Journal of Mathematical Chemistry 12(1993)147–162

k-coverable coronoid systems*

Rong-si Chen

College of Finance and Economics, Fuzhou University, Fuzhou, 350002 Fujian, PR China

and

Xiao-feng Guo

Department of Mathematics, Xinjiang University, Urumchi, 830046 Xinjiang, PR China

A coronoid system G is k-coverable if for every k (or fewer) pairwise 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, some criteria are given to determine whether or not a given coronoid system is k-coverable.

1. Introduction

The terms "benzenoid system" and "coronoid system" are defined in the usual way [1–3]. Thus, a benzenoid system (BS), also called "honeycomb system" [1], is a finite connected plane graph with no cut vertices in which each interior face is a regular hexagon of side length 1, whereas a coronoid system (CS) G can be obtained from a benzenoid system B by deleting at least one interior vertex together with the incident edges, and/or at least one interior edge such that each edge of G belongs to at least one hexagon of G and a unique non-hexagon interior face emerges. The graph depicted in fig. 1(a) is a coronoid system, while the one depicted in fig. 1(b) is not a coronoid system since it has some edges not belonging to any of its hexagons.

The unique non-hexagon interior face of a CS G is called a hole. The perimeter of the hole is called the inner perimeter of G. The perimeter of the BS from which G is obtained is called the outer perimeter of G. A hexagon of G is said to be a side hexagon of G if it has at least one edge lying on the outer or inner perimeter of G; otherwise, it is called a non-side hexagon of G.

A perfect matching, which corresponds to a Kekulé structure [4] in organic chemistry, in a graph G is a set of pairwise non-adjacent edges of G that spans the

*Supported by NSFC.

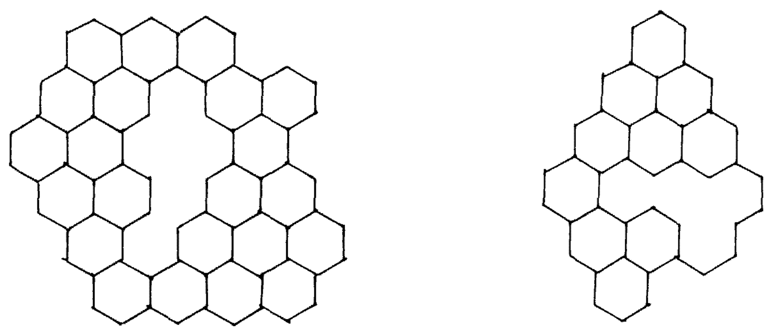


Fig. 1.

vertices of G. Let G be a BS or a CS and M a perfect matching of G. A circuit of G with h edges is said to be an M-conjugated circuit [5] if it has $h/2$ M-double bonds.

An edge of a CS G is said to be interior if it does not lie on the outer or inner perimeter of G. An interior edge of G is said to be a chord if its two end-vertices are on the outer and/or inner perimeter of G. A chord is of type I if its two end-vertices are simultaneously on the outer or inner perimeter of G. Otherwise, it is of type II (cf. fig. 5 below).

Let $K = \{s_1, s_2, \ldots, s_k\}$ $(k \geq 1)$ be a set of pairwise disjoint hexagons of a BS or CS G. $G - K$ denotes the subgraph obtained from G by deleting all the hexagons of K together with their incident edges. K is said to be a cover of G if $G - K$ has at least a perfect matching or is an empty graph. If K is a cover of G, then we will also say that hexagons $s_1, s_2, \ldots, s_k$ form a cover of G. A BS or a CS G is said to be k-coverable if for every k (or fewer) pairwise disjoint hexagons the subgraph, obtained from G by deleting all these k hexagons together with their incident edges, has at least one perfect matching.

The concept of a cover is just a graph-theoretical reformulation of the concept "generalized Clar formula" occurring in the so-called Clar aromatic sextet theory [6,7]. The problem concerning coverability is an interesting mathematical one. For any positive integer k, the criterion to determine whether or not a given BS is k-coverable is known [8–10].

THEOREM 1 [8]

A BS B is 1-coverable if and only if the perimeter of B is a conjugated circuit for some perfect matching of B.

THEOREM 2 [9]

A BS B is 2-coverable if and only if, for any side-hexagon s of B, each connected component of $B(s)$ is 1-coverable and $B - s - B(s)$ has a perfect matching;

where $B-s$ is the subgraph obtained from B by deleting the hexagon s and its incident edges, $B(s)$ is the subgraph of $B-s$ obtained by deleting the edges and vertices which do not belong to any hexagon of $B-s$.

THEOREM 3 [10]

A BS B is 3-coverable if and only if, for any side-hexagon s of B, each component of B(s) is 2-coverable and $B-s-B(s)$ has a perfect matching.

THEOREM 4 [10]

A BS B is $k(\geq 3)$-coverable if and only if B is 3-coverable. If B is a 3-coverable BS without chords, then B is a hexagon, or a T_n, or a crown (cf. fig. 7 below). If B is a 3-coverable BS with a chord e, then both $B(e)$ and $B'(e)$ are 3-coverable, where $B(e)$ and $B'(e)$ are subgraphs of B of which the union is B, and the intersection is $\{e\}$.

For a CS G, only the following result is known [9].

THEOREM 5 [9]

A CS G is 1-coverable if and only if each of its outer and inner perimeters is a conjugated circuit for some perfect matching of G.

The main purpose of this paper is to solve the problem: what is the criterion for a CS to be $k(\geq 2)$-coverable?

2. 2-coverable coronoid systems

Let G be a CS, s be a hexagon of G. The following notation is used throughout this section:

$C(G)$: the union of the outer and inner perimeters of G;

$E(G)$: the edge set of G;

$E(C)$: the set of edges on the cycle C of G;

$C(s)$: the perimeter of the hole appearing after deleting the hexahon s together with the incident edges if s is a non-side hexagon of G;

$G-s$: the subgraph of G obtained from G by deleting the hexagon s together with the incident edges.

$G(s)$: the subgraph of $G-s$ obtained by deleting the edges and vertices which do not belong to any hexagon of $G-s$.

Recall that a fixed single bond is an edge of G which does not belong to any perfect matching of G, while a fixed double bond is an edge of G which belongs to every perfect matching of G. Both fixed single bonds and fixed double bonds are called fixed bonds.

Before continuing, we cite three lemmas from ref. [9].

LEMMA 6 [9]

Let G be a BS or a CS with a fixed single bond e, M be a perfect matching of G such that the edges of M saturating the end vertices of e are not parallel. Then all the edges $e_1, \ldots, e_n$ (see fig. 2) are fixed single bonds, where e_n is on the perimeter of G.

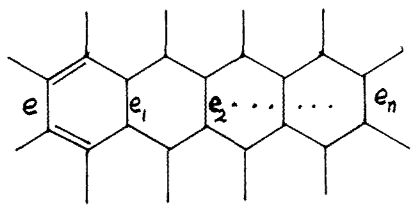


Fig. 2.

LEMMA 7 [9]

Let G be a BS or a CS with some fixed single bonds. Then at least one of them lies on the perimeter of G.

LEMMA 8 [9]

Let G be a CS without any fixed bond. Then each of the hexagons and the perimeters of G is a conjugated circuit for some perfect matching of G.

The following lemma is useful in the proof of our main theorem.

LEMMA 9

Let e be a fixed single bond of a CS G. The endpoints of e are both of degree 3. Let e_1, e_2, e_3 and e_4 be the four edges adjacent to e, as in fig. 3. If neither of e_1 and e_2 is a fixed double bond of G, then there is a perfect matching of G in which e_3 and e_4 are simultaneously double bonds.

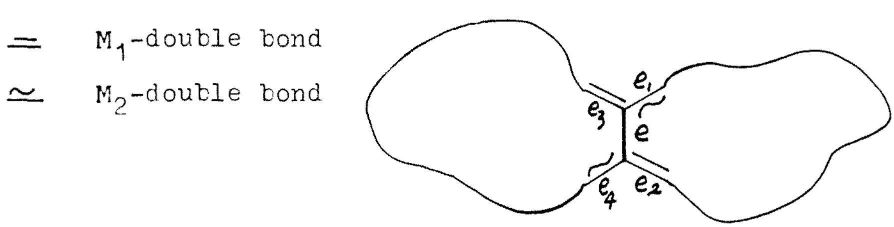


Fig. 3.

Proof

Since e is a fixed single bond and e_1 is not a fixed double bond, there is a perfect matching M_1 in which e_3 is an M_1-double bond. If e_4 is also an M_1-double bond, then M_1 is the desired perfect matching of G. Otherwise, e_2 is an M_1-double bond. Similarly, there is a perfect matching M_2 in which e_4 is an M_2-double bond, and e_1 is also an M_2-double bond if e_3 is not an M_2-double bond. The symmetric difference of M_1 and M_2, i.e. $(M_1 \cup M_2) - (M_1 \cap M_2)$, constitutes a set of pairwise disjoint $M_1(M_2)$-conjugated circuits. Let D denote the $M_1(M_2)$-conjugated circuit containing e_1 and e_3. Then D will not contain e_2 and e_4. Otherwise, D will be divided into two odd cycles containing e, contradicting that G is a bipartite graph and has no odd cycles. Now let $M = (M_2 \cup E(D)) - (M_2 \cap E(D))$. It is not difficult to see that M is a perfect matching of G in which both e_3 and e_4 are M-double bonds.

Now we are in a position to give our main theorem which provides a criterion for a CS to be 2-coverable.

THEOREM 10

A CS G is 2-coverable if and only if every pair of disjoint side hexagons of G forms a cover of G.

Proof

The necessity is evident.

We prove the sufficiency by contradiction. Assume that G satisfies the condition of the theorem and is not 2-coverable. Then there are two disjoint hexagons s' and s'' which do not form a cover of G, and at least one them, say s', is a non-side hexagon of G. In the following, we prove three conclusions which will lead to a contradiction.

CONCLUSION 1

For any side hexagon s^* of G which is disjoint with s', s^* and s' form a cover of G. In fact, we can prove a stronger one: $G(s^*)$ is 1-coverable. It is not difficult to see that each component of $G - s^* - G(s^*)$ is a path if $G - s^* - G(s^*)$ is not an empty graph. Moreover, each such path is connected to a side hexagon of G which is disjoint with s^*. Since s^* and each side hexagon which is disjoint with s^* form a cover of G, each component of $G - s^* - G(s^*)$ has a perfect matching. Therefore, $G(s^*)$ has perfect matchings. If $G(s^*)$ has no fixed bond, then each of the perimeters of $G(s^*)$ is a conjugated circuit for some perfect matching of $G(s^*)$ (lemma 8), and hence $G(s^*)$ is 1-coverable (theorem 5). Now the remaining thing to prove is that $G(s^*)$ has no fixed bond. By lemma 7, it suffices to prove that there is no fixed bond on the perimeters of $G(s^*)$. By the condition of the theorem, each of those side hexagons of $G(s^*)$ which are also side hexagons of G is a cover of $G(s^*)$ and has no fixed bond of $G(s^*)$. Thus, if $G(s^*)$ has fixed bonds on its perimeters, they are on those side hexagons of $G(s^*)$ which are not side hexagons of G. Let e be such a fixed single bond, e_1 and e_1' be the two edges which are adjacent to e and are on the perimeter of $G(s^*)$. We claim that at least one of e_1 and e_1' is a fixed double bond of $G(s^*)$. This is evident when one end vertex of e is of degree 2 in $G(s^*)$. Now suppose that both of the end vertices of e are of degree 3 in $G(s^*)$. If neither of e_1 and e_1' is a fixed double bond of $G(s^*)$, then by lemma 9 there is a perfect matching M of $G(s^*)$ such that both e^* and e^{**} are M-double bonds (see fig. 4). By

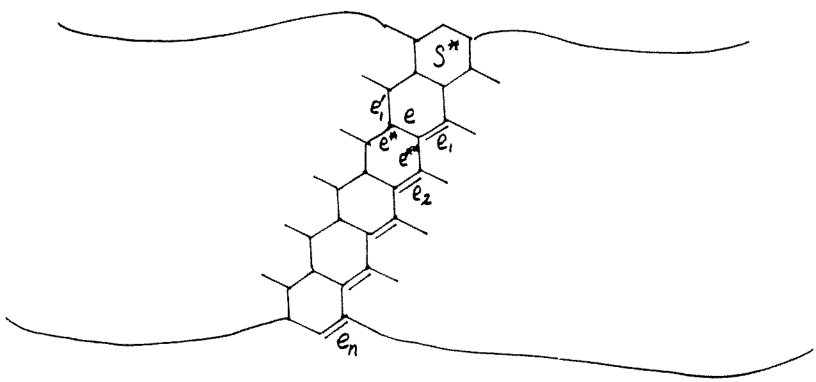


Fig. 4.

lemma 6, there will be a fixed single bond on the side hexagons of $G(s^*)$ which is also a side hexagon of G, a contradiction. Hence, at least one of e_1 and e_1', say e_1, is a fixed double bond of $G(s^*)$. By repeated use of lemma 6, we come to the conclusion that all the edges $e_2, \ldots, e_n$ (see fig. 4) are fixed double bonds of $G(s^*)$, where e_n is on the side hexagon of $G(s^*)$ which is also a side hexagon of G, again a contradiction. This implies that $G(s^*)$ has no fixed bond and is 1-coverable.

CONCLUSION 2

There is a fixed bond of $G-s'$ on $C(s')-C(G)$. By the assumption that s' and s'' do not form a cover of G, $G-s'$ is not 1-coverable. Then by theorem 5 and lemma 8, $G-s'$ has some fixed bonds. Moreover, there is at least one fixed single bond on $C(G)$ or $C(s')$ (lemma 7). By conclusion 1, any edge in $C(G)-C(s')$ is not a fixed bond since it belongs to a side hexagon of G which forms a cover of $G-s'$. Hence, the fixed bonds appear on $C(s')$. If $C(G)\cap C(s')=\emptyset$, then $C(s')=C(s')-C(G)$, and the conclusion follows. Now suppose that $C(G)\cap C(s')\neq\emptyset$. It is easy to see that if one of the edges $C(G)\cap C(s')$ is on a conjugated circuit for some perfect matching of $G-s'$, then all the edges of $C(G)\cap C(s')$ must be on the same conjugated circuit. This means that the edges of $C(G)\cap C(s')$ are simultaneously fixed bonds or not. If all the fixed bonds of $C(s')$ are on $C(G) \cap C(s')$, then all the edges of $C(G) \cap C(s')$ are fixed bonds. Furthermore, those edges of $C(G) \cap C(s')$ connected to $G(s')$ are fixed single bonds. Thus, $G - s' - G(s')$ has a unique perfect matching and $G(s')$ has perfect matchings. Since $C(G(s')) = (C(G) \cup C(s')) - (C(G) \cap C(s'))$ has no fixed bonds, $G(s')$ is 1-coverable (lemma 7, lemma 8 and theorem 5). Note that s'' is completely in $G(s')$. Thus, s' and s'' form a cover of G, contradicting our assumption. This contradiction is caused by assuming that all the fixed bonds of $C(s')$ are on $C(G) \cap C(s')$. Consequently, there is at least one fixed bond on $C(s') - C(G)$.

CONCLUSION 3

There is a fixed bond of $G - s'$ belonging to a side hexagon of G. By conclusion 2, there is a fixed bond, say e, on $C(s') - C(G)$. Without loss of generality, we may assume that e is a fixed single bond (see fig. 5). If neither e' nor e'' is a

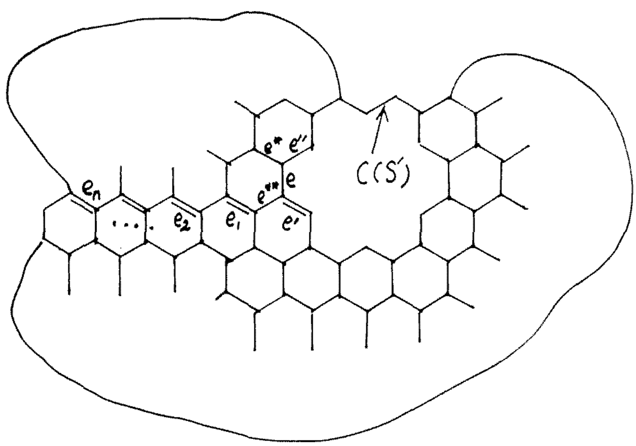


Fig. 5.

fixed double bond of $G - s'$, then by lemma 9 there is a perfect matching of $G - s'$ in which both e^* and e^{**} are double bonds. Thus, by lemma 6, a fixed single bond will be found on a side hexagon of G which is disjoint with s', a contradiction. Therefore, one of e' and e'', say e', is a fixed double bond of $G - s'$. Reasoning in a similar way as before, a series of double fixed bonds are found: $e_1, e_2, \ldots, e_n$, where e_n is on a side hexagon of G.

It is easy to see that conclusion 3 contradicts conclusion 1. This contradiction establishes the sufficiency of the theorem.

3. $k(\geq 3)$-coverable coronoid systems

In this section, we give a constructive criterion for a CS G to be $k(\geq 3)$-coverable. Let G be a CS with a chord e of type I. It is not difficult to see that G is separated by e into two parts: one is a BS, denoted by BS(e); the other is a CS, denoted by CS(e). Thus, for any chord e of type I, BS(e) and CS(e) have exactly one edge e in common (see fig. 6). A chord e of type I is said to be maximal if for any chord $e^* \neq e$ of type I, BS(e) is not a subgraph of BS(e^*). For example, the CS G shown in fig. 6 has two maximal chords of type I: e_3 and e_4.

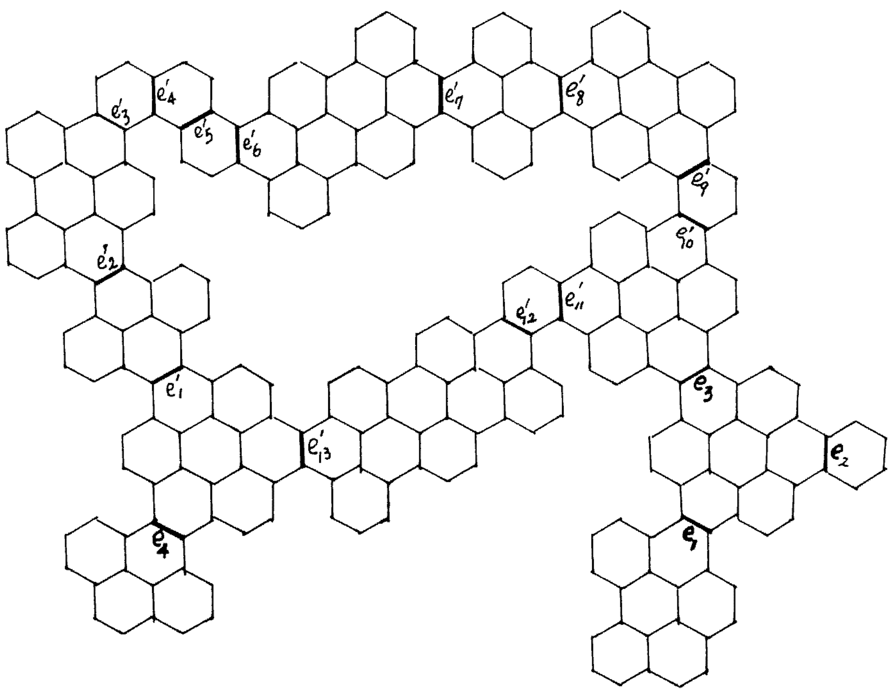
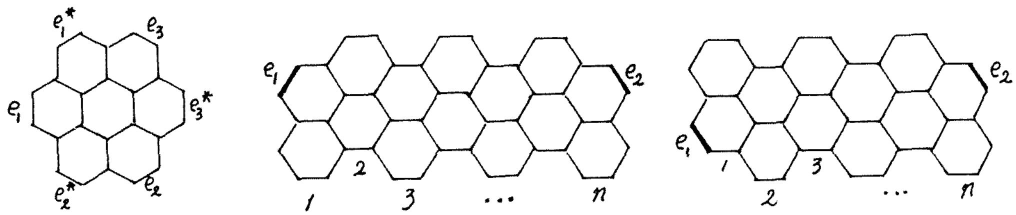


Fig. 6.

A CS G without a chord of type I is said to be a normal CS. Let G be a CS with maximal chords of type I: $e_1^*, \ldots, e_n^*$. It is clear that $G' = \mathrm{CS}(e_1^*) \cap \mathrm{CS}(e_2^*) \cap \ldots \cap \mathrm{CS}(e_n^*)$ is a normal CS. Let G be a normal CS with chords of type II arranged clockwise as follows: $e_1', e_2', \ldots, e_t'$. Denote the section of G between chords e_i' and e_{i+1}' (inclusive of e_i' and e_{i+1}') by $G(e_i', e_{i+1}')$, where $i+1$ is taken modulo t, $i = 1, 2, \ldots, t$. Then $G(e_i', e_{i+1}')$ is a BS.

The BSs depicted in fig. 7 are called a crown and a T_n ($n \geq 2$), respectively. For each T_n, we specify two edges on the perimeter as attachable edges (see fig. 7). For a crown, the six edges on the perimeter with two end vertices of degree 2 are divided into two sets $\{e_1, e_2, e_3\}$ and $\{e_1^*, e_2^*, e_3^*\}$ (see fig. 7). Two or three edges



a crown

a T_n (n is odd)

a T_n (n is even)

e_1 and e_2 are attachable edges of T_n

Fig. 7.

of them constitute an attachable combination if they belong to the same set. For example, e_1 and e_2 form an attachable combination, while e_1 and e_1^* do not. For a single hexagon, two or three mutually non-parallel and non-adjacent edges constitute an attachable combination.

LEMMA 11

Let G be a CS. If there are three side hexagons of G, s_1, s_2 and s_3 as shown in fig. 8, and vertex v is of degree 2, then G is not 2-coverable.

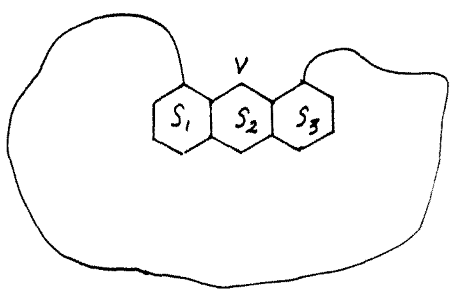


Fig. 8.

Proof

Since s_1 and s_3 do not form a cover of G, G is not 2-coverable.

LEMMA 12

Let G be a 3-coverable CS. Then any two non-side hexagons of G are disjoint.

Proof

By contradiction. If G has two non-side hexagons s' and s'' with an edge in common, then G has a subgraph as shown in fig. 9. It is easy to check that s_1, s_2 and s_3 do not form a cover of G. The lemma follows.

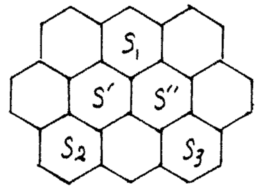


Fig. 9.

LEMMA 13

Let G be a 3-coverable CS. Then G has no such subgraph, as shown in fig. 10.

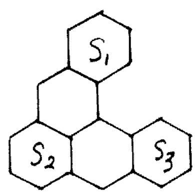


Fig. 10.

Proof

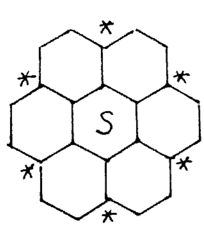
Since s_1, s_2 and s_3 do not form a cover, the graph shown in fig. 10 cannot be a subgraph of any 3-coverable CS.

LEMMA 14

Let G be a 3-coverable CS, s be a non-side hexagon of G. Then the vertices on the perimeter of the crown containing s as its centre are all on the perimeter of G.

Proof

The lemma follows from the fact that there is no hexagon on the positions, each of which has a star (see fig. 11) (lemma 13).



(Fig. 11).

LEMMA 15

Let G be a 3-coverable CS. Then G contains no such side hexagon that has exactly one pair of parallel edges on the perimeter of G (see fig. 12).

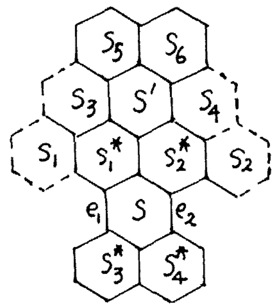


Fig. 12.

Proof

If the lemma is false, we can find a side hexagon s of G with exactly two parallel edges e_1 and e_2 on the perimeter of G (see fig. 12). Then hexagons s_1^*, s_2^*, s_3^* and s_4^* belong to G. Without loss of generality, we may assume that s is uppermost in the sense that s' is not a hexagon having the same property as s, or s' does not belong to G. By lemma 13, neither s_1 nor s_2 belongs to G. By lemma 11, none of s_3 and s_4 belongs to G. Hence, s' must belong to G (otherwise e_1 and e_2 are fixed single bonds of G, a contradiction). Since s_1^* and s_4^* form a cover of G, at least one of s_5 and s_6 belongs to G. Again by lemma 11, if one of s_5 and s_6 belongs to G, the other must belong to G too. This means that s' is a side hexagon with exactly two parallel edges on the perimeter of G, which is contrary to the selection of s. The proof is thus completed.

THEOREM 16

Let G be a normal $k(\geq 3)$-coverable CS. Then G has chords of type II: $e_1, \ldots, e_m$. Each section $G(e_i, e_{i+1})$ is either a T_n with attachable edges e_i and e_{i+1}, or a crown, or a hexagon, where e_i and e_{i+1} constitute an attachable combination.

Proof

Let G be a $k(\geq 3)$-coverable CS, s be any hexagon of G. We want to prove that s is contained in a section of G which is a T_n, or a crown, or a hexagon.

Case 1. None of the vertices of s lies on the perimeter of G, i.e. s is a non-side hexagon of G. By lemma 14, all the vertices of the crown containing s as its centre hexagon are on the perimeter of G. This implies that there are two chords of type II, say e_i and e_{i+1}, on the perimeter of the crown, and $G(e_i, e_{i+1})$ is a crown.

We claim e_i and e_{i+1} constitute an attachable combination. Let $e_i = e_1$ (cf. fig. 7). Then e_{i+1} cannot be e_j^*, $j = 1, 2, 3$. Otherwise, we can find three hexagons of G: the centre hexagon of the crown, the two hexagons of G containing the edges e_i and e_{i+1}, respectively, which do not belong to the crown. It is not difficult to check that these three hexagons do not form a cover of G, contradicting that G is 3-coverable.

Case 2. Hexagon s has exactly two vertices on the perimeter of G. Then G has a subgraph which is a T_3 (see fig. 13). Let T_n be the maximal subgraph of G containing s in the sense that there is no T_{n+1} which is a subgraph of G and contains s. By lemma 13, it is clear that there is no hexagon of G on the positions,

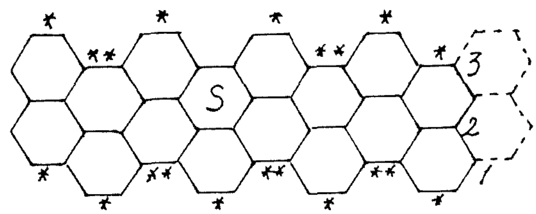


Fig. 13.

each of which has a star. By lemma 14, there is no hexagon on the positions, each of which has a double-star. There is no hexagon on position 1 (lemma 11). Again by lemma 11, if there is a hexagon on position 2, there must be a hexagon on position 3. Then we find a T_{n+1} containing s, contradicting the maximality of T_n. Therefore, there is no hexagon of G on position 2. This implies that e_1 is either a chord of G or an edge on the perimeter of G. Analogously, edge e_2 is either a chord of G or an edge on the perimeter of G. Since G is a normal CS, both e_1 and e_2 are chords of type II. Clearly, the section $G(e_1, e_2)$ is a T_n and e_1 and e_2 are attachable edges of T_n.

Case 3. Hexagon s has exactly three vertices on the perimeter of G. By lemma 11, this is impossible.

Case 4. Hexagon s has exactly four vertices on the perimeter of G. By lemma 15, these four vertices cannot be contained in two parallel edges of s. Hence, s has three consecutive edges or two non-parallel, non-incident edges on the perimeter of G.

Subcase 4.1. Hexagon s has three consecutive edges on the perimeter of G (see fig. 14). It is clear that in the case when s_2 does not belong to G, neither s_4 nor s_5 belongs to G (lemmas 11 and 15). Similarly, if s_1 does not belong to G, neither of s_6 and s_7 belongs to G. Hence, if neither of s_1 and s_2 belongs to G, e is a chord of type I, which is contrary to the fact that G is normal. Therefore, at least one of s_1 and s_2 must belong to G. Suppose that s_1 belongs to G. Then by lemma 11, one or both of s_2 and s_3 must belong to G. Thus, the hexagon s^* is one with

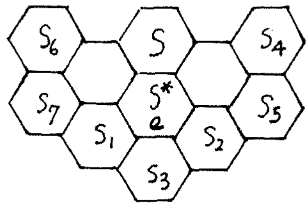


Fig. 14.

exactly two vertices on the perimeter of G, or is a non-side hexagon of G. It will be reduced to case 1 or case 2. Therefore, s^* is contained in a section of G which is a crown or a T_n. Consequently, s is contained in a crown or a T_n which is a section of G.

Subcase 4.2. Hexagon s has two non-parallel and non-incident edges on the perimeter of G (see fig. 15). By lemma 13, there is no hexagon of G on the positions, each of which has a star. By lemma 11, no hexagon of G appears on the position, each of which has a double star. If on one of the positions 1 and 2 there

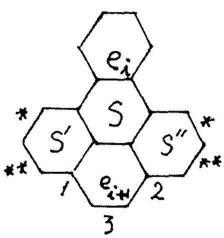


Fig. 15.

is a hexagon of G, s' or s'' will be a hexagon with three consecutive edges on the perimeter of G, and it can be reduced to subcase 4.1. Otherwise, there is a hexagon on position 3, and e_i and e_{i+1} are chords of type II, and the section $G(e_i, e_{i+1})$ is a T_2.

Case 5. Hexagon s has five vertices on the perimeter of G. If on the position with a star (see fig. 16) there is no hexagon of G, then G has no hexagon on each of the positions labelled by 1, 2, 3 and 4 (lemmas 11 and 15). Thus, G is a BS with

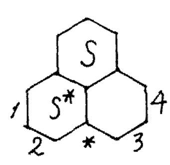


Fig. 16.

three hexagons, a contradiction. Therefore, there must be a hexagon on the position with a star, and s^* is a hexagon of G with at most four vertices on the perimeter of G. Consequently, it can be reduced to one of the above cases.

Case 6. Hexagon s has six vertices on the perimeter of G. Since G is a normal CS, s has exactly chords of type II. It is not difficult to verify that these two chords constitute an attachable combination of s.

Let T_n^- and T_n^{--} denote the subgraph of T_n obtained from T_n by deleting one and two attachable edges of T_n, respectively (see fig. 17).

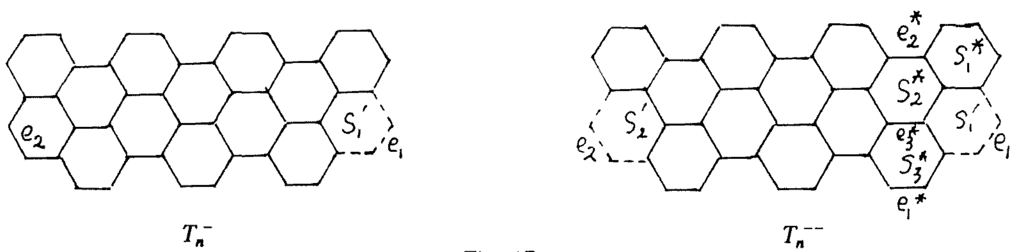


Fig. 17.

We have the following:

LEMMA 17

T_n^- and T_n^{--} are $k(\geq 3)$-coverable.

Proof

Let $K = \{s_1, \ldots, s_k\}$ be a set of $k(\geq 3)$ pairwise disjoint hexagons of T_n, where $s_i \neq s_1'$, $s_i \neq s_2'$ for $i = 1, \ldots, k$ (see fig. 17). Let M be a perfect matching of $T_n - K$. To prove that K is a cover of T_n^{--}, it suffices to prove that both e_1 and e_2 are M-double bonds. If one of the hexagons s_1^*, s_2^* and s_3^* belongs to K, then e_1 is an M-double bond. If none of them belong to K, then it is not difficult to see that edge e_1^* is an M-double bond, while edges e_2^* and e_3^* are M-single bonds. Without loss of generality, we may assume that M is a perfect matching of $T_n - K$ in which e_1 is an M-double bond. By an analogous reasoning, e_2 is an M-double bond. Hence, K is also a cover of T_n^{--}. By the arbitrariness of K, T_n^{--} is $k(\geq)$-coverable.

We can prove that T_n^- is $k(\geq 3)$-coverable in a similar way.

THEOREM 18

Let G be a normal CS with chords of type II: $e_1, \ldots, e_t$ such that each section $G(e_i, e_{i+1})$ is a T_n with attachable edges e_i and e_{i+1}, or a crown, or a hexagon, where e_i and e_{i+1} constitute an attachable combination. Then G is $k(\geq 3)$-coverable.

Proof

Let $K = \{s_1, \ldots, s_k\}$ be a set of $k(\geq 3)$ pairwise disjoint hexagons of G, $K_i = K \cap G(e_i, e_{i+1})$, $i = 1, \ldots, t$. We divide G into t separate parts according to the following regulations: (1) Each chord belongs to exactly one part. (2) If the hexagon of $G(e_i, e_{i+1})$ containing chord e_i (or e_{i+1}) belongs to K_i, then e_i (or e_{i+1}) must belong to the ith part. (3) If chord e_i does not belong to any hexagon of K, then e_i belongs to the ith part. It is clear that each part is a T_n, or a T_n^-, or a T_n^{--}, or one of the graphs depicted in fig. 18. All these are $k(\geq 3)$-coverable (theorem 4 and lemma 17). Hence, K_i is a cover of the ith part. Consequently, K is a cover of G, and G is thus $k(\geq 3)$-coverable.

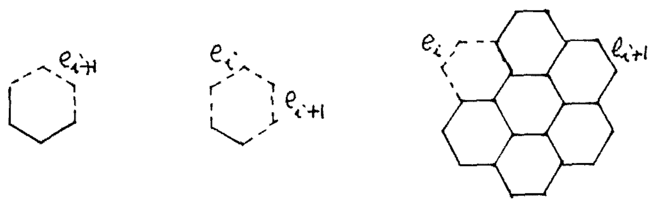


Fig. 18.

THEOREM 19

A normal CS G is $k(\geq 3)$-coverable if and only if G has chords of type II: $e_1, \ldots, e_t$ and each section $G(e_i, e_{i+1})$ is a T_n with attachable edges e_i and e_{i+1}, or a crown, or a hexagon where e_i and e_{i+1} constitute an attachable combination.

Proof

Immediate from theorems 16 and 18.

If G is not a normal CS, then G has some chords of type I. Let $e'_1, \ldots, e'_m$ be the maximal chords of type I. Then $G' = \mathrm{BS}(e'_1) \cap \mathrm{BS}(e'_2) \cap \ldots \cap \mathrm{BS}(e'_m)$ is a normal CS, as we mentioned before.

THEOREM 20

Let G be a CS with chords of type I, $e'_1, \ldots, e'_m$ be the maximal chords of type I. Then G is $k(\geq 3)$-coverable if and only if $\mathrm{BS}(e'_i)$ $(i = 1, \ldots, m)$ is a $k(\geq 3)$-coverable BS and G' is a normal $k(\geq 3)$-coverable CS.

Proof

Suppose that G is $k(\geq 3)$-coverable. Let $K = \{s_1, \ldots, s_k\}$ be a set of k pairwise disjoint hexagons of $\mathrm{BS}(e'_i)$, where e'_i is a maximal chord of type I, $i = 1, \ldots, m$. Since G is $k(\geq 3)$-coverable, $G - K$ has a perfect matching, say M. Denote the hexagon of $\mathrm{CS}(e'_i)$ containing the chord e'_i by s^*. Since s^* itself is a cover of G, BS(e_i') has perfect matchings. Hence, BS(e_i') has an even number of vertices. This implies that if e_i' is not an M-double bond, then the two end vertices of e_i' are saturated by M-double bonds which are simultaneously in CS(e_i') or BS(e_i'). Therefore, BS(e_i') $- K$ has a perfect matching: BS(e_i') $\cap M$ if e_i' is in M or the two M-double bonds saturating the end vertices of e_i' are in BS(e_i'); or BS(e_i') $\cap M \cup \{e_i'\}$ if the two M-double bonds saturating the end vertices of e_i' are in CS(e_i'). Consequently, K is a cover of BS(e_i') and thus BS(e_i') is $k(\geq 3)$-coverable. Similarly, we can prove that G' is $k(\geq 3)$-coverable.

Conversely, suppose that G' and BS(e_i') ($i = 1, \ldots, m$) are $k(\geq 3)$-coverable. By theorem 16, it is not difficult to see that e_i' must be a member of an attachable combination of a crown or a hexagon (cf. fig. 6). Now we can prove that G is $k(\geq 3)$-coverable in a similar way as in the proof of theorem 18. We omit the details.

4. General remark

A multi-CS is a CS with more than one hole. By the above results, the constructive feature of $k(\geq 3)$-coverable multi-CSs is already clear. We do not discuss the details here.

Acknowledgement

The authors would like to thank Dr. I. Gutman for his valuable comments.

References

[1] F. Harary, *Beitrage zur Graphentheorie*, ed. H. Sachs, H.-J. Voss and H. Walther, B.G. (1968).
[2] I. Gutman, Bull. Soc. Chim. Beograd 47(1982)453.
[3] J. Brunvoll, B.N. Cyvin and S.J. Cyvin, J. Chem. Inf. Comput. Sci. 27(1987)14.
[4] S.J. Cyvin and I. Gutman, *Kekulé Structures in Benzenoid Hydrocarbons* (Springer, Berlin, 1988).
[5] N. Trinajstić, *Chemical Graph Theory* (CRC Press, Boca Raton, 1983).
[6] I. Gutman, in: *Proc. 4th Yugoslav Seminar in Graph Theory*, Novi Sad (1983).
[7] N. Ohkami, A. Motoyama, T. Yamaguchi, H. Hosoya and I. Gutman, Tetrahedron 37(1980)1113.
[8] F.U. Zhang and R.S. Chen, Discr. Appl. Math. 30(1991).
[9] F.J. Zhang and M.I. Zheng, to be published.
[10] M.L. Zheng, to be published.