - a_4 - 1)$ . The subsets  $E'_7, E'_8$ , and  $E'_9$  are depicted in Figure 3(a) while the subsets  $E'_{10}, \dots, E'_{9+t'}$  are depicted in Figure 3(b). For  $l \in \{7, 8, 9\}$ , the quotient graph  $H'_l$  depends on parameter  $r_l$ , where  $r_7 = a_6, r_8 = a_2$ , and  $r_9 = a_4$ . The quotient graph  $H'_l$  is depicted in Figure 5(a) if  $r_l = 1$ , in Figure 5(b) if  $r_l = 2$ , and in Figure 5(c) if  $r_l > 2$ . On the other hand, the quotient graphs  $H'_{10}, \dots, H'_{9+t'}$  are isomorphic, so we only show  $H'_{10}$  in Figure 5(d). Using Theorem 2.1, for  $h$  odd we obtain

$$\text{Mo}(H) = \sum_{i=1}^6 \text{Mo}(H_i) + \sum_{l=7}^9 \text{Mo}(H'_l) + t' \text{Mo}(H'_{10}). \tag{4.2}$$

In order to obtain the expression to compute the Mostar index of a hollow hexagon, in the following lemmas we find the value of the Mostar index for each quotient graph in equalities (4.1) and (4.2).

Let  $\bar{H}$  be a quotient graph and  $e = uv$  and  $e' = u'v'$  two edges of  $\bar{H}$ . We say that in this quotient graph the edges  $e$  and  $e'$  are equivalent if  $w_e(e|\bar{H}) = w_{e'}(e'|\bar{H}), n_u(e|\bar{H}) = n_{u'}(e'|\bar{H}),$  and  $n_v(e|\bar{H}) = n_{v'}(e'|\bar{H})$ .

**Lemma 4.1.** *Let  $i \in \{1, \dots, 6\}$ , then  $\text{Mo}(H_i) = (2 + a_i)(4h - 4a_i - 6)$ .*

*Proof.* The following parameters for the quotient graph  $H_i$  (see Figure 4(a)), were computed in [22, Lemma 1]:

$$n_{u_i}(e_i|H_i) = 2a_i + 3, \quad n_{v_i}(e_i|H_i) = 4h - 2a_i - 3, \quad w_e(e_i|H_i) = s_e(e_i|H_i) = a_i + 2.$$

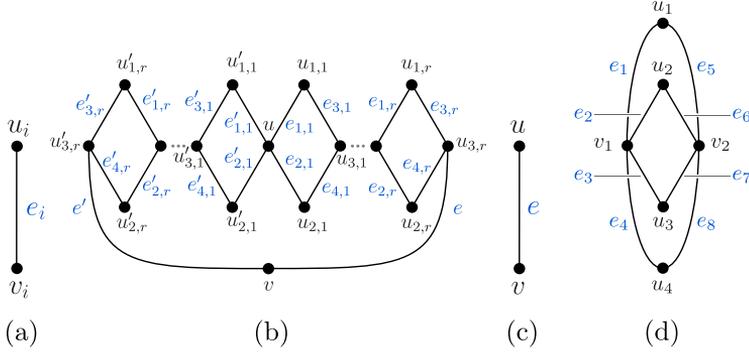


Figure 4: Quotient graphs of  $H(a_1, a_2, a_3, a_4) \in \mathcal{HH}_h$  when  $h$  is even.

Relation (3.3) implies  $h \geq a_i + 5$  for any  $i \in \{1, \dots, 6\}$ . Since

$$\text{Mo}(H_i) = w_e(e_i|H_i) |n_{u_i}(e_i|H_i) - n_{v_i}(e_i|H_i)|,$$

we are done. □

**Lemma 4.2.** *Let  $h$  be even, then  $\text{Mo}(H_7) = 16(a_1 - a_4)$ .*

*Proof.* Let  $2r = a_1 - a_4$ . If  $r = 0$  (so  $a_1 - a_4 = 0$ ), the following parameters for the quotient graph  $H_7$  (see Figure 4(c)) were computed in [22, Lemma 2]:

$$n_u(e|H_7) = n_v(e|H_7) = 2h, \quad w_e(e|H_7) = s_e(e|H_7) = 4.$$

Then  $\text{Mo}(H_7) = w_e(e|H_7) |n_u(e|H_7) - n_v(e|H_7)| = 0$ .

If  $r > 0$  (so  $a_1 - a_4 \geq 2$ ), the quotient graph  $H_7$  is shown in Figure 4(b). By the equivalence of edges found in  $H_7$ , we get the following subsets of equivalent edges:  $\{e, e'\}$ ,  $\{e_{1,1}, e'_{1,1}, e_{2,1}, e'_{2,1}\}$ , the subsets  $\{e_{3,j}, e'_{3,j}, e_{4,j}, e'_{4,j}\}$  for each  $j \in \{1, \dots, r\}$ , and the subsets  $\{e_{1,j}, e'_{1,j}, e_{2,j}, e'_{2,j}\}$  for each  $j \in \{2, \dots, r\}$  if  $r > 1$ .

The expressions for  $n_u$ ,  $n_v$ , and  $w_e$  for each edge in the quotient graph  $H_7$  were computed in [22, Lemma 2]:

$$\begin{aligned} n_v(e|H_7) &= 2h + 1, & n_{u_{3,r}}(e|H_7) &= 2h - 1, & w_e(e|H_7) &= 2, \\ n_u(e_{1,1}|H_7) &= 2h, & n_{u_{1,1}}(e_{1,1}|H_7) &= 2h, & w_e(e_{1,1}|H_7) &= 1. \end{aligned}$$

For  $j \in \{1, \dots, r\}$

$$n_{u_{3,j}}(e_{3,j}|H_7) = 2h + 3, \quad n_{u_{1,j}}(e_{3,j}|H_7) = 2h - 3, \quad w_e(e_{3,j}|H_7) = 1,$$

and if  $r > 1$ , for  $j \in \{2, \dots, r\}$

$$n_{u_{1,j}}(e_{1,j}|H_7) = 2h + 1, \quad n_{u_{3,j-1}}(e_{1,j}|H_7) = 2h - 1, \quad w_e(e_{1,j}|H_7) = 1.$$

Note that for  $r > 0$ , the parameters associated to the edges  $e_{3,j}$  for  $j \in \{1, \dots, r\}$  are equal. The same is true for the parameters associated with the edges  $e_{1,j}$  for  $j \in \{2, \dots, r\}$  when  $r > 1$ . Then

$$\begin{aligned} \text{Mo}(H_7) &= 2w_e(e|H_7) |n_v(e|H_7) - n_{u_{3,r}}(e|H_7)| + \\ &\quad 4w_e(e_{1,1}|H_7) |n_u(e_{1,1}|H_7) - n_{u_{1,1}}(e_{1,1}|H_7)| + \\ &\quad 4rw_e(e_{3,r}|H_7) |n_{u_{3,r}}(e_{3,r}|H_7) - n_{u_{1,r}}(e_{3,r}|H_7)| + \\ &\quad 4(r-1)w_e(e_{1,2}|H_7) |n_{u_{1,2}}(e_{1,2}|H_7) - n_{u_{3,1}}(e_{1,2}|H_7)| \\ &= 8 + 24r + 8(r-1) = 32r = 16(a_1 - a_4). \end{aligned} \quad \square$$

**Lemma 4.3.** *Let  $h$  be even, then  $\text{Mo}(H_{10}) = 16$ .*

*Proof.* Note that all edges  $e_1, \dots, e_8$  in  $H_{10}$  are equivalent (see Figure 4(d)). The expressions  $n_u, n_v$ , and  $w_e$  for  $e_1$  were computed in [22, Lemma 3]:

$$n_{v_1}(e_1|H_{10}) = 2h - 1, \quad n_{u_1}(e_1|H_{10}) = 2h + 1, \quad w_e(e_1|H_{10}) = 1.$$

Then  $\text{Mo}(H_{10}) = 8w_e(e_1|H_{10}) |n_{v_1}(e_1|H_{10}) - n_{u_1}(e_1|H_{10})| = 16$ . □

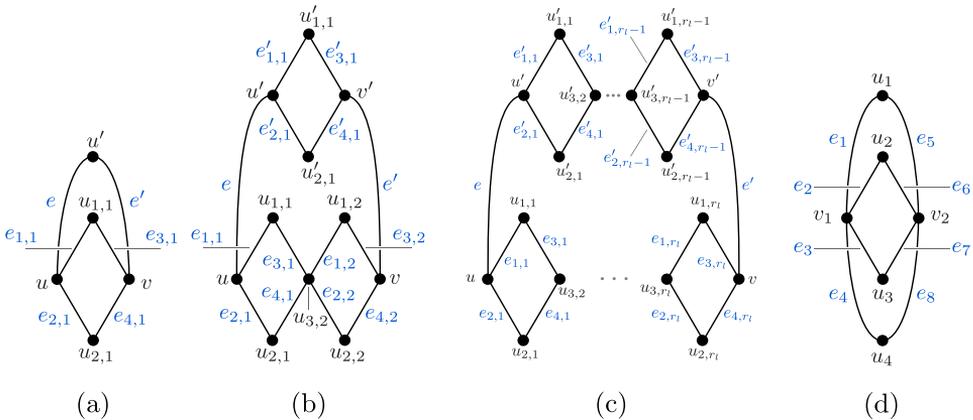


Figure 5: Quotient graphs of  $H(a_1, a_2, a_3, a_4) \in \mathcal{H}_h$  when  $h$  is odd.

**Lemma 4.4.** *Let  $h$  be odd and  $l \in \{7, 8, 9\}$ , then  $\text{Mo}(H'_l) = 16r_l + 8$ , where  $r_7 = a_6$ ,  $r_8 = a_2$ , and  $r_9 = a_4$ .*

*Proof.* Recall that  $r_7 = a_6$ ,  $r_8 = a_2$ , and  $r_9 = a_4$ . If  $r_l = 1$ , by the equivalence of edges found in the quotient graph  $H'_l$  (see Figure 5(a)), we have the following subsets of equivalent edges:  $\{e_{1,1}, e_{2,1}, e_{3,1}, e_{4,1}\}$  and  $\{e, e'\}$ . After [22, Lemma 4], the values of  $n_u, n_v$ , and  $w_e$  for the edges  $e$  and  $e_{1,1}$  are:

$$\begin{aligned} n_u(e|H'_l) &= 2h - 1, & n_{u'}(e|H'_l) &= 2h + 1, & w_e(e|H'_l) &= 2, \\ n_u(e_{1,1}|H'_l) &= 2h + 2, & n_{u_{1,1}}(e_{1,1}|H'_l) &= 2h - 2, & w_e(e_{1,1}|H'_l) &= 1. \end{aligned}$$

Then

$$\begin{aligned} \text{Mo}(H'_l) &= 2w_e(e|H'_l) |n_u(e|H'_l) - n_{u'}(e|H'_l)| + \\ & 4w_e(e_{1,1}|H'_l) |n_u(e_{1,1}|H'_l) - n_{u_{1,1}}(e_{1,1}|H'_l)| = 24. \end{aligned}$$

If  $r_l = 2$  (see Figure 5(b)), we have the following subsets of equivalent edges in  $H'_l$ :  $\{e'_{1,1}, e'_{2,1}, e'_{3,1}, e'_{4,1}\}$ ,  $\{e_{1,1}, e_{2,1}, e_{3,2}, e_{4,2}\}$ ,  $\{e_{1,2}, e_{2,2}, e_{3,1}, e_{4,1}\}$ , and  $\{e, e'\}$ . After [22, Lemma 4], the values of  $n_u$ ,  $n_v$ , and  $w_e$  for the edges  $e$ ,  $e_{1,1}$ ,  $e_{1,2}$ , and  $e'_{1,1}$  are:

$$\begin{aligned} n_u(e|H'_l) &= 2h - 1, & n_{u'}(e|H'_l) &= 2h + 1, & w_e(e|H'_l) &= 2, \\ n_u(e_{1,1}|H'_l) &= 2h + 2, & n_{u_{1,1}}(e_{1,1}|H'_l) &= 2h - 2, & w_e(e_{1,1}|H'_l) &= 1, \\ n_{u_{3,2}}(e_{1,2}|H'_l) &= 2h + 1, & n_{u_{1,2}}(e_{1,2}|H'_l) &= 2h - 1, & w_e(e_{1,2}|H'_l) &= 1, \\ n_{u'}(e'_{1,1}|H'_l) &= 2h + 1, & n_{u'_{1,1}}(e'_{1,1}|H'_l) &= 2h - 1, & w_e(e'_{1,1}|H'_l) &= 1. \end{aligned}$$

Then

$$\begin{aligned} \text{Mo}(H'_l) &= 2w_e(e|H'_l) |n_u(e|H'_l) - n_{u'}(e|H'_l)| + \\ & 4w_e(e_{1,1}|H'_l) |n_u(e_{1,1}|H'_l) - n_{u_{1,1}}(e_{1,1}|H'_l)| + \\ & 4w_e(e_{1,2}|H'_l) |n_{u_{3,2}}(e_{1,2}|H'_l) - n_{u_{1,2}}(e_{1,2}|H'_l)| + \\ & 4w_e(e'_{1,1}|H'_l) |n_{u'}(e'_{1,1}|H'_l) - n_{u'_{1,1}}(e'_{1,1}|H'_l)| = 40. \end{aligned}$$

Finally, if  $r_l > 2$  (see Figure 5(c)), by the equivalence of edges found in  $H'_l$  we have the following subsets of equivalent edges:

$$\begin{aligned} & \{e, e'\}, \{e_{1,1}, e_{2,1}, e_{3,r_l}, e_{4,r_l}\}, \{e'_{1,1}, e'_{2,1}, e'_{3,r_l}, e'_{4,r_l}\}, \\ & \{e_{3,1}, e_{4,1}, e_{1,r_l}, e_{2,r_l}, e_{i,j} : i = 1, \dots, 4, j = 2, \dots, r_l - 1\}, \\ & \{e'_{3,1}, e'_{4,1}, e'_{1,r_l-1}, e'_{2,r_l-1}, e'_{i,j} : i = 1, \dots, 4, j = 2, \dots, r_l - 2\}. \end{aligned}$$

In [22, Lemma 4], the following values of  $n_u$ ,  $n_v$  and  $w_e$  for the edges  $e$ ,  $e_{1,1}$ ,  $e_{3,1}$ ,  $e'_{1,1}$ , and  $e'_{3,1}$  were computed:

$$\begin{aligned} n_u(e|H'_l) &= 2h - 1, & n_{u'}(e|H'_l) &= 2h + 1, & w_e(e|H'_l) &= 2, \\ n_u(e_{1,1}|H'_l) &= 2h + 2, & n_{u_{1,1}}(e_{1,1}|H'_l) &= 2h - 2, & w_e(e_{1,1}|H'_l) &= 1, \\ n_{u_{1,1}}(e_{3,1}|H'_l) &= 2h - 1, & n_{u_{3,2}}(e_{3,1}|H'_l) &= 2h + 1, & w_e(e_{3,1}|H'_l) &= 1, \\ n_{u'}(e'_{1,1}|H'_l) &= 2h + 1, & n_{u'_{1,1}}(e'_{1,1}|H'_l) &= 2h - 1, & w_e(e'_{1,1}|H'_l) &= 1, \\ n_{u'_{1,1}}(e'_{3,1}|H'_l) &= 2h - 1, & n_{u'_{3,2}}(e'_{3,1}|H'_l) &= 2h + 1, & w_e(e'_{3,1}|H'_l) &= 1. \end{aligned}$$

Then

$$\begin{aligned} \text{Mo}(H'_l) &= 2w_e(e|H'_l) |n_u(e|H'_l) - n_{u'}(e|H'_l)| + \\ & 4w_e(e_{1,1}|H'_l) |n_u(e_{1,1}|H'_l) - n_{u_{1,1}}(e_{1,1}|H'_l)| + \\ & 4(r_l - 1)w_e(e_{3,1}|H'_l) |n_{u_{1,1}}(e_{3,1}|H'_l) - n_{u_{3,2}}(e_{3,1}|H'_l)| + \\ & 4w_e(e'_{1,1}|H'_l) |n_{u'}(e'_{1,1}|H'_l) - n_{u'_{1,1}}(e'_{1,1}|H'_l)| + \\ & 4(r_l - 2)w_e(e'_{3,1}|H'_l) |n_{u'_{1,1}}(e'_{3,1}|H'_l) - n_{u'_{3,2}}(e'_{3,1}|H'_l)| \\ & = 16r_l + 8. \end{aligned}$$

□

**Lemma 4.5.** *Let  $h$  be odd, then  $\text{Mo}(H'_{10}) = 32$ .*

*Proof.* By the equivalence of edges found in  $H'_{10}$  (see Figure 5(d)), we have the following two subsets of equivalent edges:  $\{e_1, e_2, e_3, e_4\}$  and  $\{e_5, e_6, e_7, e_8\}$ . In [22, Lemma 6], the following values of  $n_u$ ,  $n_v$ , and  $w_e$  for the edges  $e_1$  and  $e_5$  were computed:

$$\begin{aligned} n_{v_1}(e_1|H'_{10}) &= 2h - 1, & n_{u_1}(e_1|H'_{10}) &= 2h + 1, & w_e(e_1|H'_{10}) &= 1, \\ n_{v_2}(e_5|H'_{10}) &= 2h + 3, & n_{u_1}(e_5|H'_{10}) &= 2h - 3, & w_e(e_5|H'_{10}) &= 1. \end{aligned}$$

Then

$$\begin{aligned} \text{Mo}(H'_{10}) &= 4w_e(e_1|H'_{10}) |n_{v_1}(e_1|H'_{10}) - n_{u_1}(e_1|H'_{10})| + \\ & 4w_e(e_5|H'_{10}) |n_{v_2}(e_5|H'_{10}) - n_{u_1}(e_5|H'_{10})| = 32. \quad \square \end{aligned}$$

The expression to compute the Mostar index of a hollow hexagon  $H(a_1, a_2, a_3, a_4) \in \mathcal{HH}_h$  is the main result of this section.

**Theorem 4.6.** *Let  $h \geq 8$  and  $H = H(a_1, a_2, a_3, a_4) \in \mathcal{HH}_h$ , then*

$$\text{Mo}(H) = \sum_{i=1}^6 (2 + a_i)(4h - 4a_i - 6) + 8h + 24(a_1 - a_4) - b(h),$$

where  $b(h) = 48$  if  $h$  is even and  $b(h) = 24$  if  $h$  is odd.

*Proof.* If  $h$  is even, using equality (4.1) and Lemmas 4.1, 4.2, and 4.3 we obtain

$$\begin{aligned} \text{Mo}(H) &= \sum_{i=1}^6 \text{Mo}(H_i) + 3 \text{Mo}(H_7) + t \text{Mo}(H_{10}) \\ &= \sum_{i=1}^6 (2 + a_i)(4h - 4a_i - 6) + 3(16)(a_1 - a_4) + \frac{h - 6 - 3(a_1 - a_4)}{2} (16) \\ &= \sum_{i=1}^6 (2 + a_i)(4h - 4a_i - 6) + 8h + 24(a_1 - a_4) - 48. \end{aligned}$$

If  $h$  is odd, using equality (4.2) and Lemmas 4.1, 4.4, and 4.5 we obtain

$$\begin{aligned} \text{Mo}(H) &= \sum_{i=1}^6 \text{Mo}(H_i) + \sum_{l=7}^9 \text{Mo}(H'_l) + t' \text{Mo}(H'_{10}) \\ &= \sum_{i=1}^6 (2 + a_i)(4h - 4a_i - 6) + \\ & 16(a_6 + a_2 + a_4) + 24 + \frac{3(a_1 - a_4 - 1)}{2} (32). \end{aligned}$$

By relations (3.1), (3.2), and (3.3), it is easy to see that  $2(a_2 + a_4 + a_6) = h - 3(a_1 - a_4)$ . Then

$$\begin{aligned} \text{Mo}(H) &= \sum_{i=1}^6 (2 + a_i)(4h - 4a_i - 6) + 8h - 24(a_1 - a_4) + 24 + 48(a_1 - a_4 - 1) \\ &= \sum_{i=1}^6 (2 + a_i)(4h - 4a_i - 6) + 8h + 24(a_1 - a_4) - 24. \quad \square \end{aligned}$$

## 5 Extremal hollow hexagons with respect to the Mostar index

In this section we find the extremal values of the Mostar index over the set  $\mathcal{HH}_h$ .

Given  $H = H(a_1, a_2, a_3, a_4) \in \mathcal{HH}_h$ , the parameters are related by relations (3.1), (3.2), and (3.3). Also, we assume that  $1 \leq a_2 \leq a_4 \leq a_1 \leq a_3$ . Recall that  $h$  and  $a_1 - a_4$  have the same parity. Then we assume that  $1 \leq a_2 \leq a_4 \leq a_1 \leq a_3 \leq \frac{h-4}{2}$  if  $h$  is even, and  $1 \leq a_2 \leq a_4 < a_1 \leq a_3 \leq \frac{h-5}{2}$  if  $h$  is odd. The upper bounds for  $a_3$  are easily justified after (3.3) and the fact that  $a_1, a_2$ , and  $a_4$  are at least 1. So, when  $h$  is even,  $h = a_1 + 2a_2 + 2a_3 + a_4 \geq 4 + 2a_3$  explains the bound. Proceed in a similar manner for the odd case, but remember that  $a_1 > 1$ , hence  $a_1 \geq 2$ .

We denote by  $\text{Mo}(a_1, a_2, a_3, a_4)$  the Mostar index of  $H = H(a_1, a_2, a_3, a_4)$ . By Theorem 4.6, we have

$$\text{Mo}(a_1, a_2, a_3, a_4) = \sum_{i=1}^6 g(a_i, h) + 24(a_1 - a_4) + 8h - b(h),$$

where  $b(h) = 48$  if  $h$  is even,  $b(h) = 24$  if  $h$  is odd, and  $g(x, h) = (2 + x)(4h - 4x - 6)$ .

In order to determine the extremal values for the Mostar index, we need to solve the following integer programming problems:

$$\begin{array}{ll} \underset{(a_1, a_2, a_3, a_4) \in \mathbb{Z}^4}{\text{minimize}} & \text{Mo}(a_1, a_2, a_3, a_4) \quad | \quad \underset{(a_1, a_2, a_3, a_4) \in \mathbb{Z}^4}{\text{maximize}} \quad \text{Mo}(a_1, a_2, a_3, a_4) \\ \text{subject to} & \begin{aligned} a_1 + a_2 - a_4 &= a_5, \\ a_3 + a_4 - a_1 &= a_6, \\ a_1 + 2(a_2 + a_3) + a_4 &= h, \\ 1 \leq a_2 \leq a_4 \leq a_1 \leq a_3 &\leq \left\lfloor \frac{h-4}{2} \right\rfloor. \end{aligned} \end{array}$$

To solve them, we decrease or increase by one unit the values of the variables successively, respecting the constraints, so that the value of the objective function decreases (for the minimum problem) or increases (for the maximum problem).

The following technical lemmas will be used to prove the main results of this section.

**Lemma 5.1.** *Let  $h \geq 10$  and  $1 < a_2 \leq a_4 \leq a_1 \leq a_3 < \left\lfloor \frac{h-4}{2} \right\rfloor$ , then*

$$\text{Mo}(a_1, a_2 - 1, a_3 + 1, a_4) < \text{Mo}(a_1, a_2, a_3, a_4).$$

*Proof.* Using relations (3.1), (3.2), and (3.3) we obtain

$$\begin{aligned} \Delta_g &= \text{Mo}(a_1, a_2 - 1, a_3 + 1, a_4) - \text{Mo}(a_1, a_2, a_3, a_4) \\ &= g(a_2 - 1, h) - g(a_2, h) + g(a_3 + 1, h) - g(a_3, h) + \\ &\quad g(a_5 - 1, h) - g(a_5, h) + g(a_6 + 1, h) - g(a_6, h) \\ &= 16(a_2 - a_4 + a_1 - a_3 - 1) < 0. \end{aligned} \quad \square$$

**Lemma 5.2.** *Let  $1 \leq a_2 < a_4 \leq a_1 \leq a_3 < \left\lfloor \frac{h-4}{2} \right\rfloor$ , then*

$$\text{Mo}(a_1 - 1, a_2, a_3 + 1, a_4 - 1) < \text{Mo}(a_1, a_2, a_3, a_4).$$

*Proof.* Since there are no changes in parameters  $a_2$  and  $a_5$ , using relations (3.2) and (3.3) we obtain

$$\begin{aligned} \Delta_g &= \text{Mo}(a_1 - 1, a_2, a_3 + 1, a_4 - 1) - \text{Mo}(a_1, a_2, a_3, a_4) \\ &= g(a_1 - 1, h) - g(a_1, h) + g(a_3 + 1, h) - g(a_3, h) + \\ &\quad g(a_4 - 1, h) - g(a_4, h) + g(a_6 + 1, h) - g(a_6, h) \\ &= 16(a_1 - a_3 - 1) < 0. \end{aligned} \quad \square$$

**Lemma 5.3.** *Let  $h \geq 10$  and  $1 \leq a_2 \leq a_4 < a_1 \leq a_3$ .*

*If  $a_1 - a_4 \geq 4$ , then*

$$\text{Mo}(a_1 - 1, a_2 + 1, a_3 - 1, a_4 + 1) > \text{Mo}(a_1, a_2, a_3, a_4).$$

*If  $a_1 - a_4 = 3$ , then*

$$\text{Mo}(a_1 - 1, a_2 + 1, a_3 - 1, a_4 + 1) = \text{Mo}(a_1, a_2, a_3, a_4).$$

*Proof.* Using relations (3.1), (3.2), and (3.3) we obtain

$$\begin{aligned} \Delta &= \text{Mo}(a_1 - 1, a_2 + 1, a_3 - 1, a_4 + 1) - \text{Mo}(a_1, a_2, a_3, a_4) \\ &= g(a_1 - 1, h) - g(a_1, h) + g(a_4 + 1, h) - g(a_4, h) + \\ &\quad g(a_2 + 1, h) - g(a_2, h) + g(a_5 - 1, h) - g(a_5, h) + \\ &\quad g(a_3 - 1, h) - g(a_3, h) + g(a_6 + 1, h) - g(a_6, h) - 48 \\ &= 24(a_1 - a_4 - 3). \end{aligned} \quad \square$$

**Theorem 5.4.** *Let  $h \geq 12$  and  $\mathcal{HH}_h$  be the set of hollow hexagons with  $h$  hexagons. The hollow hexagon with the minimal value of the Mostar index is*

- (1)  $H = H(1, 1, \frac{h-4}{2}, 1)$  if  $h$  is even,
- (2)  $H = H(2, 1, \frac{h-5}{2}, 1)$  if  $h$  is odd.

*Proof.* Let's consider each case separately, first for the even case and then for the odd case.

- (1) Let  $h \geq 12$  be even and  $H(a_1, a_2, a_3, a_4) \in \mathcal{HH}_h$  with  $1 \leq a_2 \leq a_4 \leq a_1 \leq a_3 \leq \frac{h-4}{2}$ . Note that  $a_2 + a_3 = \frac{h-a_1-a_4}{2} \leq \frac{h-2}{2}$ . If  $a_2 + a_3 = \frac{h-2}{2}$ , then  $a_1 + a_4 = 2$ . Thus  $a_2 = a_1 = a_4 = 1, a_3 = \frac{h-4}{2}$ , as required.

Now, assume that  $a_3 + a_2 < \frac{h-2}{2}$ . If  $a_2 > 1$ , it follows that  $a_3 + a_2 - 1 < \frac{h-4}{2}$ . By Lemma 5.1,  $\text{Mo}(a_1, a_2, a_3, a_4) > \text{Mo}(a_1, 1, a_3 + a_2 - 1, a_4)$ . We may then consider hollow hexagons of the form  $H(a_1, 1, a_3, a_4)$  where  $1 \leq a_4 \leq a_1 \leq a_3 \leq \frac{h-4}{2}$ . If  $a_3 = \frac{h-4}{2}$ , then  $a_1 + a_4 = 2$ ; consequently  $a_1 = a_4 = 1$  and we are done. If  $a_3 < \frac{h-4}{2}$ , using repeatedly Lemma 5.2, we end up with one of the following situations:

- (a)  $\text{Mo}(a_1, 1, a_3, a_4) > \text{Mo}(a_1 + a_3 - \frac{h-4}{2}, 1, \frac{h-4}{2}, a_4 + a_3 - \frac{h-4}{2})$ . We may then consider hollow hexagons of the form  $H = (a_1, 1, \frac{h-4}{2}, a_4)$ , but in this case  $a_1 + a_4 = 2$ , so  $a_1 = a_4 = 1$ .

- (b)  $\text{Mo}(a_1, 1, a_3, a_4) > \text{Mo}(a_1 - a_4 + 1, 1, a_3 + a_4 - 1, 1)$ . If  $a_4 = a_1$  we are done. Otherwise, we may consider hollow hexagons of the form  $H = H(a_1, 1, a_3, 1)$  where  $1 < a_1 \leq a_3 < \frac{h-4}{2}$ . Using relations (3.1), (3.2), and (3.3), we calculate the difference

$$\text{Mo}\left(1, 1, \frac{h-4}{2}, 1\right) - \text{Mo}(a_1, 1, a_3, 1) = -2(a_1 - 1)(8a_3 - 5a_1 + 9) < 0.$$

- (2) Let  $h \geq 13$  be odd and  $H(a_1, a_2, a_3, a_4) \in \mathcal{HH}_h$ . It implies  $1 \leq a_2 \leq a_4 < a_1 \leq a_3 \leq \frac{h-5}{2}$ . Note that  $a_2 + a_3 = \frac{h-a_1-a_4}{2} \leq \frac{h-3}{2}$ . If  $a_2 + a_3 = \frac{h-3}{2}$ , then  $a_1 + a_4 = 3$ . Thus  $a_1 = 2, a_2 = a_4 = 1, a_3 = \frac{h-5}{2}$ , as required.

Now, assume that  $a_3 + a_2 < \frac{h-3}{2}$ . If  $a_2 > 1$ , it follows that  $a_3 + a_2 - 1 < \frac{h-5}{2}$ . By Lemma 5.1,  $\text{Mo}(a_1, a_2, a_3, a_4) > \text{Mo}(a_1, 1, a_3 + a_2 - 1, a_4)$ . We may then consider the hollow hexagons of the form  $H(a_1, 1, a_3, a_4)$  where  $1 \leq a_4 < a_1 \leq a_3 \leq \frac{h-5}{2}$ . If  $a_3 = \frac{h-5}{2}$ , then  $a_1 + a_4 = 3$ ; consequently  $a_1 = 2, a_4 = 1$  and we are done. If  $a_3 < \frac{h-5}{2}$ , using repeatedly Lemma 5.2, we end up with one of the following situations:

- (a)  $\text{Mo}(a_1, 1, a_3, a_4) > \text{Mo}(a_1 + a_3 - \frac{h-5}{2}, 1, \frac{h-5}{2}, a_4 + a_3 - \frac{h-5}{2})$ . We may then consider hollow hexagons of the form  $H = H(a_1, 1, \frac{h-5}{2}, a_4)$ , but in this case  $a_1 + a_4 = 3$ , so  $a_1 = 2, a_4 = 1$ .
- (b)  $\text{Mo}(a_1, 1, a_3, a_4) > \text{Mo}(a_1 - a_4 + 1, 1, a_3 + a_4 - 1, 1)$ . If  $a_1 = a_4 + 1$  we are done. Otherwise, we may consider hollow hexagons  $H = H(a_1, 1, a_3, 1)$  where  $2 < a_1 \leq a_3 < \frac{h-5}{2}$ . Then

$$\text{Mo}\left(2, 1, \frac{h-5}{2}, 1\right) - \text{Mo}(a_1, 1, a_3, 1) = 2(a_1 - 2)(5a_1 - 8a_3) < 0. \quad \square$$

In Figure 6 the hollow hexagons with minimal value of the Mostar index are depicted.

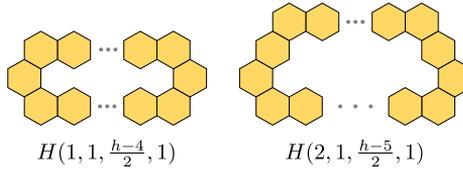


Figure 6: Hollow hexagons with minimal value of Mostar index.

**Theorem 5.5.** Let  $h \geq 12$  be even and  $\mathcal{HH}_h$  be the set of hollow hexagons with  $h$  hexagons. The hollow hexagon with the maximal value of the Mostar index is

- (1)  $H = H\left(\frac{h+6}{6}, \frac{h-6}{6}, \frac{h+6}{6}, \frac{h-6}{6}\right)$ , if  $h \equiv 0 \pmod{6}$ ,
- (2)  $H = H\left(\frac{h+4}{6}, \frac{h-8}{6}, \frac{h+10}{6}, \frac{h-8}{6}\right)$ , if  $h \equiv 2 \pmod{6}$ ,
- (3)  $H = H\left(\frac{h+8}{6}, \frac{h-10}{6}, \frac{h+8}{6}, \frac{h-4}{6}\right)$ , if  $h \equiv 4 \pmod{6}$ .

*Proof.* Let  $H(a_1, a_2, a_3, a_4) \in \mathcal{HH}_h$  with  $1 \leq a_2 \leq a_4 \leq a_1 \leq a_3 \leq \frac{h-4}{2}$ . Recall that in this case  $a_1 - a_4$  is an even non-negative integer. If  $a_1 - a_4 \geq 4$ , we may apply repeatedly Lemma 5.3 until we obtain

$$\text{Mo}(a_1, a_2, a_3, a_4) < \text{Mo}(a_1 - x, a_2 + x, a_3 - x, a_4 + x),$$

where  $x = \frac{a_1 - a_4}{2} - 1$ . Note that  $a_1 - x = a_4 + x + 2$ . So, if  $a_1 - a_4 \geq 2$ , we may consider hollow hexagons of the form  $H(a_1, a_2, a_3, a_1 - 2)$ . In this case,  $h = 2(a_1 + a_2 + a_3) - 2$  and  $a_2 \leq a_1 - 2 \leq a_3 - 2$ . Consider the following cases:

E.1.1  $a_2 = a_1 - 2 = a_3 - 2$ . In this case,  $h \equiv 0 \pmod 6 \geq 12$ ,  $a_2 = a_4 = \frac{h-6}{6}$ ,  $a_1 = a_3 = \frac{h+6}{6}$ , and we obtain hollow hexagons in affirmation (1).

E.1.2  $a_2 = a_1 - 2 = a_3 - 3$ . In this case,  $h \equiv 2 \pmod 6 \geq 14$ ,  $a_2 = a_4 = \frac{h-8}{6}$ ,  $a_1 = \frac{h+4}{6}$ ,  $a_3 = \frac{h+6}{6}$ , and we obtain hollow hexagons in affirmation (2).

E.1.3  $a_2 + 1 = a_1 - 2 = a_3 - 2$ . In this case,  $h \equiv 4 \pmod 6 \geq 16$ ,  $a_1 = a_3 = \frac{h+8}{6}$ ,  $a_2 = \frac{h-10}{6}$ ,  $a_4 = \frac{h-4}{6}$ , and we obtain hollow hexagons in affirmation (3).

E.1.4  $a_2 = a_1 - 2 = a_3 - 4$ . In this case,  $h \equiv 4 \pmod 6 \geq 16$ ,  $a_1 = \frac{h+2}{6}$ ,  $a_3 = \frac{h+14}{6}$ , and  $a_2 = a_4 = \frac{h-10}{6}$ . Affirmation (3) holds, since the difference

$$\begin{aligned} \Delta &= \text{Mo}\left(\frac{h+8}{6}, \frac{h-10}{6}, \frac{h+8}{6}, \frac{h-4}{6}\right) - \\ &\quad \text{Mo}\left(\frac{h+2}{6}, \frac{h-10}{6}, \frac{h+14}{6}, \frac{h-10}{6}\right) \\ &= 16 > 0. \end{aligned}$$

E.1.5  $a_2 + 2 = a_1 - 2 = a_3 - 2$ . In this case,  $h \equiv 2 \pmod 6 \geq 20$ ,  $a_1 = a_3 = \frac{h+10}{6}$ ,  $a_2 = \frac{h-14}{6}$ , and  $a_4 = \frac{h-2}{6}$ . Affirmation (2) holds, since the difference

$$\begin{aligned} \Delta &= \text{Mo}\left(\frac{h+4}{6}, \frac{h-8}{6}, \frac{h+10}{6}, \frac{h-8}{6}\right) - \\ &\quad \text{Mo}\left(\frac{h+10}{6}, \frac{h-14}{6}, \frac{h+10}{6}, \frac{h-2}{6}\right) \\ &= 16 > 0. \end{aligned}$$

E.1.6  $a_2 = a_1 - 2, a_3 - a_1 \geq 3$ . Since  $h = 4a_1 + 2a_3 - 6 \geq 10$  and  $a_3 \geq a_1 + 3$ , the difference

$$\begin{aligned} \Delta &= \text{Mo}(a_1 + 1, a_1 - 1, a_3 - 2, a_1 - 1) - \text{Mo}(a_1, a_1 - 2, a_3, a_1 - 2) \\ &= 2(g(a_1 + 1, h) - g(a_1, h)) + 2(g(a_1 - 1, h) - g(a_1 - 2, h)) + \\ &\quad g(a_3 - 2, h) - g(a_3, h) + g(a_3 - 4, h) - g(a_3 - 2, h) \\ &= 16(2a_3 - 2a_1 - 3) > 0. \end{aligned}$$

If we repeat this operation until we obtain a hollow hexagons with  $a_2 = a_1 - 2$  and  $a_3 - a_1 \leq 2$ , using one of the cases E.1.1, E.1.2, or E.1.4 we obtain the result.

E.1.7  $a_3 = a_1$ ,  $a_1 - a_2 \geq 5$ . Since  $h = 4a_1 + 2a_2 - 2 \geq 10$  and  $a_1 \geq a_2 + 5 \geq 6$ , the difference

$$\begin{aligned} \Delta &= \text{Mo}(a_1 - 1, a_2 + 2, a_1 - 1, a_1 - 3) - \text{Mo}(a_1, a_2, a_1, a_1 - 2) \\ &= 3(g(a_1 - 1, h) - g(a_1, h)) + 2(g(a_2 + 2, h) - g(a_2, h)) \\ &\quad + g(a_1 - 3, h) - g(a_1 - 2, h) \\ &= 32(a_1 - a_2 - 2) > 0. \end{aligned}$$

If we repeat this operation until we obtain a hollow hexagons with  $a_1 = a_3$  and  $a_1 - a_2 \leq 4$ , using one of the cases E.1.1, E.1.3, or E.1.5, we obtain the result.

E.1.8  $a_2 - 2 < a_1 < a_3$ . We may apply repeatedly Lemma 5.1 until

$$\text{Mo}(a_1, a_2, a_3, a_1 - 2) < \text{Mo}(a_1, a_1 - 2, a_3 - a_1 + a_2 + 2, a_1 - 2),$$

or until

$$\text{Mo}(a_1, a_2, a_3, a_1 - 2) < \text{Mo}(a_1, a_2 + a_3 - a_1, a_1, a_1 - 2).$$

In the first case, considering hollow hexagons of the form  $H(a_1, a_1 - 2, a_3, a_1 - 2)$ , the result follows from cases E.1.1, E.1.2, E.1.4, or E.1.6. In the second case, considering hollow hexagons of the form  $H(a_1, a_2, a_1, a_1 - 2)$ , the result follows from cases E.1.1, E.1.3, E.1.5, or E.1.7.

To complete the proof in the case  $h$  even, we consider hollow hexagons of the form  $H(a_1, a_2, a_3, a_1)$ . Here  $h = 2(a_1 + a_2 + a_3)$  and  $a_2 \leq a_1 \leq a_3$ . Consider the following cases:

E.2.1  $a_2 = a_1 = a_3$ . In this case,  $h \equiv 0 \pmod{6} \geq 12$ ,  $a_1 = a_2 = a_3 = a_4 = \frac{h}{6}$ . We obtain

$$\text{Mo}\left(\frac{h+6}{6}, \frac{h-6}{6}, \frac{h+6}{6}, \frac{h-6}{6}\right) - \text{Mo}\left(\frac{h}{6}, \frac{h}{6}, \frac{h}{6}, \frac{h}{6}\right) = 24 > 0.$$

E.2.2  $a_2 = a_1 = a_3 - 1$ . In this case,  $h \equiv 2 \pmod{6} \geq 14$ ,  $a_1 = a_2 = a_4 = \frac{h-2}{6}$ , and  $a_3 = \frac{h+4}{6}$ . We obtain

$$\text{Mo}\left(\frac{h+4}{6}, \frac{h-8}{6}, \frac{h+10}{6}, \frac{h-8}{6}\right) - \text{Mo}\left(\frac{h-2}{6}, \frac{h-2}{6}, \frac{h+4}{6}, \frac{h-2}{6}\right) = 24 > 0.$$

E.2.3  $a_2 + 1 = a_1 = a_3$ . In this case,  $h \equiv 4 \pmod{6} \geq 16$ ,  $a_1 = a_3 = a_4 = \frac{h+2}{6}$ ,  $a_2 = \frac{h-4}{6}$ . We obtain

$$\text{Mo}\left(\frac{h+8}{6}, \frac{h-10}{6}, \frac{h+8}{6}, \frac{h-4}{6}\right) - \text{Mo}\left(\frac{h+2}{6}, \frac{h-4}{6}, \frac{h+2}{6}, \frac{h+2}{6}\right) = 24 > 0.$$

E.2.4  $a_2 = a_1 = a_3 - 2$ . In this case,  $h \equiv 4 \pmod{6} \geq 16$ ,  $a_1 = a_2 = a_4 = \frac{h-4}{6}$ , and  $a_3 = \frac{h+8}{6}$ . We obtain

$$\text{Mo}\left(\frac{h+8}{6}, \frac{h-10}{6}, \frac{h+8}{6}, \frac{h-4}{6}\right) - \text{Mo}\left(\frac{h-4}{6}, \frac{h-4}{6}, \frac{h+8}{6}, \frac{h-4}{6}\right) = 40 > 0.$$

E.2.5  $a_2 + 2 = a_1 = a_3$ . In this case,  $h \equiv 2 \pmod{6} \geq 20$ ,  $a_1 = a_3 = a_4 = \frac{h+4}{6}$ , and  $a_2 = \frac{h-8}{6}$ . We obtain

$$\text{Mo} \left( \frac{h+4}{6}, \frac{h-8}{6}, \frac{h+10}{6}, \frac{h-8}{6} \right) - \text{Mo} \left( \frac{h+4}{6}, \frac{h-8}{6}, \frac{h+4}{6}, \frac{h+4}{6} \right) = 40 > 0.$$

E.2.6  $a_2 = a_1$ ,  $a_3 - a_1 \geq 3$ . Since  $h = 4a_1 + 2a_3 \geq 10$  and  $a_3 \geq a_1 + 3$ , the difference

$$\begin{aligned} \Delta &= \text{Mo}(a_1 + 1, a_1 + 1, a_3 - 2, a_1 + 1) - \text{Mo}(a_1, a_1, a_3, a_1) \\ &= 4(g(a_1 + 1, h) - g(a_1, h)) + 2(g(a_3 - 2, h) - g(a_3, h)) \\ &= 16(2a_3 - 2a_1 - 3) > 0. \end{aligned}$$

If we repeat this operation until we obtain a hollow hexagons with  $a_3 - a_1 \leq 2$ , using one of the cases E.2.1, E.2.2, or E.2.4, we obtain the result.

E.2.7  $a_3 = a_1$ ,  $a_1 - a_2 \geq 3$ . Since  $h = 4a_1 + 2a_2 \geq 10$  and  $a_1 \geq a_2 + 3 \geq 4$ , the difference

$$\begin{aligned} \Delta &= \text{Mo}(a_1 - 1, a_2 + 2, a_1 - 1, a_1 - 1) - \text{Mo}(a_1, a_2, a_1, a_1) \\ &= 4(g(a_1 - 1, h) - g(a_1, h)) + 2(g(a_2 + 2, h) - g(a_2, h)) \\ &= 16(2a_1 - 2a_2 - 3) > 0. \end{aligned}$$

If we repeat this operation until we obtain a hollow hexagons with  $a_1 - a_2 \leq 2$ , using one of the cases E.2.1, E.2.3, or E.2.5, we obtain the result.

E.2.8  $a_2 < a_1 < a_3$ . We may apply repeatedly Lemma 5.1 until

$$\text{Mo}(a_1, a_2, a_3, a_1) < \text{Mo}(a_1, a_1, a_3 - a_1 + a_2, a_1),$$

or until

$$\text{Mo}(a_1, a_2, a_3, a_1) < \text{Mo}(a_1, a_2 + a_3 - a_1, a_1, a_1).$$

In the first case, considering hollow hexagons of the form  $H(a_1, a_1, a_3, a_1)$  the result follows from cases E.2.1, E.2.2, E.2.4, or E.2.6. In the second case, considering hollow hexagons of the form  $H(a_1, a_2, a_1, a_1)$ , the result follows from cases E.2.1, E.2.3, E.2.5, or E.2.7.  $\square$

In Figure 7 the hollow hexagons with maximal value of the Mostar index for  $h \in \{12, 14, 16\}$  are depicted.

In our next result we find maximal hollow hexagons with respect to Mostar index when  $h$  is odd and greater than 13. In the case of  $h = 13$ , there exist only two hollow hexagons  $H(2, 1, 4, 1)$  and  $H(3, 1, 3, 2)$  with  $\text{Mo}(2, 1, 4, 1) = 1010 < \text{Mo}(3, 1, 3, 2) = 1026$ .

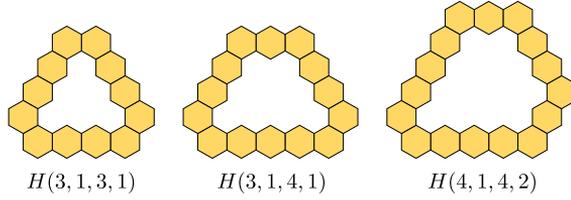


Figure 7: Hollow hexagons with maximal value of Mostar index for  $h \in \{12, 14, 16\}$ .

**Theorem 5.6.** Let  $h \geq 15$  be odd and  $\mathcal{HH}_h$  be the set of hollow hexagons with  $h$  hexagons. The hollow hexagons with the maximal value of the Mostar index are

- (1)  $H\left(\frac{h+11}{6}, \frac{h-13}{6}, \frac{h+11}{6}, \frac{h-7}{6}\right)$  and  $H\left(\frac{h+5}{6}, \frac{h-7}{6}, \frac{h+5}{6}, \frac{h-1}{6}\right)$ , if  $h \equiv 1 \pmod 6$ ,
- (2)  $H\left(\frac{h+9}{6}, \frac{h-9}{6}, \frac{h+9}{6}, \frac{h-9}{6}\right)$  and  $H\left(\frac{h+3}{6}, \frac{h-3}{6}, \frac{h+3}{6}, \frac{h-3}{6}\right)$ , if  $h \equiv 3 \pmod 6$ ,
- (3)  $H\left(\frac{h+7}{6}, \frac{h-11}{6}, \frac{h+13}{6}, \frac{h-11}{6}\right)$  and  $H\left(\frac{h+1}{6}, \frac{h-5}{6}, \frac{h+7}{6}, \frac{h-5}{6}\right)$  if  $h \equiv 5 \pmod 6$ .

*Proof.* Let  $H(a_1, a_2, a_3, a_4) \in \mathcal{HH}_h$  with  $1 \leq a_2 \leq a_4 < a_1 \leq a_3 \leq \frac{h-5}{2}$ . Since  $h$  is odd,  $a_1 - a_4$  is an odd non-negative integer. If  $a_1 - a_4 \geq 5$ , we may apply repeatedly Lemma 5.3 until we obtain a hollow hexagon with  $a_1 = a_4 + 3$ . Then we may consider hollow hexagons of the form  $H(a_1, a_2, a_3, a_1 - 3)$ . Also, by Lemma 5.3, we have that

$$\text{Mo}(a_1 - 1, a_2 + 1, a_3 - 1, a_1 - 2) = \text{Mo}(a_1, a_2, a_3, a_1 - 3).$$

Then we may consider hollow hexagons of the form  $H(a_1, a_2, a_3, a_1 - 1)$ . In this case,  $h = 2(a_1 + a_2 + a_3) - 1$  and  $a_2 + 1 \leq a_1 \leq a_3$ . Consider the following cases:

- O.1  $a_2 + 1 = a_1 = a_3$ . In this case,  $h \equiv 3 \pmod 6 \geq 15$ ,  $a_1 = a_3 = \frac{h+3}{6}$ ,  $a_2 = a_4 = \frac{h-3}{6}$ , and we obtain hollow hexagons in affirmation (2).
- O.2  $a_2 + 1 = a_1 = a_3 - 1$ . In this case,  $h \equiv 5 \pmod 6 \geq 17$ ,  $a_1 = \frac{h+1}{6}$ ,  $a_2 = a_4 = \frac{h-5}{6}$ ,  $a_3 = \frac{h+7}{6}$ , and we obtain hollow hexagons in affirmation (3).
- O.3  $a_2 + 2 = a_1 = a_3$ . In this case,  $h \equiv 1 \pmod 6 \geq 19$ ,  $a_1 = a_3 = \frac{h+5}{6}$ ,  $a_2 = \frac{h-7}{6}$ ,  $a_4 = \frac{h-1}{6}$ , and we obtain hollow hexagons in affirmation (1).
- O.4  $a_2 + 1 = a_1 = a_3 - 2$ . In this case,  $h \equiv 1 \pmod 6 \geq 19$ ,  $a_1 = \frac{h-1}{6}$ ,  $a_2 = a_4 = \frac{h-7}{6}$ ,  $a_3 = \frac{h+11}{6}$ . Affirmation (1) holds, since the difference

$$\begin{aligned} \Delta &= \text{Mo}\left(\frac{h+5}{6}, \frac{h-7}{6}, \frac{h+5}{6}, \frac{h-1}{6}\right) - \text{Mo}\left(\frac{h-1}{6}, \frac{h-7}{6}, \frac{h+11}{6}, \frac{h-7}{6}\right) \\ &= 16 > 0. \end{aligned}$$

- O.5  $a_2 + 3 = a_1 = a_3$ . In this case,  $h \equiv 5 \pmod 6 \geq 17$ ,  $a_1 = a_3 = \frac{h+7}{6}$ ,  $a_2 = \frac{h-11}{6}$ , and  $a_4 = \frac{h+1}{6}$ . Affirmation (3) holds, since the difference

$$\begin{aligned} \Delta &= \text{Mo}\left(\frac{h+1}{6}, \frac{h-5}{6}, \frac{h+7}{6}, \frac{h-5}{6}\right) - \text{Mo}\left(\frac{h+7}{6}, \frac{h-11}{6}, \frac{h+7}{6}, \frac{h+1}{6}\right) \\ &= 16 > 0. \end{aligned}$$

O.6  $a_2 + 1 = a_1, a_3 - a_1 \geq 3$ . Since  $h = 4a_1 + 2a_3 - 3$  and  $a_3 \geq a_1 + 3 \geq 5$ , the difference

$$\begin{aligned} \Delta &= \text{Mo}(a_1 + 1, a_1, a_3 - 2, a_1) - \text{Mo}(a_1, a_1 - 1, a_3, a_1 - 1) \\ &= 16(2a_3 - 2a_1 - 3) > 0. \end{aligned}$$

If we repeat this operation until we obtain a hollow hexagons with  $a_2 + 1 = a_1$  and  $a_3 - a_1 \leq 2$ , using one of the cases O.1, O.2, or O.4 we obtain the result.

O.7  $a_3 = a_1, a_1 - a_2 \geq 4$ . Since  $h = 4a_1 + 2a_2 - 1$  and  $a_1 \geq a_2 + 4 \geq 5$ , the difference

$$\begin{aligned} \Delta &= \text{Mo}(a_1 - 1, a_2 + 2, a_1 - 1, a_1 - 2) - \text{Mo}(a_1, a_2, a_1, a_1 - 1) \\ &= 16(2a_1 - 2a_2 - 5) > 0. \end{aligned}$$

If we repeat this operation until we obtain a hollow hexagons with  $a_1 = a_3$  and  $a_1 - a_2 \leq 3$ , using one of cases O.1, O.3, or O.5 we obtain the result.

O.8  $a_2 + 1 < a_1 < a_3$ . We may apply repeatedly Lemma 5.1 until

$$\text{Mo}(a_1, a_1 - 1, a_3 - a_1 + a_2 + 1, a_1 - 1) > \text{Mo}(a_1, a_2, a_3, a_1 - 1)$$

or until

$$\text{Mo}(a_1, a_2, a_3, a_1) > \text{Mo}(a_1, a_2 + a_3 - a_1, a_1, a_1 - 1).$$

In the first case, considering hollow hexagons of the form  $H(a_1, a_1 - 1, a_3, a_1 - 1)$ , the result follows from cases O.1, O.2, O.4, or O.6. In the second case, considering hollow hexagons of the form  $H(a_1, a_2, a_1, a_1 - 1)$ , the result follows from cases O.1, O.3, O.5, or O.7. □

In Figure 8 the hollow hexagons with maximal value of the Mostar index for  $h \in \{15, 17, 19\}$  are depicted.

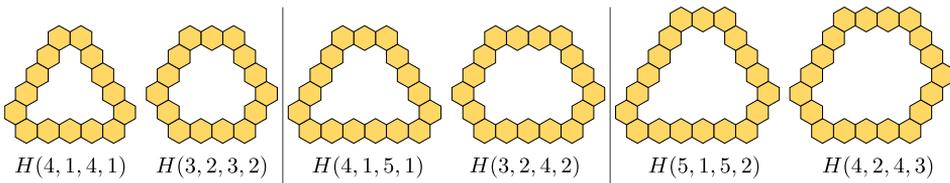


Figure 8: Hollow hexagons with maximal value of Mostar index for  $h \in \{15, 17, 19\}$ .

## 6 Conclusions

In this work, we use the cut method to compute the Mostar index of hollow hexagons. For this purpose, we employed the  $c$ -partition described in [22] to reduce a hollow hexagon with  $h$  hexagons into smaller strength-weighted quotient graphs. Once this is done, we compute the aforementioned index of each quotient graph. In Theorem 4.6, we obtain an expression for the Mostar index of a hollow hexagon with  $h$  hexagons. Using the obtained

expression, we find the extreme values of the Mostar index over the set  $\mathcal{HH}_h$  by solving the corresponding integer programming problems.

As a future work, it would be possible to find expressions for the edge-Mostar and total Mostar indices of hollow hexagons by using the same  $c$ -partition. On the other hand, hollow hexagons are the simplest primitive coronoid systems. An important problem to solve would be to find the expressions to calculate the Szeged and Mostar indices of any primitive coronoid system.

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## References

- [1] M. Arockiaraj, F. J. H. Campena, A. B. Greeni, M. U. Ghani, S. Gajavalli, F. Tchier and A. Z. Jan, QSPR analysis of distance-based structural indices for drug compounds in tuberculosis treatment, *Heliyon* **10** (2024), e23981, doi:10.1016/j.heliyon.2024.e23981, <https://doi.org/10.1016/j.heliyon.2024.e23981>.
- [2] M. Arockiaraj, J. Clement and K. Balasubramanian, Topological indices and their applications to circumscribed donut benzenoid systems, kekulenes and drugs, *Polycyclic Aromatic Compounds* **40** (2020), 280–303, doi:10.1080/10406638.2017.1411958, <https://doi.org/10.1080/10406638.2017.1411958>.
- [3] M. Arockiaraj, J. Clement and N. Tratnik, Mostar indices of carbon nanostructures and circumscribed donut benzenoid systems, *Int. J. Quantum Chem.* **119** (2019), e26043, doi:10.1002/qua.26043, <https://doi.org/10.1002/qua.26043>.
- [4] M. Arockiaraj, J. Clement, N. Tratnik, S. Mushtaq and K. Balasubramanian, Weighted Mostar indices as measures of molecular peripheral shapes with applications to graphene, graphyne and graphdiyne nanoribbons, *SAR and QSAR in Environmental Research* **31** (2020), 187–208, doi:10.1080/1062936X.2019.1708459, <https://doi.org/10.1080/1062936X.2019.1708459>.
- [5] M. Arockiaraj, S. Klavžar, J. Clement, S. Mushtaq and K. Balasubramanian, Edge distance-based topological indices of strength-weighted graphs and their application to coronoid systems, carbon nanocones and SiO<sub>2</sub> nanostructures, *Mol. Inform.* **38** (2019), 1900039, doi:10.1002/minf.201900039, <https://doi.org/10.1002/minf.201900039>.
- [6] S. Brezovnik and N. Tratnik, General cut method for computing Szeged-like topological indices with applications to molecular graphs, *Int J. Quantum Chem.* **121** (2020), e26530, doi:10.1002/qua.26530, <https://doi.org/10.1002/qua.26530>.
- [7] S. J. Cyvin, J. Brunvoll, R. S. Chen, B. N. Cyvin and F. J. Zhang, *Theory of Coronoid Hydrocarbons II*, volume 62 of *Lecture Notes in Chemistry*, Springer-Verlag, Berlin, 1994, doi:10.1007/978-3-642-50157-9, <https://doi.org/10.1007/978-3-642-50157-9>.
- [8] S. J. Cyvin, J. Brunvoll and B. N. Cyvin, *Theory of Coronoid Hydrocarbons*, volume 54 of *Lecture Notes in Chemistry*, Springer-Verlag, Berlin, 1991, doi:10.1007/978-3-642-51110-3, <https://doi.org/10.1007/978-3-642-51110-3>.
- [9] S. J. Cyvin, J. Brunvoll, B. N. Cyvin, J. L. Bergan and E. Brendsdal, The simplest coronoids: hollow hexagons, *Struct. Chem.* **2** (1991), 555–566, doi:10.1007/BF00673438, <https://doi.org/10.1007/BF00673438>.

- [10] J. C. Dearden, *The use of topological indices in QSAR and QSPR modeling: Applications in Pharmaceutical, Chemical, Food, Agricultural and Environmental Sciences*, Springer International Publishing, 2017.
- [11] K. Deng and S. Li, On the extremal values for the Mostar index of trees with given degree sequence, *Appl. Math. Comput.* **390** (2021), 11, doi:10.1016/j.amc.2020.125598, id/No 125598, <https://doi.org/10.1016/j.amc.2020.125598>.
- [12] F. Diederich and H. A. Staab, Benzenoid versus annulenoïd aromaticity: Synthesis and properties of kekulene, *Angew. Chem.* **17** (1978), 372–374.
- [13] T. Došlić, I. Martinjak, R. Škrekovski, S. T. Spužević and I. Zubac, Mostar index, *J. Math. Chem.* **56** (2018), 2995–3013, doi:10.1007/s10910-018-0928-z, <https://doi.org/10.1007/s10910-018-0928-z>.
- [14] D. J. H. Funhoff and H. A. Staab, Cyclo[d.e.d.e.d.e.d.e.d.e]decakisbenzene, a new cycloarene, *Angew. Chem.* **25** (1986), 742–744.
- [15] N. Ghanbari and S. Alikhani, Mostar index and edge Mostar index of polymers, *Comput. Appl. Math.* **40** (2021), Id/No 260, 21 pp., doi:10.1007/s40314-021-01652-x, <https://doi.org/10.1007/s40314-021-01652-x>.
- [16] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes* **27** (1994), 9–15.
- [17] I. Gutman and S. J. Cyvin, *Introduction to the Theory Benzenoid Hydrocarbons*, Springer-Verlag, Berlin, 1989.
- [18] H. Hosoya, Topological index. a newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.* **44** (1971), 2332–2339, doi:10.1246/bcsj.44.2332, <https://doi.org/10.1246/bcsj.44.2332>.
- [19] S. Huang, S. Li and M. Zhang, On the extremal Mostar indices of hexagonal chains, *MATCH Commun. Math. Comput. Chem.* **84** (2020), 249–271.
- [20] S. A. K. Kirmani, P. Ali and F. Azam, Topological indices and QSPR/QSAR analysis of some antiviral drugs being investigated for the treatment of COVID-19 patients, *Int. J. Quantum Chem.* **121** (2021), e26594, doi:10.1002/qua.26594, <https://doi.org/10.1002/qua.26594>.
- [21] H. Liu, L. Song, Q. Xiao and Z. Tang, On edge Mostar index of graphs, *Iran. J. Math. Chem.* **11** (2020), 95–106, doi:10.22052/ijmc.2020.221320.1489, <https://doi.org/10.22052/ijmc.2020.221320.1489>.
- [22] C. Lopera and R. Cruz, Szeged index of hollow hexagons, *Int J. Quantum Chem.* **119** (2023), e27231, doi:10.1002/qua.27231, <https://doi.org/10.1002/qua.27231>.
- [23] D. Ž. Đoković, Distance-preserving subgraphs of hypercubes, *J. Comb. Theory, Ser. B* **14** (1973), 263–267, doi:10.1016/0095-8956(73)90010-5, [https://doi.org/10.1016/0095-8956\(73\)90010-5](https://doi.org/10.1016/0095-8956(73)90010-5).
- [24] H. A. Staab and F. Diederich, Cycloarenes, a new class of aromatic compounds, I. synthesis of kekulene, *Chem. Ber.* **116** (1983), 3487–3503, doi:10.1002/cber.19831161021, <https://doi.org/10.1002/cber.19831161021>.
- [25] H. A. Staab and M. Sauer, Cycloarene, eine neue klasse aromatischer verbindungen, iv. versuche zur synthese des Cyclo[d.e.d.e.d.e.d.e]nonakisbenzens und des Cyclo[d.e.d.e.d.e.d.e.d.e]decakisbenzens, *Liebigs Ann. Chem.* **1984** (1984), 742–760, doi:10.1002/jlac.198419840411, <https://doi.org/10.1002/jlac.198419840411>.
- [26] A. Tepfeh, Extremal bicyclic graphs with respect to Mostar index, *Appl. Math. Comput.* **355** (2019), 319–324, doi:10.1016/j.amc.2019.03.014, <https://doi.org/10.1016/j.amc.2019.03.014>.

- [27] R. Todeschini, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.
- [28] R. Todeschini and V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley-VCH, Weinheim, 2009.
- [29] N. Tratnik, Computing the Mostar index in networks with applications to molecular graphs, *Iran. J. Math. Chem.* **12** (2021), 1–18, doi:10.22052/ijmc.2020.240316.1526, <https://doi.org/10.22052/ijmc.2020.240316.1526>.
- [30] H. Wang and M. Liu, The upper bound of the edge mostar index with respect to bicyclic graphs, *Mathematics* **11** (2023), 2506, doi:10.3390/math11112506, <https://doi.org/10.3390/math11112506>.
- [31] H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* **69** (1947), 17–20, doi:10.1021/ja01193a005, <https://doi.org/10.1021/ja01193a005>.
- [32] P. Winkler, Isometric embeddings in products of complete graphs, *Discrete Appl. Math.* **7** (1984), 221–225, doi:10.1016/0166-218X(84)90069-6, [https://doi.org/10.1016/0166-218X\(84\)90069-6](https://doi.org/10.1016/0166-218X(84)90069-6).