K-Coverable Polyhex Graphs

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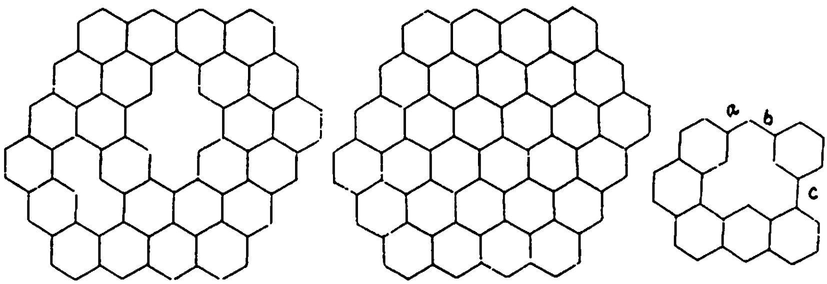
ABSTRACT. A polyhex graph is either a hexagonal system or a coronoid system. A polyhex graph G is said to be k-coverable if for any k mutually disjoint hexagons the subgraph obtained from G by deleting all these k hexagons together with their incident edges has at least one perfect matching. In this paper a constructive criterion is given to determine whether or not a given polyhex graph is k-coverable. Furthermore, a simple method is developed which allows us to determine whether or not there exists a k-coverable polyhex graph with exactly h hexagons.

1 Introduction

The terms "hexagonal system" and "coronoid system" are defined in the usual way. A hexagonal system [1], also called hexagonal animal [2], is a finite connected plane graph with no cut-vertices in which every interior region is bounded by a regular hexagon of side length 1. A coronoid system G [3] is a subgraph of a hexagonal system H which can be obtained from H by deleting at least one interior vertex of H (i.e. vertex not lying on the perimeter of H) together with its incident edge, and/or at least one interior edge (i.e. edge not lying on the perimeter of H) such that each edge of G belongs to at least one hexagon of G. The graph depicted in Figure 1a is a coronoid system, the hexagonal system from which it is obtained is shown in Figure 1b. While Figure 1c shows a graph which is not a coronoid system since it has three edges a, b, and c that do not belong to any of its hexagons.



From the definitions of hexagonal system and coronoid system it is clear that for a hexagonal system each interior region is bounded by a regular hexagon of side length 1, while for a coronoid system there is at least one interior region bounded by a polygon of more than six sides, this interior region is said to be a hole. If a coronoid system has only one hole, it is said to be a single coronoid system; otherwise, it is said to be a multiple coronoid system. The coronoid system depicted in Figure 1a is a multiple coronoid system.

A polyhex graph is either a hexagonal system or a coronoid system.

A perfect matching of a graph G is a set of disjoint edges such that each vertex of G is exactly an end vertex of some edge of the set. Perfect matchings of polyhex graphs coincide with what are called Kekulé structures in organic chemistry [4].

Let $N = \{s_1, \ldots, s_k\}$ be a set of k (a positive integer) mutually disjoint hexagons of a polyhex graph G, $G - N$ denote the subgraph of G obtained from G by deleting all the hexagons of N together with their incident edges. N is said to be a cover of G if $G - N$ is an empty graph (i.e. the unique graph without vertex and edge), or has at least one perfect matching. For a given positive integer k a polyhex graph G is said to be k-coverable if every set N of k (or fewer) mutually disjoint hexagons of G is a cover of G or there are not k mutually disjoint hexagons in G.

By the definition of k-coverable polyhex graph the following propositions are evident.

Proposition 1.1. *Let G be a k-coverable polyhex graph for a given positive integer k. Then G is also $(k-u)$-coverable, where u is a given positive integer such that $1 \leq u \leq k-1$.*

Proposition 1.2. *Let $\alpha(G)$ denote the maximum cardinality of the sets of mutually disjoint hexagons of a polyhex graph G. Then G is k-coverable for any given positive integer $k > \alpha(G)$.*

A cover of a polyhex graph is just what is called generalized Clar formula of the corresponding benzenoid or coronoid hydrocarbon in aromatic sextet theory [5,6]. The problem concerning coverability of polyhex graphs is an interesting mathematical problem. Necessary and sufficient conditions for a polyhex graph to be 1- and 2-coverable are known [7-10]. Criterions for a benzenoid system and a single coronoid system to be $k(\geq 3)$-coverable were reported in [9] and [10], respectively. Note that in ref. 10 the term "coronoid system" actually refers to "single coronoid system". Our work will fill the gap: when a multiple coronoid system is $k(\geq 3)$-coverable. Furthermore, a simple method is developed to determine whether or not there exist a k-coverable polyhex graph with exactly h (a positive integer) hexagons.

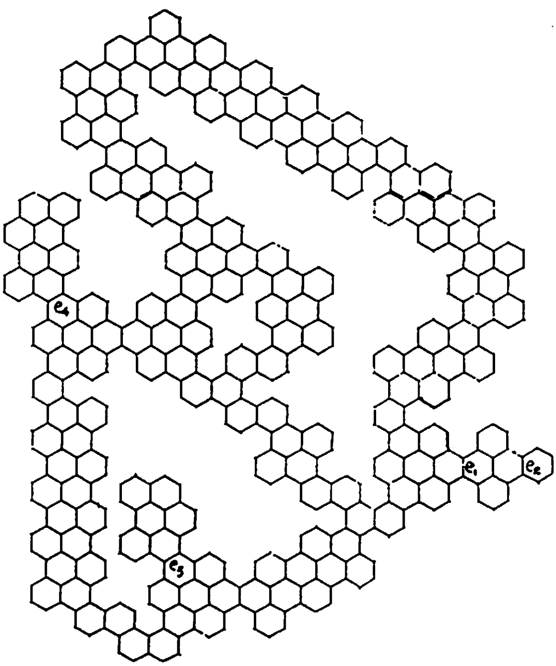


Figure 2. A k-coverable multiple coronoid system

2 k-Coverable Polyhex Graphs

First we need some more terminology. For a coronoid system the perimeter of each hole is said to be an inner perimeter, while the perimeter of the hexagonal system from which it is obtained is said to be the outer perimeter. Thus a single coronoid system has one outer perimeter and one inner perimeter, a multiple coronoid system has more than one inner perimeter.

Both outer and inner perimeters are called perimeters. Let e be an edge of a coronoid system G. If e does not lie on the perimeters of G, but two end vertices of e lie on the perimeter of G, then e is said to be a chord of G. If the two end vertices of e are simultaneously on the outer perimeter of G, or on the same perimeter of a hole, e is said to be of type I. Otherwise, e is said to be of type II. The reader is referred to Figure 2 for an illustration. For the coronoid system shown in Figure 2, e_1, e_2, e_3 and e_4 are of type I, and all the other chords are of type II.

The hexagonal systems depicted in Figure 3 are designated as a crown and a T_n (n is an integer not less than two), respectively. For each T_n we specify two edges on the perimeter to form an attachable set (see Figure 3). Each crown has six edges on its perimeter with two end vertices of degree two. They are divided into two attachable set each of which has three non-parallel edges (see Figure 3). Similarly, for a single hexagon three non-parallel and non-adjacent edges form an attachable set. Thus as a crown a single hexagon has two attachable sets.

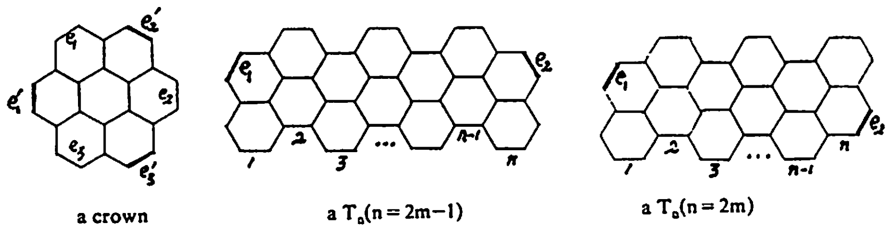


Figure 3

A subgraph G' of a polyhex graph G is said to be normal if it satisfies:

1. G' is a crown, or a T_n (n is an integer not less than 2), or a single hexagon;
2. G' contains at least one and at most three chords of G such that these chords form a subset of the attachable set of G';
3. deleting of these chords will separate G' from G.

For example, the single coronoid system shown in Figure 4 has seven normal subgraphs. Among them there are one crown, one single hexagon and five T_3's.

It is not difficult to see that any two normal subgraphs have at most one edge in common which is a chord of G. A polyhex graph G is said to have a normal decomposition if G has normal subgraphs $G_1, \ldots, G_t$ such that each hexagon of G belongs to exactly one $G_i (i = 1, \dots, t)$. The coronoid depicted in Figure 4 has a normal decomposition.

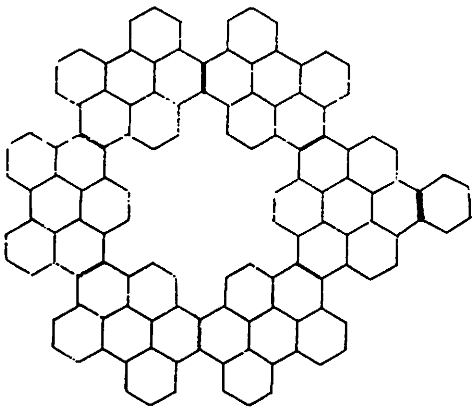


Figure 4

Note that when G itself is a T_n, or a crown, or a single hexagon, we also say that G is a normal subgraph of itself. Hence a T_n, or a crown, or a single hexagon has evidently a normal decomposition.

A hexagon of a polyehex graph is said to be external if it has at least one edge on the perimeter (inner or outer); otherwise, it is said to be internal.

Lemma 2.1. *Let G be a k-coverable polyhex graph for a given positive integer $k \geq 3$. Then*

(1) G cannot have three consecutive vertices on its perimeter such that the first and the last ones are of degree three and the second one is of degree two (see Figure 5(a)).

(2) G has no subgraph as shown in Figure 5(b).

(3) Any two internal hexagons of G are disjoint.

(4) The vertices on the perimeter of any crown which is a subgraph of G are on the perimeter of G.

(5) G has no such external hexagon that has exactly two parallel edges on the perimeter of G.

Proof:

(1) If there are three consecutive vertices v_1, v_2 and v_3 on the perimeter as shown in Figure 5(a), then $\{s_1, s_2\}$ is not a cover of G, and G is not 2-coverable, contradicting that G is k-coverable for a given positive integer $k \geq 3$.

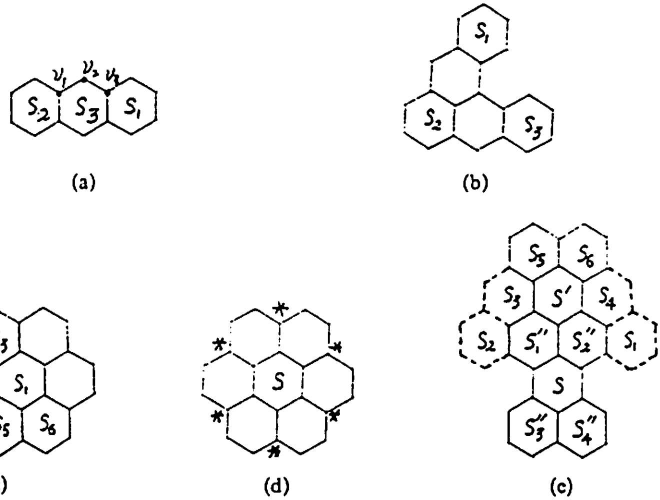


Figure 5

(2) If G has such a subgraph as shown in Figure 5(b) then $\{s_1, s_2, s_3\}$ is not a cover of G, again a contradiction.

(3) If G has two internal hexagons s_1 and s_2 with an edge in common, then G has a subgraph consisting of five hexagons s_3, s_2, s_4, s_5 and s_6. (see Figure 5(c)) It is impossible by (2).

(4) By (2) there is no hexagon on the positions each of which has a star (see Figure 5(d). Hence all the vertices of the crown must be on the perimeter of G.

(5) Let s be an external hexagon with exactly two parallel edges on the perimeter (see Figure 5(e)). We may further assume that s is uppermost in the sense that s' does not belong to G, or s' does not have the same property as s. By (2) neither of s_1 and s_2 belongs to G. Again neither of s_3 and s_4, belongs to G by (1). If s' does not belong to G, $\{s\}$ is not a cover of G, a contradiction. Hence s' must be in G. since s_1'' and s_4'' form a cover of G, at least one of s_5 and s_6 belongs to G. If one of them is in G, then the other must also be in G (by (1)). Then s' is an external hexagon possessing the same property as s, contradicting the selecting of s.

Let G' be a subgraph of G. We use the symbol $G - G'$ to denote the subgraph of G which is obtained from G by deleting all the vertices and edges of G' except those edges which are chords of G. For example, suppose that G is the coronoid system depicted in Figure 4, G' is the crown of G

then $G - G'$ will be a disconnected graph consisting of two components as shown in Figure 6.

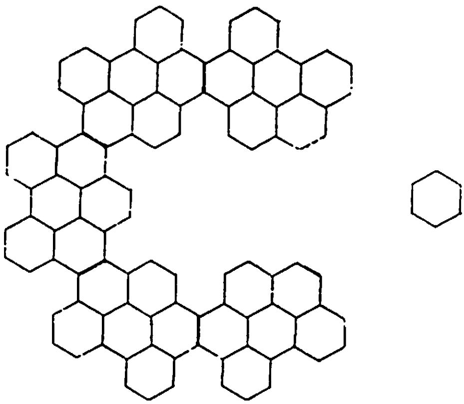


Figure 6

Theorem 2.2. *Let G be a k-coverable polyhex graph for a given positive integer $k \geq 3$. Then G has a normal decomposition.*

Proof: It suffices to prove that each hexagon s of G is contained in a normal subgraph of G. We distinguish six cases according to how may vertices of s lie on the perimeter of G.

Case 1 s has no vertex on the perimeter of G. This means that s is an internal hexagon of G. Let the crown containing s as its center be G'. By Lemma 2.1(4) all the vertices on the perimeter of G' are also on the perimeter of G. This implies that the intersection of G' and $G - G'$, i.e. $(G - G') \cap G'$ is a set consisting of some isolated edges on the perimeter of G'. Now we prove that $(G - G') \cap G'$ is a subset of an attachable set of G'. First $|(G - G') \cap G'| < 4$, otherwise, a pair of e_i and e'_i $(1 \leq i \leq 3)$ belongs to $(G - G') \cap G'$ (cf. Figure 3), which contradicts Lemma 2.1(2). If $(G - G') \cap G'$ contains both e_i and e'_j for some $1 \leq i, j \leq 3$,then either $(G - G') \cap G'$ contains a pair of e_i and e'_i for some $1 \leq i \leq 3$, or a pair of e_i and e'_{i+1} (where $i+1$ is taken modelo 3) or a pair of e_i and e'_{i+2} (where $i+2$ is take modulo 3) for some $1 \leq i \leq 3$. The first two cases contradict Lemma 2.1(2) as mentioned above. For the last case the two hexagons in $G - G'$ containing e_i and e'_{i+2} respectively together with s will not form a cover of G, which contradicts the fact that G is k-coverable for a given positive integer $k \geq 3$. Therefore, $(G - G') \cap G'$ is a subset of an attachable set of the crown G' containing s as its centre. Consequently, G' is a normal subgraph of G by the definition of normal subgraph.

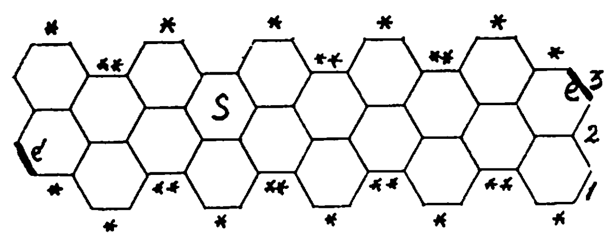


Figure 7

Case 2 s has exactly two vertices on the perimeter of G. It is clear that G has a subgraph which is a T_3 (see Figure 7) Let T_m be the maximal subgraph of G containing s in the sense that no other T_n which is a subgraph of G and contains T_m. By Lemma 2.1(2) there is no hexagon of G on each position with a star. There is no hexagon of G on the positions each of which has a double star (Lemma 2.1(4)). Thus there is no hexagon of G on position 1 (Lemma 2.1(1)). If there is a hexagon on position 2, there must also be a hexagon on position 3 (Lemma 2.1(1)). But this contradicts the maximality of T_m. Hence it is the only possibility that there is a hexagon of G on position 3. This means that edge e is either on the perimeter of G or a member of the attachable set of T_m. The same is true of edge e'. Let $G' = T_m$. If $G \neq G'$, then $(G - G') \cap G' = \{e\}$ or $\{e'\}$ or $\{e, e'\}$. It is a subset of the attachable set of T_m. Consequently, G' is a normal subgraph of G.

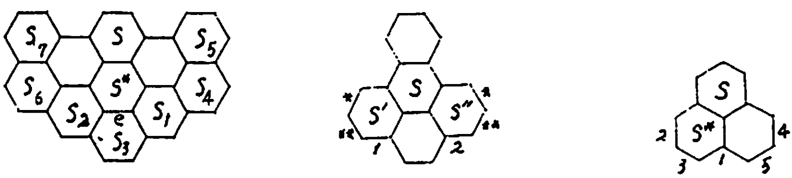
Case 3 s has exactly three vertices on the perimeter of G. By Lemma 2.1(1) this is impossible.

Case 4 s has exactly four vertices on the perimeter of G. By Lemma 2.1(5) these four vertices cannot appear on two parallel edges of s. We distinguish two subcases.

Subcase 4.1 s has three consecutive edges on the perimeter of G (see Figure 8.1). If s_1 is not in G, neither s_4 nor s_5 belongs to G (Lemma 2.1(1) and (5)). Analogously, if s_2 is not in G, neither of s_6 and s_7 belongs to G. Hence if neither of s_1 and s_2 is in G, s is contained in a T_2. Let $G' = T_2$. If $G \neq T_2$, then $(G - G') \cap G' = \{e\}$ is a subset of the attachable set of T_2. Therefore, G' is a normal subgraph of G. If at least one of s_1 and s_2 belongs to G, we may assume that s_1 is in G. By Lemma 2.1(1) one or both of s_2 and s_3 must belong to G. In the former case s^* is a hexagon with exactly two vertices on the perimeter of G. In the latter case s^* is an internal hexagon of G. By the conclusions of case 1 and case 2, s^*, and therefore s, is contained in a normal subgraph of G.

Subcase 4.2 s has two non-parallel and non-adjacent edges on the perimeter of G (see Figure 8.2). By Lemma 2.1(2) there is no hexagon of G on each position with a star. There is no hexagon on each position with a double star (Lemma 2.1(1)). If on neither of positions 1 and 2 there is a hexagon of

G, then it is not difficult to see that s is contained in a normal subgraph of G which is a T_2. Now suppose that at least on one of the positions 1 and 2 there is a hexagon of G. Then s' or s'' will be a hexagon with exactly three consecutive edges on the perimeter of G. By the conclusion of subcase 4.1, s' (or s''), and therefore s, is contained in a normal subgraph of G.



(1) (2) (3)

Figure 8

Case 5 s has five vertices on the perimeter of G. If there is no hexagon of G on position 1 (see Figure 8.3), then there is no hexagon on positions 2,3,4, and 5. (Lemma 2.1(1) and (5)). This means that G is a benzenoid system consisting of three hexagons and has no perfect matching, a contradiction. Hence there must be a hexagon on position 1. Now s^* is a hexagon with at most four vertices on the perimeter of G. By the conclusions of cases 1 to 4, s^*, and therefore s, is contained in a normal subgraph of G.

Case 6 s has six vertices on the perimeter of G. Then G consists of a single hexagon. The conclusion holds.

When confined to hexagonal systems or single coronoid systems, we have the following corollaries which can be regarded as the main results in [9] and [10].

Corollary 2.3 [9]. *Let G be a k-coverable benzenoid system without chords for a given positive integer $k \geq 3$. Then G is a crown, or a T_n, or a hexagon.*

Corollary 2.4 [10]. *Let G be a k-coverable single coronoid system without chords of type I for a given positive integer $k \geq 3$. The chords of type II are denoted by $e_1, e_2, \ldots, e_t$ such that the section of G between chords e_i and e_{i+1} inclusive, designated by $G(e_i, e_{i+1})$, will not contain any other chords of G except e_i and e_{i+1}, $i = 1, 2, \ldots, t$, where $i+1$ is taken modulo t. Then $G(e_i, e_{i+1})$ is a normal subgraph of G for $i = 1, 2, \ldots, t$.*

For each k-coverable polyhex graph G we construct a plane graph G^*: the vertex set of G^* is the set of normal subgraphs of G, two vertices of G^* are adjacent if and only if the corresponding normal subgraphs of G have an edge in common. It is clear that G^* is a tree when G is a k-coverable hexagonal system, and G^* is a cycle when G is a k-coverable single coronoid without chords of type I. For a k-coverable single coronoid system G with some chords of type I, G^* is a cycle with some pendent paths. When G is a k-coverable multiple coronoid, G^* is a plane graph with multiple cycles.

We have already known that a crown, a T_n and a single hexagon are k-coverable for a given positive integer $k \geq 3$. Furthermore, it is not difficult to verify that the subgraph of a crown obtained by deleting some edge(s) which belong to an attachable set of the crown is still k-coverable for a give positive integer $k \geq 3$. The same is true of T_n. Based on this fact, we have the following.

Theorem 2.5. *Let G be a polyhex graph. If G has a normal decomposition. then G is k-coverable for a given positive integer $k \geq 3$.*

As a direct consequence of Theorem 2.2 and 2.5 we get a criterion for a polyhex graph to be k-coverable for a given positive integer $k \geq 3$.

Theorem 2.6. *For a given positive integer $k \geq 3$ a polyhex graph G is k-coverable if and only if G has a normal decomposition.*

Remark: Let G be a 3-coverable polyhex graph. Taking $k = 3$ in the above theorem, the necessity of the theorem ensures that G has a normal decomposition. Then by the sufficiency of the above theorem for $k = 4$, G is also 4-coverable. In a similar way we come to the conclusion that if G is 3-coverable then G is k-coverable for all positive integer not less than 3. On the other hand, by Proposition 1.1 G is also 1-coverable and 2-coverable. Therefore, if G is 3-coverable then G is coverable for all positive integers $k = 1, 2, 3, \ldots$. We make convention that in the following if we say that G is k-coverable without pointing out the concrete value of k, it means that k is taken all positive integers.

3 Realization Of k-Coverable Polyhex Graphs With H Hexagons

From previous section the constructive feature of k-coverable polyhex graphs is clear. Now we concentrate ourselves to the problem: whether or not there exists a k-coverable polyhex graph with exactly h (a positive integer) hexagons.

As a common knowledge it is much easier to draw a polygon than a polyhex graph. By setting up a correspondence between polyhex graphs and polygons, we transfer the problem of determining whether or not there is a k-coverable polyhex graph with h (a positive integer) hexagons to a problem of drawing a polygon with some properties. From section 2 we know that a k-coverable coronoid system with some chords of type I can be separated into two parts: one is a k-coverable coronoid system without chords of type I, and the other consists of some k-coverable hexagonal systems (cf. Figure 2). It is not difficult to see that for any positive integer h there exists a k-coverable benzenoid system with h hexagons. For example, a single zigzag chain (i.e. a cata-condensed hexagonal system with h

normal subgraphs which are all single hexagons, cf. [11]) is a required one. Furthermore, the answer is not unique. When $h = 2n$ ($n \geq 2$), T_n is a k-coverable hexagonal system with h hexagons. When $h = 2n+1$ ($n \geq 5$), the hexagonal system with two normal subgraphs, one being a T_{n-3} and the other being a crown; or one being a T_n and the other being a single hexagon, is also a required k-coverable hexagonal system. In the following we will confine ourselves to k-coverable coronoid systems without chords of type I, and start from single coronoid systems.

3.1 Realization Of k-Coverable Single Coronoid Systems

Let C be the hole of a k-coverable single coronoid system. Edges $e_1, e_2, \ldots, e_m$ be the chords of type II each of which has an end vertex v_i ($i = 1, 2, \ldots, m$) on the perimeter of C such that $v_1, v_2, \ldots, v_m$ appear clockwise. We denote the normal subgraph between e_i and e_{i+1} ($i+1$ is taken modulo m) by $G(i, i+1)$ ($i = 1, 2, \ldots, m$). It is easy to see that for $G(i, i+1) = T_{2t_i}$, there is a unique hexagon with three consecutive vertices of degree two on the perimeter of C (cf. Figure 9, hexagon s is such one). We refer to this hexagon as the characteristic hexagon of the corresponding T_{2t_i}. We construct a polygon corresponding to G in this way: place a vertex in the centre of characteristic hexagon of each normal subgraph $G(j, j+1) = T_{2t_j}$ and denote it by v_j^*; connect v_j and v_j^*, v_j^* and v_{j+1}, for each $G(j, j+1) = T_{2t_j}$ connect v_i and v_{i+1} for $G(i, i+1) = T_{2t_i+1}$ or a crown, or a hexagon. Denote the resultant polygon by $P(G)$. It is evident from the construction that a T_{2t+1} contributes a side to $P(G)$ whose length is $3t+1$ or $3t+2$. In the former case T_{2t+1} is said to be regular, in the latter case it is said to be irregular. For a T_{2t} it contributes two consecutive sides to $P(G)$, their lengths are 2 and $3t-1$, or $3t-1$ and 2 (clockwise). Similarly, in the former case T_{2t} is said to be regular, and in the latter case it is said to be irregular (cf. Figure 9). For a single hexagon which is a normal subgraph of G, it contributes a side of length 1 or 2 to $P(G)$, and is said to be regular or irregular. Similarly, a crown is said to be regular or irregular depending on whether the length of the side contributed by it is 4 or 5. It is not difficult to see that the inner angles of $P(G)$ are $2\pi/3$, or π, or $4\pi/3$; and the lengths of sides of $P(G)$ can be expressed as $3t-2$, or $3t-1$ ($t \geq 1$). A side with length $3t-2$ is contributed by a regular T_n with odd n (a regular crown, a regular single hexagon) .For a side with length $3t-1$ it may be contributed by a T_n with even n, or an irregular T_n with odd n (an irregular crown, an irregular single hexagon). In the former case the side is referred to as E-type, and in the latter case as O-type. The relation between sides and angles of $P(G)$ can be described in detail as shown in Chart I.

A k-covrerable single coronoid system G and its corresponding polygon $P(G)$ are shown in Figure 9.

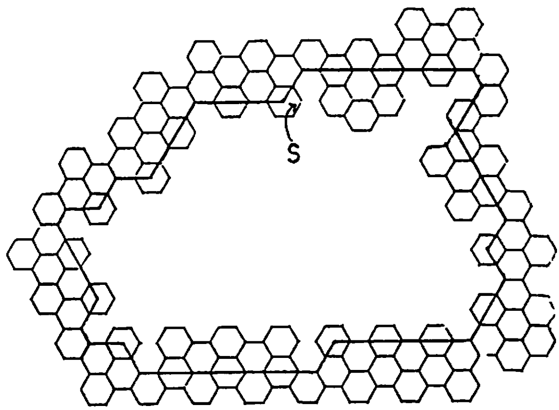


Figure 9

Now suppose that P is a polygon satisfying the following rules.

(1) Any inner angle of P is $2\pi/3$, or π, or $4\pi/3$.

(2) Let a be a side of P. Then $|a| \equiv 1 \pmod 3$, or $|a| \equiv 2 \pmod 3$.

(3) The sides with $|a| \equiv 2 \pmod 3$ is divided into two classes: one referred to as E-type, and the other as O-type.

(4) The relation between angles and sides is given in Chart I.

(5) A side of E-type is always a side of an angle of $4\pi/3$.

Anglc \ |b| / |a|		3t−2	3t−1	
			E−typc	O−typc
3t−2		$2\pi/3$	$2\pi/3$	π
3t−1	E−typc	$2\pi/3$	$4\pi/3$	π
	O−typc	π	π	$4\pi/3$

Chart I (a and b denote two consecutive sides of P)

Note that the above rules are just those that are satisfied by $P(G)$.

For each polygon P obeying above rules, we can construct a corresponding k-coverable single coronoid system in the following way.

(1) Let b be a side with $|b| \equiv 1 \pmod 3$, i.e. $|b| = 3t - 2$. If $t = 1$, let b correspond to a regular single hexagon; if $t = 2$, let b correspond to a regular crown or a regular T_{2t-1} (i.e. T_3); if $t > 2$, let it correspond to a regular T_{2t-1}.

(2) Let two consecutive sides a_1 and a_2 of E-type together with the inner angle between them correspond to a T_{2m}, where $m = \max\{t, r\}$, $|a_1| = 3t - 1$, $|a_2| = 3r - 1$. (note the inner angle between a_1 and a_2 must be $4\pi/3$ by Rules 4 and 5).

(3) Let c be a side of O-type. Then $|c| = 3t - 1$. If $t = 1$, let c correspond to an irregular single hexagon; if $t = 2$, let c correspond to an irregular crown or an irregular T_{2t-1} (i.e: T_3); if $t > 2$, let it correspond to an irregular T_{2t-1}.

Suppose that G is a k-coverable single coronoid system without chords of type I. G has h hexagon and u normal subgraphs $G_1, G_2, \ldots, G_u$, G_i has h_i hexagons ($i = 1, 2, \ldots, u$). Then $(h_1, h_2, \ldots, h_u)$ is an integer partition of h, and $h_i = 1$, or 7, or $4t_i$ ($t_i \geq 1$), or $4t_i - 2$ ($t_i \geq 2$). Let the corresponding polygon be $P(G)$. The side length sequence of $P(G)$ can be obtained from $(h_1, h_2, \ldots, h_u)$ in this way: if $h_i = 4t_i$ ($t_i \geq 1$), substitute h_i by 2^e and $(3ti - 1)^e$, or $(3ti - 1)^e$ and 2^e; if $h_i = 4t_i - 2$ ($t_i \geq 2$), substitute h_i by $(3t_i - 1)^o$ or $3t_i - 2$. It is evident that the resultant sequence has $u + n$ ($h_i = 4t_i$) numbers, where $n(h_i = 4t_i)$ denotes the number of h_i's with $h_i = 4t_i$; if $h_i = 1$, substitute it by 1 or 2; if $h_i = 7$, substitute it by 4 or 5. Note that a number with a superscript e indicates that the corresponding side of $P(G)$ is of E-type, while a number with a superscript o indicates that the corresponding side is of O-type.

We are now in the position to describe our method to determine whether or not there is a k-coverable single coronoid system without chords of type I and with exactly h hexagons, and find out all such coronoid systems, if any.

Step 1 Find out the set of integer partitions of h:
$\{(h_1, h_2, \ldots, h_u) | \Sigma h_i = h,\ h_i = 1, 7, 4t_i\ (t_i \geq 1), \text{ or } 4t_i - 2\ (t_i \geq 2),\ u \geq 6\}$
(Note: the inequality $u \geq 6$ is obtained from inner angle sum rule of polygons.)

Step 2 For each partition $(h_1, h_2, \ldots, h_u)$ find out the set N of all corresponding number sequences.

Step 3 For each number sequence of N check whether or not there is a polygon satisfying the rules in Chart I, and find out the corresponding k-coverable single coronoid system, if any.

3.2 Realization Of k-Coverable Multiple Coronoid Systems

As mentioned in section 2, each k-coverable polyhex graph G corresponds to a plane graph G^*: the vertex sat of G^* is the set of normal subgraphs of G, two vertices of G^* are adjacent if and only if the corresponding normal subgraphs of G have an edge in common. If G is a k-coverable multiple coronoid system without chords of type I, G^* is a plane graph with multiple cycles. Hence the constructing of a k-coverable multiple coronoid system can be regarded as a series of constructing of k-coverable single coronoid systems. For example, constructing the multiple coronoid G depicted in Figure 10 can be reduced to constructing of three single coronoid system G_1, G_2, and G_3. In the following we outline the method to determine whether or not there exists a k-coverable multiple coronoid system with h hexagons.

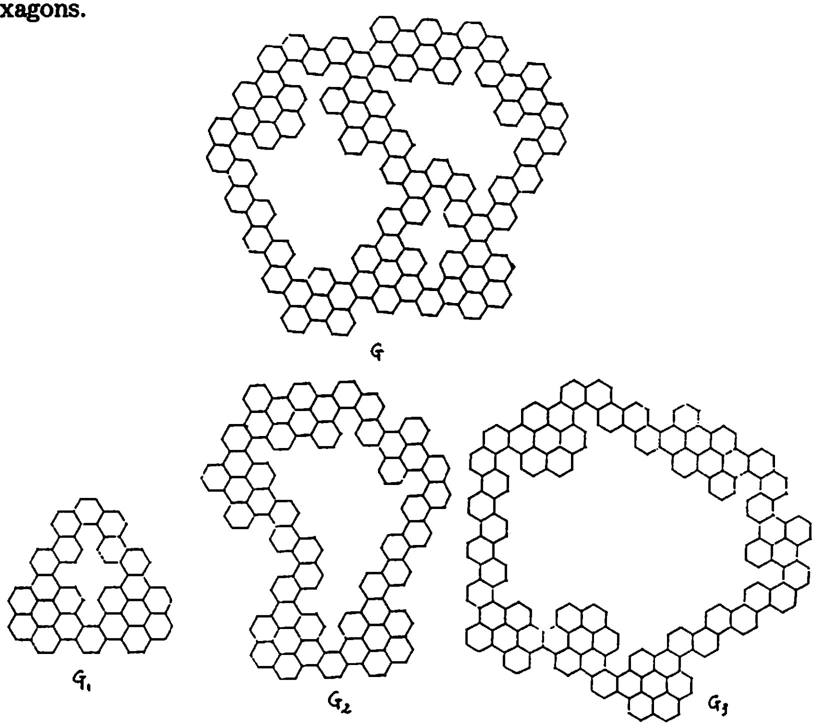


Figure 10

Suppose that $(h_1, h_2, \ldots, h_r)$ is an integer partition of h with $r \geq 2$.

Step 1 Determine the set Z_1 of k-coverable single coronoid systems with h_1 hexagons. If $Z_1 = \phi$, check another integer partition of h. If $Z_1 \neq \phi$, go to next step.

Step 2 Take a k-coverable coronoid system from Z_1. Denote the corresponding partition by $(h_{11}, h_{12}, \ldots, h_{1u})$. If there exist i and t such that

$h_{1i}, h_{1\ i+t} \in \{1,7\}$ $(1 \leq i, i+t \leq u)$ go to next step. Otherwise, check another k-coverable coronoid system in Z_1 until there is no one left in Z_1 and stop.

Step 3 Find an integer partition of h_2: $(h_{21}, h_{22}, \ldots, h_{2v})$. Determine the set Z_2 of k-coverable single coronoid system such that the corresponding partition is $(h_{11}, h_{12}, \ldots, h_{1i}, h_{21}, h_{22}, \ldots, h_{2v}, h_{1i+t}, h_{1i+t+1}, \ldots, h_{1u})$. If $Z_2 = \phi$, check another integer partition of h_2. If $Z_2 \neq \phi$, go to next step.

Step 4 Take a k-coverable coronoid system from Z_2. Rewrite the partition as $(h_{21}, h_{22}, \ldots, h_{2d})$. If there exist i and t such that $h_{2i}, h_{2i+t} \in \{1,7\}$ $(1 \leq i, i+t \leq d)$ go to next step. Otherwise, check another k-coverable coronoid system in Z_2 until there is no one left in Z_2, and stop.

Step 5 Find an integer partition of h_3: $(h_{31}, h_{32}, \ldots, h_{3e})$. Determine the set Z_3 of k-coverable single coronoids with partition $(h_{21}, h_{22}, \ldots, h_{2i}, h_{31}, h_{32}, \ldots, h_{3e}, h_{2i+t}, h_{2i+t+1}, \ldots, h_{2d})$. If so, go to next step. Otherwise, check another integer partition of h_3.

We need not to go further, that is enough. The remaining steps are just repetition of steps 4 and 5 by replacing h_j by h_{j+1}. In the following we give an example as an illustration.

Suppose $h = 77$. $(h_1, h_2, h_3) = (22, 30, 25)$ is an integer partition of h. In step 1 we find a k-coverable single coronoid system G_1 with $h_1 = 22$ hexagons (see Figure 10). In step 2 we denote the corresponding partition of G_1 by $(h_{11}, h_{12}, \ldots, h_{1,10}) = (1,7,1,1,1,1,1,1,1,7)$, and find $i = 3$, $t = 4$ such that $h_i = h_3 = h_{i+t} = h_7 = 1$. In step 3 we give an integer partition for $h_2 = 30$: $(h_{21}, h_{22}, \ldots, h_{2,15}) = (1,1,1,1,1,1,4,1,1,1,8,1,6,1,1)$, and find a k-coverable single coronoid system G_2 with partition $(h_{11}, h_{12}, h_{13}, h_{21}, h_{22}, \ldots, h_{2,15}, h_{17}, h_{18}, h_{19}, h_{1,10}) = (1,7,1,1,1,1,1,1,1,4,1,1,1,8,1,6,1,1,1,1,1,7)$ (see Figure 10). In step 4 we rewrite the partition as $(h_{21}, h_{22}, \ldots, h_{2,22})$, and find $i = 15$, $t = 7$ such that $h_{2i} = h_{2,15} = 1$ and $h_{2,i+t} = h_{2,22} = 7$. In step 5 an integer partition is given for $h_3 = 25$: $(h_{31}, h_{32}, \ldots, h_{3,14}) = (1,1,1,1,7,1,1,1,1,1,1,1,1,16)$ and find a k-coverable single coronoid system G_3 (see Figure 10) with partition $(h_{21}, h_{22}, \ldots, h_{2,15}, h_{31}, h_{32}, \ldots, h_{3,14}, h_{2,22}) = (1,7,1,1,1,1,1,1,1,4,1,1,1,8,1,1,1,1,1,7,1,1,1,1,1,1,1,1,6)$. Consequently, the union of G_1, G_2 and G_3, i.e. G (see Figure 10) is a k-coverable multiple coronoid with $h = 77$ hexagons.

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References

[1] H. Sachs, Perfect matchings in hexagonal systems, Combinatorica **4(1)** (1984), 89–99.

[2] F. Harary, The cell growth problem and its attempted solutions, Beitrage zur Graphentheorie (Int. Koll. Manebach, 9–12. Mai 1967), ed. H. Sachs, H.-J. Voss and H. Walther. B.G. Teubner Verlagsgesellschaft Leipzig 1968, 49–60.

[3] S. J. Cyvin, J. Brunvoll and B. N. Cyvin, Theory of Coronoid Hydrocardons, *Lecture Notes in Chemistry* **54**, Springer-Verlag (1991).

[4] I. Gutman and S.J. Cyvin, Introduction to the Theory of Benzenoid Hydrocarbons, Springer-Verlag (1989).

[5] I. Gutman, Covering hexagonal system with hexagons, in: Proceedings of the Fourth Yugoslav Seminar on Graph Theory, Novi Sad (1983), 151–160.

[6] N. Ohkami, A. Motoyama, T. Yamaguchi, H. Hosoya and I. Gutman, Graph-theoretical analysis of the Clar's aromatic sextet — mathematical properties of the set of the Kekulé patterns and the sextet polynomial for polycyclic aromatic hydrocarbons, *Tetrahedron* **37** (1981) 1113–1122.

[7] Zhang FJ and Chen RS, When each hexagon of a hexagonal system covers it, *Discrete Applied Math.* **30** (1991), 63–75.

[8] Zhang FJ and Zheng ML, Generalized hexagonal system with each hexagon being resonant, *Discrete Applied Math.* **36** (1992), 67–73.

[9] Zheng ML, K-coverable hexagonal systems, Rutcor Research Report #20–88, Rutgers University, New Brunswick, N.J. U.S.A.

[10] Chen RS and Guo XF, K-coverable coronoid systems, J. Mathematical Chemistry **12** (1993), 147–162.

[11] S.J. Cyvin and I. Gutman, Kekulé Structures in Benzenoid hydrocarbons, *Lecture Notes in Chemistry* **46**, Springer-Verlag (1988).