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-cendensed 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 subpolicies".

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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.

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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 $k_{max}(h) = \max\{k(H)$: H is simply-connected cata-condensed and has h hexagons$\}$. If H is the empty graph, then define $k(H)=1$.

Fig. 1. Three hexagons in mode L_1 and in mode L_2.

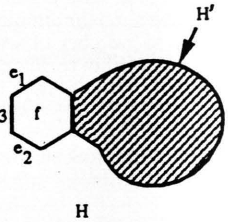


Fig. 2. Edges e_1, e_2, and e_2 in a leaf hexagon f.

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 $k_{max}(h)$ 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-

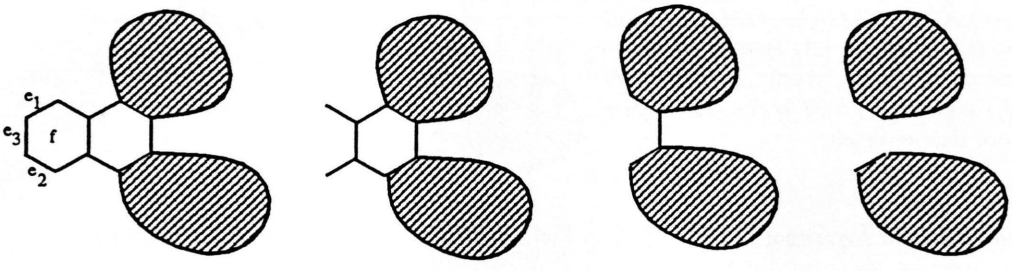


Fig. 3. Deleting e_3 together with its vertices, then deleting sequentially all pendant edges with their vertices and the incident edges and then the edges not belonging to any hexagon in the remaining graph.

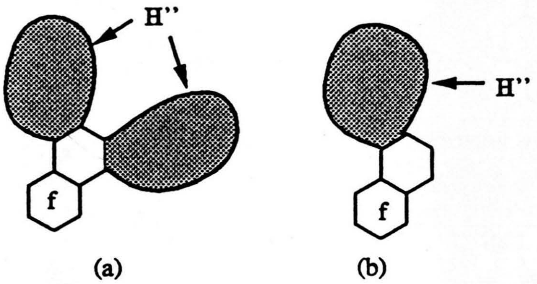


Fig. 4. The number of vertices not contained in H'' or f is 0 or 2.

nected component. By the induction hypothesis, the conclusion is true for each connected component of H''. Thus k_2 is equal to the product of the numbers of resonant sets in each of its connected components. On the other hand, the number of resonant set of H which contain f is also equal to this product. Therefore $k_2 = r_2$ and $k(H)$ is equal to the number of resonant sets of H. □

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* $k(H) < k_{max}(h)$.

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

(see Fig. 5b). Then $k(H') = k(H_1) \times k(H_2) + k(H'_1) \times k(H'_2)$. Since $k(H_i) > k(H'_i)$ $(i=1, 2)$ 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. □

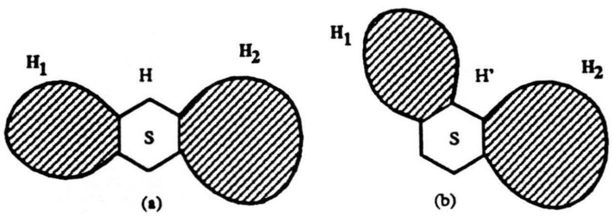


Fig. 5. A polyhex H with a hexagon in mode L_2 does not have maximum $k(H)$.

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 $k_{\max}(h)$ efficiently.

Let $\mathscr{H}(h)$ 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 $\mathscr{H}(h)$ for $h=1, 2, \ldots$ together with a distinguished leaf as its root. See Fig. 6 for an illustration.

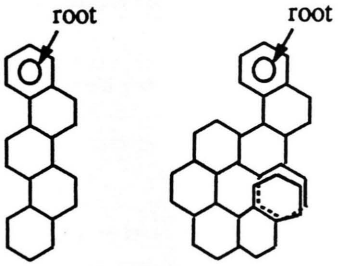
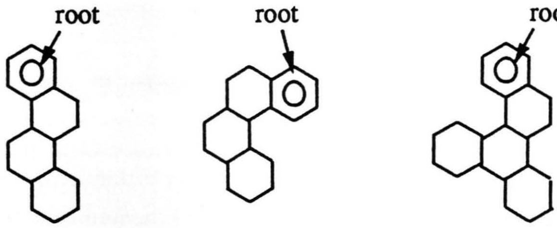


Fig. 6. Rooted symply-connected cata-condensed polyhexes.

Let $\mathscr{H}^r(h)$ 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.



(5,3) (5,3) (9,5)

Fig. 7. Feasible pairs.

Let $(f_{h,j}^0, f_{h,j}^1)$ $(j = 1, 2, \ldots, d_h)$ be all feasible pairs for a given h. In Table 1, all feasible pairs are given for h up to 8.

By Theorem 4, $k_{\max}(h) = \max\{k(H)\colon H \in \mathscr{H}(h)\}$. Thus $k_{\max}(h) = \max\{k(H)\colon H \in \mathscr{H}^r(h)\}$. By Theorem 3,

$$k_{\max}(h) = \max_j (f_{h,j}^0 + f_{h,j}^1) . \qquad (1)$$

Table 1. Feasible paris.

Number of hexagons	Feasible pairs
1	(1, 1)
2	(2, 1)
3	(3, 2)
4	(5, 3) (5, 4)
5	(8, 5) (9, 5) (8, 6)
6	(13, 8) (14, 9) (14, 8) (13, 10) (14, 10) (13, 9)
7	(21, 13) (23, 14) (22, 14) (23, 13) (24, 14) (22, 13) (21, 16) (23, 18) (22, 16) (21, 15) (23, 15)
8	(34, 21) (37, 23) (36, 22) (36, 23) (38, 24) (35, 22) (37, 21) (41, 23) (38, 22) (36, 21) (38, 23) (34,26) (37, 28) (36, 28) (36, 26) (38, 28) (35, 26) (34, 24) (37, 27) (36, 24) (34, 25) (37, 25) (37, 25) (41, 25)

A *non-dominated pair* $(f^0_{h,j}, f^1_{h,j})$ is a feasible pair for which no other feasible pair $(f^0_{h,i}, f^1_{h,i})$ satisfies the two conditions: $f^0_{h,i} \geq f^0_{h,j}$ and $f^0_{h,i} + f^1_{h,i} \geq f^0_{h,j} + f^1_{h,j}$; otherwise the pair $(f^0_{h,j}, f^1_{h,j})$ is dominated.

Let $(k^0_{h,j}, k^1_{h,j})$ $(j = 1, 2, \ldots, n_h)$ 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 gioven h. For non-dominated pairs, we have the following theorem.

Theorem 5:

$$k_{\max}(h) = \max_j (k^0_{h,j} + k^1_{h,j}).$$

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 $(k^0_{h,j}, k^1_{h,j})$ be a non-dominated pair with $h > 1$. Then there are two non-dominated pairs $(k^0_{h-t,i}, k^1_{h-t,i})$ and $(k^0_{t,l}, k^1_{t,l})$ with $t \leq h/2$ such that $k^0_{h,j} = k^0_{h-t,i} \times k^0_{t,l} + k^1_{h-t,i} \times k^1_{t,l}$ and $k^1_{h,j} = k^0_{h-t,i} \times k^0_{t,l}$.*

Proof: Let H be a cata-condensed polyhex with root r which corresponds to $(k^0_{h,j}, k^1_{h,j})$. Let r' be the hexagon of H adjacent to r. Let H^0 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^0 (see Figure 8). Without loss of generality, let H_1 have t hexagons with $t \geq h/2$. Let $(f^0_{t,l}, f^1_{t,l})$ and $(f^0_{h-t,i}, f^1_{h-t,i})$ be the two feasible pairs which correspond to H_1 and H_2 (with root r') respectively. Then $k^0_{h,j} = f^0_{h-t,i} \times f^0_{t,l} + f^1_{h-t,i} \times f^1_{t,l}$ and $k^1_{h,j} = f^0_{h-t,i} \times f^0_{t,l}$. If both of $(f^0_{t,l}, f^1_{t,l})$ and $(f^0_{h-t,i}, f^1_{h-t,i})$ are non-dominated pairs, the theorem is proved. Otherwise, without loss of generality let $(f^0_{t,l}, f^1_{t,l})$ be dominated. Then there is a non-dominated pair $(k^0_{t,m}, k^1_{t,m})$ with

$$k^0_{t,m} \geq f^0_{t,l} \tag{2}$$

and

$$k^0_{t,m} + k^1_{t,m} \geq f^0_{t,l} + f^1_{t,l} \tag{3}$$

Let H'_1 be the cata-condensed polyhex with root r'' which corresponds to $(k^0_{t,m}, k^1_{t,m})$. 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 $(f^0_{h,q}, f^1_{h,q})$ with $f^0_{h,q} = f^0_{h-t,i} \times k^0_{t,m} + f^1_{h-t,l} \times k^1_{t,m}$ and $f^1_{h,q} = f^0_{h-t,i} \times k^0_{t,m}$.

By (2), $f^1_{h,q} = f^0_{h-t,i} \times k^0_{t,m} \geq k^1_{h,j}$. Also $f^0_{h,q} - k^0_{h,j} = f^0_{h-t,i} \times (k^0_{t,m} - f^0_{t,l}) - f^1_{h-t,i} \times (f^1_{t,l} - k^1_{t,m})$. If $(f^1_{t,l} - k^1_{t,m}) \leq 0$, then $f^0_{h,q} - k^0_{h,j} \geq 0$. If $(f^1_{t,l} - k^0_{t,m}) > 0$, by (3) $(k^0_{t,m} - f^0_{t,l}) \geq (f^1_{t,l} - k^1_{t,m}) > 0$. By noting that $f^0_{h-t,i} \geq f^1_{h-t,i}$, $f^0_{h,q} - k^0_{h,j} \geq 0$. Note that (2) and (3) cannot be equalities at the same time. Thus $f^1_{h,q} \geq k^1_{h,j}$ and $f^0_{h,q} - k^0_{h,j} \geq 0$ cannot be equalities at the same time. This means that $(k^0_{h,j}, k^1_{h,j})$ is a dominated pair, a contradiction. □

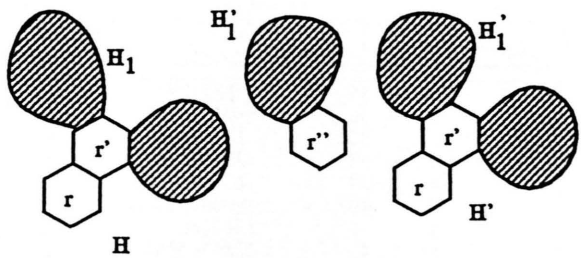


Fig. 8. Properties of non-dominated pairs.

Table 2. Non-dominated pairs of numbers of Kekulé structures

Number of hexagons	Non-dominated pairs
1	(1, 1)
2	(2, 1)
3	(3, 2)
4	(5, 4)
5	(9, 5)
6	(14, 10)
7	(24, 14) (23, 18)
8	(41, 25)
9	(66, 41) (65, 45)
10	(107, 82) (110,70)

Table 3. Application of the algorithm to small polyhexes.

Number of hexagons	Non-dominated pairs	All possible pairs calculated in (a)
1	(1, 1)	
2	(2, 1)	(2, 1)
3	(3, 2)	(3, 2)
4	(5, 4)	(5, 3), (5, 4)
5	(9, 5)	(9, 5), (8, 6)
6	(14, 10)	(14, 9), (14, 10), (13,9)

Table 4. Maximum number of Kukulé structures in simply-connected cata-condensed polyhexes with up to 100 hexagons.

h	$k_{max}(h)$	h	$k_{max}(h)$	h	$k_{max}(h)$
1	2	35	62212949	68	1231897292057784
2	3	36	104076573	69	2038292210457080
3	5	37	173169326	70	3425842818396369
4	9	38	288667101	71	5643905891795528
5	14	39	476880266	72	9427590804955560
6	24	40	800699454	73	15652773101103923
7	41	41	1319360447	74	26157207185004072
8	66	42	2210390934	75	43223119007212370
9	110	43	3669617993	76	72358101542007927
10	189	44	6100902003	77	119559022626893228
11	305	45	10104225566	78	200456254965800130
12	510	46	17012572857	79	331523467397042234
13	863	47	27963021326	80	552887059941957612
14	1425	48	46730211414	81	915893526665956910
15	2345	49	77723628299	82	1536549175733221566
16	3987	50	129649151874	83	2534281527098181854
17	6515	51	214222610438	84	4233916640677609590
18	10905	52	359261197551	85	7023536059728802112
19	18254	53	592810520174	86	11750792545044484446
20	30135	54	993399265662	87	19398634366045651280
21	49913	55	1645851650042	88	32480841022894787688
22	84546	56	2742311644086	89	53692500778754237402
23	138170	57	4539590744474	90	89909376480858669720
24	231117	58	7627440899358	91	148890403826259171221
25	386222	59	12575135816912	92	248216656107898447698
26	640830	60	20988331387026	93	410975377106181750830
27	1061039	61	34861727711192	94	690396813978436787229
28	1785078	62	58329989470488	95	1137323310636894449516
29	2931008	63	96179842466492	96	1900590864338462363070
30	4927011	64	161206731413568	97	3154203262239665593703
31	8176976	65	266499675718616	98	5271576673574081091684
32	13562472	66	445851954457908	99	8712238463081024061065
33	22512977	67	738886382963081	100	14579893080588254598747
34	37891224				

Now we are ready to state the algorithm for computing non-dominated pairs as well as $k_{max}(h)$.

Algorithm:

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

Recursive step: Increase h by 1. (a) Compute all possible pairs of values $(k^0_{h-t,i} \times k^0_{t,l} + k^1_{h-t,i} \times k^1_{t,l}, k^0_{h-t,i} \times k^0_{t,l})$ with $t \leq h/2$ and (b) keep all non-dominated pairs; calculate $k_{max}(h) = \max\{k^0_{h,i} + k^1_{h,i}\}$. 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 $k_{max}(h)$ Kekulé structures.

5. Computational Results and Conclusions

Values of $k_{max}(h)$ 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 $k_{max}(h)$ 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 $k_{max}(h)$ coincide those conjectured by Cyvin [9] for $13 \leq h \leq 20$ except in the cases $h=17$ and $h=20$. These values of $k_{max}(h)$ coincide with those given by John [17] for $h \leq 22$. 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

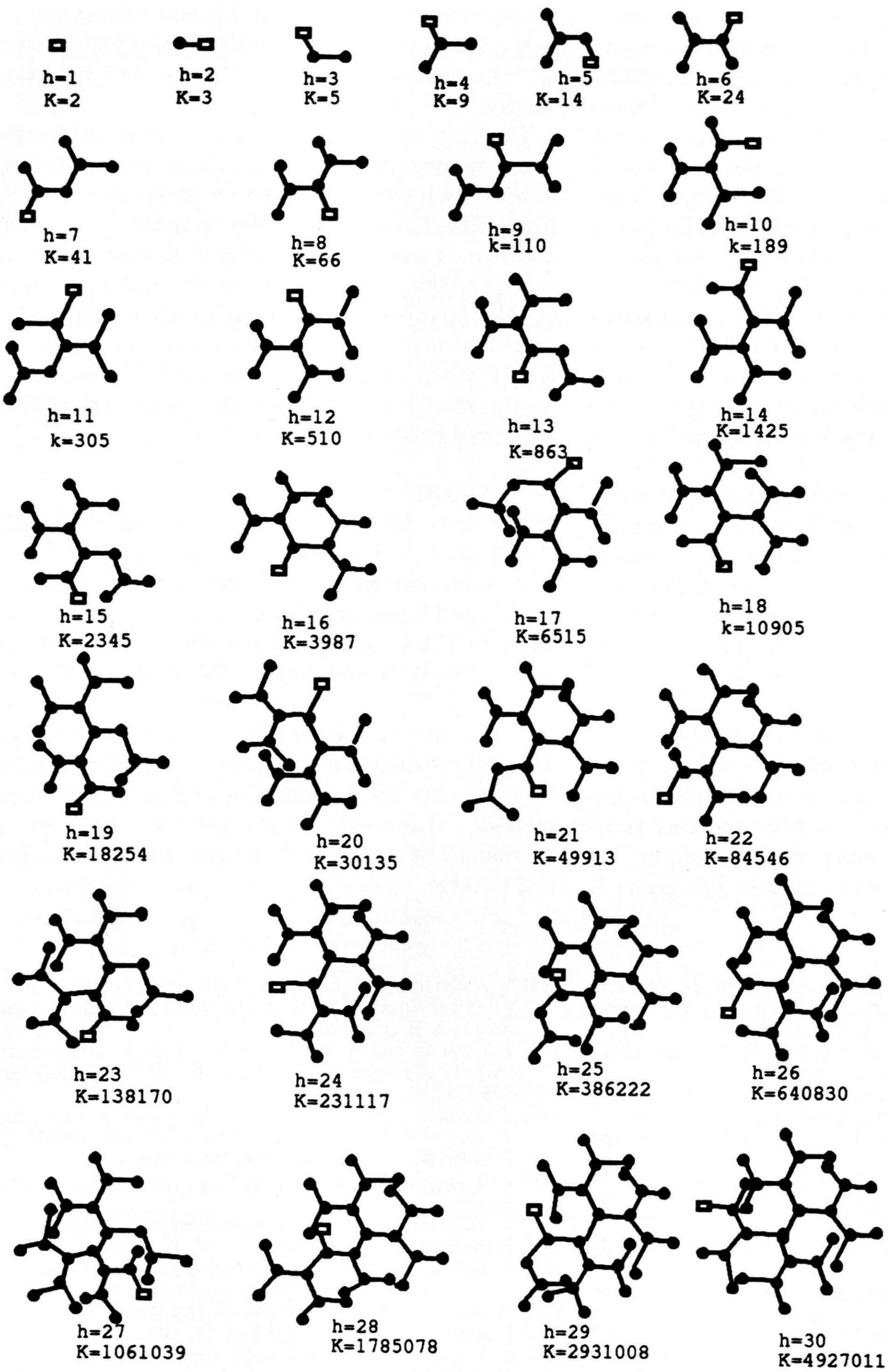


Fig. 9. The dualist graphs of simply-connected cata-condensed polyhexes with maximum number of Kekulé structures and up to 30 hexagons.

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_k are not always maximum (e.g. for $h=15$, 2306 is reported while $k_{max}(15) = 2345$, for $h = 31$, 8 143 397 is reported while $k_{max}(31) = 8\,176\,976$, 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 $k_{max}(h)$ 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 $f^0_{h,i} \geq f^0_{h,j}$ and $f^0_{h,i}+f^1_{h,i} \geq f^0_{h,j}+f^1_{h,j}$ are implied by the conditions $f^0_{h,i} \geq f^0_{h,j}$ and $f^1_{h,i} \geq f^1_{h,j}$ 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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