The Maximum Number of Kekulé Structures of Cata-condensed Polyhexes

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Let \( H \) denote a simply-connected cata-condensed polyhex. It is shown that if \( H \) has three hexagons in a row it does not have a maximum number of Kekulé structures. Otherwise, its number of Kekulé structures is equal to its number of sets of disjoint hexagons (including the empty set). These results lead to an efficient algorithm to determine simply-connected cata-condensed polyhexes with a maximum number of Kekulé structures. A table of such values of \( H \) with up to 100 hexagons is provided.

Key words: Polyhex; Cata-condensed; Kekulé structure; Resonant set; Dualist graph.

1. Introduction

Kekulé structures in polyhexes, or particular classes of polyhexes such as cata-condensed or pericondensed benzenoids, coronoids or helicenes have been extensively studied [1–14]. Indeed, a whole book by Cyvin and Gutman [14] is devoted to that topic. It is also discussed at length in several surveys of two recent volumes on *Advances in the theory of benzenoid hydrocarbons* [15, 16] and in numerous papers cited there.

Polyhexes which have a minimum or maximum number of Kekulé structures are of particular interest as they correspond to highly reactive or stable molecules. Lower and upper bounds on the number of Kekulé structures of simply-connected cata-condensed polyhexes have been given by Gutman [5], Cyvin, Chen [9, 10] and John [17]. It is conjectured [16] that the sharpest of these bounds, due to John [17], is also valid for all benzenoids. For that case, an upper bound which is not very sharp has been derived by Gutman and Cioslowski [4]. Empirical evidence (e.g. [18]) supports the often stated conjecture that a simply-connected cata-condensed benzenoid (polyhex) has the maximum number of Kekulé structures among all benzenoids (polyhexes) with the same number of hexagons.

Cyvin [9] gives a table of maximum number of Kekulé structures for simply-connected cata-condensed polyhexes with up to 12 hexagons, obtained by complete enumeration. He also conjectures some values for such polyhexes with up to 20 hexagons. In this paper, we consider again the problem of finding the maximum number of Kekulé structures in simply-connected cata-condensed polyhexes (i.e., simply-connected cata-condensed benzenoids or helicenes). Several properties of this class of polyhexes are first described. They are then used to obtain a simple algorithm to determine the maximum number of Kekulé structures in simply-connected cata-condensed polyhexes with a given number \( h \) of hexagons. Values of this number for \( h \) up to 100 are provided, as well as dualist graphs for the corresponding polyhexes with \( h \) up to 30. The algorithm makes use of lists of non-dominated numbers of sets of resonant hexagons including or not the root hexagon. This allows exclusion of many possibilities and computation of values for large \( h \) in moderate computing time. This type of dominance argument can be viewed as an application of Bellman’s optimality principle in Dynamic Programming [19, 20]: “an optimal policy can only contain optimal sub-policies”.

2. Definitions

A polyhex is a connected graph consisting of regular hexagons such that any two hexagons are either disjoint or have a bond in common and no three hexagons have a common bond. A polyhex is planar if it can be embedded in the plane.
A hole of a polyhex is a circuit larger than a hexagon in which each bond belongs to only one hexagon. A polyhex is simply-connected if it has no holes except its boundary. A polyhex $H$ is cata-condensed if it contains no inner vertices (a vertex is an inner vertex if it does not belong to any hole or to the boundary of $H$). A leaf of a polyhex is a hexagon which has only one neighbor hexagon.

The dualist graph of a polyhex $H$ is obtained by associating a vertex to each hexagon of $H$ and joining vertices corresponding to hexagons with a common bond. For simply-connected cata-condensed polyhexes, the dualist graph is a tree.

The empty graph is defined as the graph with no vertices or edges. A connected component of a graph $G$ is a maximal connected subgraph contained in $G$.

The degree of a vertex of a graph $G$ is the number of edges containing that vertex. A pendant bond (or edge) of a graph $G$ is an edge with one end vertex of degree 1.

A bond of a polyhex $H$ is fixed if it belongs to all Kekulé structures of $H$ or to none of them.

A set of disjoint hexagons of a polyhex $H$ is resonant if the subgraph obtained by deleting from $H$ all vertices of these hexagons has a perfect matching (or Kekulé structure) or is the empty graph. Hexagons in a resonant set are said to be mutually resonant. By convention, when $H$ is Kekulean the empty set is considered to be a resonant set.

A hexagon of a cata-condensed polyhex is in mode $L_1$ or $L_2$ if it has two neighbor hexagons with their mutual positions as shown in Fig. 1a and b, i.e., the three hexagons are not in a row or in a row respectively.

Let $k(H)$ denote the number of Kekulé structures (or perfect matchings) of $H$ and $k_{\text{max}}(h) = \max \{k(H): H \text{ is simply-connected cata-condensed and has } h \text{ hexagons}\}$. If $H$ is the empty graph, then define $k(H) = 1$.

### 3. Basic Properties

In this section, we present several properties of simply-connected cata-condensed polyhexes. These properties are the base of the method for computing $k_{\text{max}}(h)$ which will be given in the next section.

It is known that for cata-condensed planar polyhexes there is a one-to-one mapping between resonant sets and Kekulé structures [21]. This result holds for all simply-connected cata-condensed polyhexes as shown next.

**Theorem 1**: Let $H$ be a simply-connected cata-condensed polyhex. Then $k(H)$ is equal to the number of resonant sets of $H$.

**Proof**: By induction on the number of hexagons of $H$. When $H$ has only one hexagon, then it has two resonant sets (one of which is the empty set) and two Kekulé structures. Let $f$ be a leaf of $H$ (such a hexagon exists for $H$ is simply-connected and cata-condensed). Let $e_1$ and $e_2$ be the two bonds of $f$ with their end vertices contained in $f$ only and not adjacent between themselves, as shown in Figure 2. Let $e_3$ be the bond of $f$ which is adjacent to $e_1$ and $e_2$. Let $k_1$ (resp. $k_2$) be the number of Kekulé structures which contain $e_1$ and $e_2$ (resp. contain $e_3$). Then $k(H) = k_1 + k_2$. Let $r_1$ (resp. $r_2$) be the number of resonant sets which do not contain (resp. contain) $f$. Let $H' = H - \{e_1, e_2\}$. Then $k_1 = k(H')$ and $r_1$ is the number of resonant sets of $H'$. By the induction hypothesis, $k_1 = r_1$. Deleting $e_3$ together with its end vertices from $H$, then deleting sequentially all pendant edges together with their vertices and the incident edges and then all bonds which do not belong to any hexagon in the remaining graph (but not their vertices), a graph $H''$ is obtained (see Figure 3). $H''$ may have several connected components and each of them is a simply-connected cata-condensed polyhex or is the empty graph. Clearly $k_2$ is equal to $k(H'')$, and $k(H'')$ is equal to the product of the number of Kekulé structures in each of its con-
After deleting $e_3$ together with its end vertices, then deleting sequentially all pendant edges with their vertices and the incident edges and then the edges not belonging to any hexagon in the remaining graph.

Fig. 3. Deleting $e_3$ together with its vertices, then deleting sequentially all pendant edges with their vertices and the incident edges and then the edges not belonging to any hexagon in the remaining graph.

Fig. 4. The number of vertices not contained in $H''$ or $f$ is 0 or 2.

Theorem 2: Let $H$ be a simply-connected cata-condensed polyhex without three hexagons in a row. Then any set of disjoint hexagons of $H$ is resonant.

Proof: By induction on the number of hexagons of $H$. When $H$ has a single hexagon, it is resonant. Let $f$ be a leaf of $H$. Let $H'$ be the polyhex formed by all hexagons of $H$ except $f$ and $H''$ be the graph formed by all hexagons of $H$ except $f$ and its neighbor hexagon. Note that $H''$ may have two connected components or be empty. Let $S$ be a set of disjoint hexagons of $H$. If $S$ is empty, then it is resonant. If $S$ does not contain $f$, then $S$ is a resonant set of $H'$ by the induction hypothesis. Thus $S$ is resonant in $H$. If $f$ is in $S$, then $S' = S - \{f\}$ is contained in $H''$. Since $H$ has no hexagons in $L_2$ mode, the number of vertices not contained in $H''$ and $f$ is 0 or 2 (see Fig. 4a and b). If it is 2, then the two vertices not in $f$ and $H''$ are adjacent. By the induction hypothesis for each connected component of $H''$, the deletion of the vertices of hexagons in $S'$ from $H''$ results in a graph which is either the empty graph or has a Kekulé structure. Thus $S$ is resonant in $H$.

Note that this theorem is not valid for polyhexes in general. Theorems 1 and 2 imply the following result.

Theorem 3: Let $H$ be a simply-connected cata-condensed polyhex without three hexagons in a row. Then $k(H)$ is equal to the number of sets of disjoint hexagons of $H$.

We next show that a class of polyhexes does not contain any one with a maximum number of Kekulé structures.

Theorem 4: Let $H$ be a simply-connected cata-condensed polyhex with $h$ hexagons. If $H$ has a hexagon in mode $L_2$, i.e. has three hexagon in a row, then $k(H) < k_{\text{max}}(h)$.

Proof: Let $S$ be a hexagon of $H$ which is in mode $L_2$. Then all hexagons of $H$ except $S$ form two cata-condensed polyhexes. Let one of these be denoted by $H_1$ and the other by $H_2$ (see Fig. 5a). Let $H'_1$ (resp. $H'_2$) be the subgraph obtained by deleting from $H_1$ (resp. $H_2$) the vertices of $S$. Then $k(H) = k(H'_1) \times k(H'_2) + k(H_2) \times k(H_1)$. Let $H'$ be the cata-condensed polyhex which is equal to $H$ except that $S$ is in mode $L_1$. 

\[ \text{Theorem 2: Let } H \text{ be a simply-connected cata-condensed polyhex without three hexagons in a row. Then any set of disjoint hexagons of } H \text{ is resonant.} \]

\[ \text{Proof: By induction on the number of hexagons of } H. \text{ When } H \text{ has a single hexagon, it is resonant. Let } f \text{ be a leaf of } H. \text{ Let } H' \text{ be the polyhex formed by all hexagons of } H \text{ except } f \text{ and } H'' \text{ be the graph formed by all hexagons of } H \text{ except } f \text{ and its neighbor hexagon. Note that } H'' \text{ may have two connected components or be empty. Let } S \text{ be a set of disjoint hexagons of } H. \text{ If } S \text{ is empty, then it is resonant. If } S \text{ does not contain } f, \text{ then } S \text{ is a resonant set of } H' \text{ by the induction hypothesis. Thus } S \text{ is resonant in } H. \text{ If } f \text{ is in } S, \text{ then } S' = S - \{f\} \text{ is contained in } H''. \text{ Since } H \text{ has no hexagons in } L_2 \text{ mode, the number of vertices not contained in } H'' \text{ and } f \text{ is 0 or 2 (see Fig. 4a and b). If it is 2, then the two vertices not in } f \text{ and } H'' \text{ are adjacent. By the induction hypothesis for each connected component of } H'', \text{ the deletion of the vertices of hexagons in } S' \text{ from } H'' \text{ results in a graph which is either the empty graph or has a Kekulé structure. Thus } S \text{ is resonant in } H. \]

Note that this theorem is not valid for polyhexes in general. Theorems 1 and 2 imply the following result.

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\[ \text{Proof: Let } S \text{ be a hexagon of } H \text{ which is in mode } L_2. \text{ Then all hexagons of } H \text{ except } S \text{ form two cata-condensed polyhexes. Let one of these be denoted by } H_1 \text{ and the other by } H_2 \text{ (see Fig. 5a). Let } H'_1 \text{ (resp. } H'_2) \text{ be the subgraph obtained by deleting from } H_1 \text{ (resp. } H_2) \text{ the vertices of } S. \text{ Then } k(H) = k(H'_1) \times k(H'_2) + k(H_2) \times k(H_1). \text{ Let } H' \text{ be the cata-condensed polyhex which is equal to } H \text{ except that } S \text{ is in mode } L_1. \]
Then \( k(H) = k(H_1) \times k(H_2) + k(H') \times k(H_2) \). Since \( k(H_1) > k(H'_1) \) for \( i = 1, 2 \) as no bonds of a cata-condensed polyhex are fixed, \( k(H - k(H) = (k(H_1) - k(H'_1) \times (k(H_2) - k(H'_2)) > 0 \), i.e., \( k(H') > k(H) \). The proof is completed.

4. Non-dominated Pairs and Algorithm

By Theorem 3, instead of computing \( k(H) \) we can calculate the number of sets of disjoint hexagons of \( H \). Keeping this in mind, we first introduce the definition of rooted simply-connected cata-condensed polyhex and then the definition of feasible pairs and non-dominated pairs of integers. By exploiting non-dominated pairs, we are able to compute \( k_{\text{max}}(h) \) efficiently.

Let \( \mathcal{H}(h) \) be the set of simply-connected cata-condensed polyhexes with \( h \) hexagons which have no hexagons in mode \( L_2 \), i.e. no three hexagons in a row.

A rooted simply-connected cata-condensed polyhex is a polyhex belonging to \( \mathcal{H}(h) \) for \( h = 1, 2, \ldots \) together with a distinguished leaf as its root. See Fig. 6 for an illustration.

Let \( \mathcal{H}'(h) \) be the set of rooted simply-connected cata-condensed polyhexes with \( h \) hexagons. The number of Kekulé structures of a rooted simply-connected cata-condensed polyhex \( H \) is the same as \( k(H) \), without consideration of which hexagon is the root.

A feasible pair \( (f_h^0, f_h^1) \) is a pair of integers such that there is a rooted simply-connected cata-condensed polyhex \( H \) with root \( r \) and \( h \) hexagons for which the number of sets of disjoint hexagons not containing (resp. containing) \( r \) is equal to \( f_h^0 \) (resp. \( f_h^1 \)). There may be many feasible pairs corresponding to the same \( h \). For example, for \( h = 1 \) there is only one feasible pair, i.e. \( (1, 1) \); for \( h = 2 \) there is again only one feasible pair, i.e. \( (2, 1) \); for \( h = 3 \) there is only one feasible pair also, i.e. \( (3, 2) \); for \( h = 4 \) there are two feasible pairs, i.e. \( (5, 3) \) and \( (5, 4) \). In Fig. 7, some feasible pairs are given along with the corresponding rooted simply-connected cata-condensed polyhexes. Note that a feasible pair may correspond to more than one rooted simply-connected cata-condensed polyhex.

Let \( (f_h^0, f_h^1) \) be all feasible pairs for a given \( h \). In Table 1, all feasible pairs are given for \( h \) up to 8.

By Theorem 4, \( k_{\text{max}}(h) = \max \{ k(H) : H \in \mathcal{H}(h) \} \).

Thus \( k_{\text{max}}(h) = \max \{ k(H) : H \in \mathcal{H}'(h) \} \).

By Theorem 3,

\[
 k_{\text{max}}(h) = \max_j \left( f_h^0 + f_h^1 \right) .
\]
A non-dominated pair \((f_{h,j}^0, f_{h,j}^1)\) is a feasible pair for which no other feasible pair \((f_{h,j}^{0'}, f_{h,j}^{1'})\) satisfies the two conditions: \(f_{0,j}^0 \geq f_{h,j}^{0'} \) and \(f_{h,j}^0 + f_{h,j}^1 \geq f_{h,j}^{0'} + f_{h,j}^{1'}\); otherwise the pair \((f_{h,j}^0, f_{h,j}^1)\) is dominated.

Let \((k_{h,j}^0, k_{h,j}^1)\) \((j = 1, 2, \ldots, n_h)\) be all non-dominated pairs for a given \(h\). In Table 2, all non-dominated pairs are given for \(h\) up to 10.

The two tables clearly show that the number of non-dominated pairs is much less than the number of feasible pairs for a given \(h\). For non-dominated pairs, we have the following theorem.

**Theorem 5:**

\[
 k_{\text{max}}(h) = \max(k_{h,j}^0 + k_{h,j}^1).
\]

**Proof:** This follows immediately from (1) and the definition of non-dominated pairs.

The following theorem provides a recursive method to compute non-dominated pairs.

**Theorem 6:** Let \((k_{h,j}^0, k_{h,j}^1)\) be a non-dominated pair with \(h > 1\). Then there are two non-dominated pairs \((k_{h-t,j}^0, k_{h-t,j}^1)\) and \((k_{h-t,j}^1, k_{h-t,j}^0)\) with \(t \leq h/2\) such that \(k_{h,j}^0 = k_{h-t,j}^0 \times k_{t,j}^0 + k_{h-t,j}^1 \times k_{t,j}^1\) and \(k_{h,j}^1 = k_{h-t,j}^1 \times k_{t,j}^0 + k_{h-t,j}^0 \times k_{t,j}^1\).

**Proof:** Let \(H\) be a cata-condensed polyhex with root \(r\) which corresponds to \((k_{h,j}^0, k_{h,j}^1)\). Let \(r'\) be the hexagon of \(H\) adjacent to \(r\). Let \(H' \equiv H - r\) be the cata-condensed polyhex consisting of all hexagons of \(H\) except \(r\). Let \(H_1\) and \(H_2\) be the two cata-condensed polyhexes such that their intersection is \(r'\) and their union is \(H'\) (see Figure 8). Without loss of generality, let \(H_1\) have \(t\) hexagons with \(t \geq h/2\). Let \((f_{t,1}^0, f_{t,1}^1)\) and \((f_{h-t,1}^0, f_{h-t,1}^1)\) be the two feasible pairs which correspond to \(H_1\) and \(H_2\) (with root \(r'\)) respectively. Then \(k_{h,j}^0 = f_{t,1}^0 \times f_{h-t,1}^0 + f_{t,1}^1 \times f_{h-t,1}^1\) and \(k_{h,j}^1 = f_{t,1}^1 \times f_{h-t,1}^0 + f_{t,1}^0 \times f_{h-t,1}^1\). If both of \((f_{t,1}^0, f_{t,1}^1)\) and \((f_{h-t,1}^0, f_{h-t,1}^1)\) are non-dominated pairs, the theorem is proved. Otherwise, without loss of generality let \((f_{t,1}^1, f_{t,1}^0)\) be dominated. Then there is a non-dominated pair \((k_{t,m}^0, k_{t,m}^1)\) with

\[
 k_{t,m}^0 \geq f_{t,1}^0 \tag{2}
\]

and

\[
 k_{t,m}^0 + k_{t,m}^1 \geq f_{t,1}^0 + f_{t,1}^1 \tag{3}
\]

Let \(H'_1\) be the cata-condensed polyhex with root \(r'\) which corresponds to \((k_{t,m}^0, k_{t,m}^1)\). Let \(H'\) be the rooted simply-connected cata-condensed polyhex with root \(r\) obtained from \(H\) by replacing \(H_1\) by \(H'_1\) such that \(r'\) coincides with \(r\) (see Figure 8). Then \(H'\) corresponds to a feasible pair \((f_{h,j}^0, f_{h,j}^1)\) with \(f_{h,j}^0 = f_{h-t,1}^0 \times k_{t,m}^0 + f_{h-t,1}^1 \times k_{t,m}^1\) and \(f_{h,j}^1 = f_{h-t,1}^0 \times k_{t,m}^1 + f_{h-t,1}^1 \times k_{t,m}^0\).

By (2), \(f_{h,j}^0 = f_{h-t,1}^0 \times k_{t,m}^0 \geq k_{h,j}^0\). Also \(f_{h,j}^1 - k_{h,j}^0 = f_{h-t,1}^1 \times (k_{t,m}^0 - f_{t,1}^0) - f_{h-t,1}^0 \times (f_{t,1}^1 - k_{t,m}^1)\). If \((f_{t,1}^1 - k_{t,m}^1) \leq 0\), then \(f_{h,j}^1 - k_{h,j}^0 \geq 0\). If \((f_{t,1}^1 - k_{t,m}^1) > 0\), by (3) \((k_{t,m}^0 - f_{t,1}^0) \geq (f_{t,1}^1 - k_{t,m}^1) > 0\). By noting that \(f_{h-t,1}^1 \geq f_{h-t,1}^0\), \(f_{h,j}^0 - k_{h,j}^0 \geq 0\). Note that (2) and (3) cannot be equalities at the same time. Thus \(f_{h,j}^0 \geq k_{h,j}^0\) and \(f_{h,j}^1 - k_{h,j}^0 \geq 0\) cannot be equalities at the same time. This means that \((k_{h,j}^0, k_{h,j}^1)\) is a dominated pair, a contradiction.
Now we are ready to state the algorithm for computing non-dominated pairs as well as $k_{\text{max}}(h)$.

Algorithm:

Initial step: $(k_{1,1}^0, k_{1,1}^1) = (1, 1)$ and $k_{\text{max}}(1) = 2$.

Recursive step: Increase $h$ by 1. (a) Compute all possible pairs of values $(k_{h-t,i}^0, k_{h-t,i}^1)$ with $t \leq h/2$ and (b) keep all non-dominated pairs; calculate $k_{\text{max}}(h) = \max \{k_{h-t,i}^0 + k_{h-t,i}^1\}$. Iterate as long as the maximum number of hexagons considered has not been reached.

Table 3 illustrates the recursive step for $h$ up to 6.

Observe that if we keep track of where the current non-dominant pairs come from, then we are able to draw cata-condensed polyhexes which have $k_{\text{max}}(h)$ Kekulé structures.

5. Computational Results and Conclusions

Values of $k_{\text{max}}(h)$ for $h$ up to 100 are given in Table 4. They were obtained using a code in C and SUN SPARC station IPX; computing time was of 34.5 minutes. Further values of $k_{\text{max}}(h)$ for $h$ between 101 and 150 were obtained in 12 hours and 53 minutes of computing time. A list of these values is available from the authors. It is worth noting that in our code all variables are of integer type. To accommodate large numbers, these are encoded in several computer words.

In Fig. 9, are drawn the dualist graphs of cata-condensed polyhexes with up to 30 hexagons whose number of Kekulé structures is maximum. The square in each tree indicates the root hexagon. Observe that the values of $k_{\text{max}}(h)$ coincide those conjectured by Cyvin [9] for $13 \leq h \leq 20$ except in the cases $h = 17$ and $h = 20$. These values of $k_{\text{max}}(h)$ coincide with those given by John [17] for $h < 22$. Cyvin [9] also conjectured that cata-condensed polyhexes with maximum number of Kekulé structures have maximum branching (or, in other words, their dualist graphs have a maximum number of vertices of degree 3). Gutman [22] studied two families of cata-condensed.
Fig. 9. The dualist graphs of simply-connected cata-condensed polyhexes with maximum number of Kekulé structures and up to 30 hexagons.
polyhexes with maximum branching and a large number of Kekulé structures. He obtained recursive formulae to compute their number of Kekulé structures for those values of \( h \) for which they exist (these values of \( h \) decrease in frequency when \( h \) augments). As observed by an anonymous referee, the numbers of Kekulé structures for the Gutman benzenoids denoted by \( Y_h \) are not always maximum (e.g. for \( h = 15 \), 2306 is reported while \( k_{\text{max}}(15) = 2345 \), for \( h = 31 \), 8143397 is reported while \( k_{\text{max}}(31) = 8176976 \), etc.). This does not disprove Cyvin's conjecture cited above. Moreover a further conjecture of Cyvin [9] that for \( h = 1 + 3i \), \( i \) a positive integer, there is a simply-connected cata-condensed polyhex \( H \) with \( k(H) \) maximum which is fully resonant is confirmed for all \( h \leq 150 \).

After submission of this paper, we learned about related work of Balaban, Liu, Cyvin, and Klein [23, 24]. These authors independently obtained values of \( k_{\text{max}}(h) \) for \( h \leq 60 \) using also an enumerative algorithm exploiting dominance between cata-condensed polyhexes. The method used by Balaban et al. [24] differs however, from that of this paper as mergings of two cata-condensed polyhexes together with an additional hexagon are considered instead of mergings of two cata-condensed polyhexes sharing a common hexagon. It appears that the latter method leads to consider less pairs of undominated cata-condensed polyhexes than does the former one. Moreover the definition of dominated pairs used in this paper is stronger, as conditions \( f_{h,i}^0 \geq f_{h,j}^0 \) and \( f_{h,i}^0 + f_{h,i}^1 \geq f_{h,j}^0 + f_{h,j}^1 \) are implied by the conditions \( f_{h,i}^0 \geq f_{h,j}^0 \) and \( f_{h,i}^1 \geq f_{h,j}^1 \) used by Balaban et al. [24] but not conversely.

The main open problems on polyhexes with maximum number of Kekulé structures appear to be: (i) prove that cata-condensed polyhexes described in Fig. 9 belong to infinite families the members of which always have a maximum number of Kekulé structures (some candidate families are described in Balaban et al. [24]); (ii) prove that among all polyhexes only some cata-condensed polyhexes have maximum number of Kekulé structures (this has been verified by enumeration for small \( h \), but some new ideas seem to be needed for a mathematical proof).

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