Journal of Mathematical Chemistry 17 (1995) 15–33

Hamiltonian circuits, Hamiltonian paths and branching graphs of benzenoid systems

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Received 21 January 1993; revised 15 July 1994

A benzenoid system H is a finite connected subgraph of the infinite hexagonal lattice without cut bonds and non-hexagonal interior faces. The branching graph G of H consists of all vertices of H of degree 3 and bonds among them. In this paper, the following results are obtained:

(1) A necessary condition for a benzenoid system to have a Hamiltonian circuit.
(2) A necessary and sufficient condition for a benzenoid system to have a Hamiltonian path.
(3) A characterization of connected subgraphs of the infinite hexagonal lattice which are branching graphs of benzenoid systems.
(4) A proof that if a disconnected subgraph G of the infinite hexagonal lattice given along with the positions of its vertices is the branching graph of a benzenoid system H, then H is unique.

1. Introduction

A *Hamiltonian circuit (path)* of a graph G is a circuit (path) containing all vertices of G. The problems of deciding if a graph has a Hamiltonian circuit or a Hamiltonian path are NP-complete [1] even for planar graphs with all vertex degrees equal to 3 [2]. Hamiltonian circuits have attracted mathematicians for well over a hundred years [3–8].

In the fast few years, the problems of finding a Hamiltonian circuit or a Hamiltonian path in chemical graphs, and particularly in benzenoid systems, have been discussed in several papers [9–15]. The complexity of both problems for benzenoid systems is still unknown. The first problem is also related to the study of topological structures of benzenoid hydrocarbons [17] and the conjugated-circuit model [18], for the Hamiltonian circuits represent the largest possible conjugated circuits. In [10], it is claimed that traceability (a graph is called traceable if it has a Hamiltonian path) must be among the factors that determine what kinds of structure it is possible or impossible to form by intra-molecular crosslinking of a linear polymer.

A benzenoid system is defined to be a connected finite subgraph of the infinite hexagonal lattice which has no cut vertices or non-hexagonal interior faces (see fig. 1). A *perfect matching or 1-factor* (Kekulé structure in chemical language) of a graph is a set of disjoint edges covering all vertices. In order to facilitate the search

Fig. 1. Benzenoid systems.

for a Hamiltonian circuit (or a Hamiltonian path), Kirby [10] introduced the *branching graph* of a benzenoid system. It is defined as the subgraph consisting of all vertices of degree 3 and bonds among them (see fig. 2). The branching graph is closely related to 2-factors of a benzenoid system of H and 1-factors of the branching graph of H [15] (a 2-factor of a graph is a set of disjoint circuits covering all vertices). The branching graph is also related to the Hamiltonian circuit (path) problem for benzenoid systems. This is based on the following observation: a benzenoid system H has a Hamiltonian circuit if and only if there is a perfect matching in its branching graph such that the delection from H of the edges in this perfect matching but not of their end vertices results in a connected graph (actually it is a circuit). For further information, see the recent survey (with new results) [16].

In this paper, we first present a necessary condition for a benzenoid system to have a Hamiltonian circuit. Next we give a necessary and sufficient condition for a benzenoid system to have a Hamiltonian path, based on the branching graph and similar to the existence condition for Hamiltonian circuits cited above. Then we answer the following question: which connected subgraphs of the infinite hexagonal lattice are branching graphs of benzenoid systems. We also prove that if a disconnected subgraph G of the infinite hexagonal lattice given with the positions of its vertices is the branching graph of a benzenoid system H then H is unique. To completely characterize which graphs are branching graphs of benzenoid systems seems to be hard, for at least we need to know which graphs can be embedded in the infinite hexagonal lattice.

2. Hamiltonian circuits and Hamiltonian paths

Several necessary conditions are known for a benzenoid system H to have a Hamiltonian circuit. For example, if H has Hamiltonian circuit then the number of its internal vertices is divisible by 4 [19, p. 235]. Another necessary condition for H to have a Hamiltonian circuit is that H has no fixed bonds, i.e., each of its bonds

H G

Fig. 2. The branching graph G of a benzenoid system H.

belongs to some perfect matching of H. In [20], a linear algorithm to determine all fixed bonds of a benzenoid system is proposed. Another fast algorithm for finding fixed bonds of benzenoid systems is given in [21].

In this section, we first state a necessary condition for a benzenoid system to have a Hamiltonian circuit. Before stating this condition, we recall the following definition [18]. A *conjugated circuit* of a benzenoid system H is a circuit C such that the bonds of C are alternatively in and out of a perfect matching of H. By this definition, each circuit in a 2-factor of H is a conjugated circuit.

In [22], it was shown that a conjugated circuit in benzenoid hydrocarbons has length $4k + 2$ where k is a positive integer.

THEOREM 1

Let H be a benzenoid system. If H has a Hamiltonian circuit then the number of circuits in any 2-factor of H is odd.

Proof

Let $F = \{C_1, C_2, \ldots, C_r\}$ be a 2-factor of H with circuits $C_1, C_2, \ldots, C_r$ and let C_0 be a Hamiltonian circuit of H. Then for $i = 1, 2, \ldots, r$, the length $|C_i|$ of C_i is of the form $4k_i + 2$ where k_i is a positive integer. Thus $\sum_{i=1}^{r} 4k_i + 2r = 4k_0 + 2$. Therefore $2(r-1)$ is divisible by 4, i.e., r is odd. □

Figure 3 shows two benzenoid systems with their 2-factors. By theorem 1, they have no Hamiltonian circuits. All three necessary conditions mentioned above together are not sufficient for a benzenoid system to have a Hamiltonian circuit, as illustrated by fig. 4.

In [23], a necessary and sufficient condition for a benzenoid system H to have a Hamiltonian circuit is given: H has a Hamiltonian circuit if and only if there is a subset E' of the edge set E of H whose deletion one by one from the border of H (or of the resulting subgraph) gives a catacondensed benzenoid. Unfortunately it does not seem easy to derive from this condition an algorithm to find such a circuit. The following is another necessary and sufficient condition for a benzenoid system to have a Hamiltonian circuit (due to Kirby [10] and already mentioned before).

THEOREM 2 (KIRBY)

Let H be a benzenoid system and G its branching graph. Then H has a Hamiltonian circuit if and only if G has a perfect matching M such that the removal from H of the bonds of M but not of their end vertices results in a connected graph.

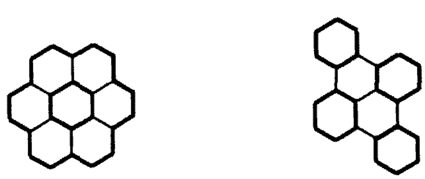


Fig. 3. The number of circuits in a 2-factor is even; the benzenoid systems have no Hamiltonian circuits.

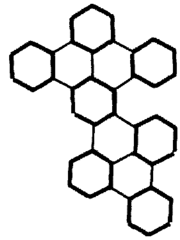


Fig. 4. H has no fixed bonds; the number of circuits in a 2-factor is odd and the number of internal vertices of H is divisible by 4; but H has no Hamiltonian circuit.

By the above theorem, an exact algorithm to find a Hamiltonian circuit in a benzenoid system H if there is one works as follows: generate sequentially all perfect matchings of the branching graph of H and check each time if the removal of the bonds in the current perfect matching from H results in a connected graph. If it is the case, then this graph is a Hamiltonian circuit of H.

This algorithm does not have a polynomial time complexity, but it at least provides a systematic way to generate a Hamiltonian circuit of a benzenoid system if there is one. Ways to generate all perfect matchings of a benzenoid system are given in [24–26]; they are easily extended to the generation of all perfect matchings of a branching graph.

We next state a necessary and sufficient condition for a benzenoid system to have a Hamiltonian path. This result has been conjectured by Kirby [10].

An *almost-perfect matching* M' of a graph is a set of disjoint edges covering all its vertices but two.

THEOREM 3

Let H be a benzenoid system and G its branching graph. Then H has a Hamiltonian path if and only if G has an almost-perfect matching M' such that the deletion from H of the bonds of M' but not of their end vertices results in a connected graph.

Proof

If H has a Hamiltonian path P, let H' be the graph obtained by deleting from H the bonds of P but not their end vertices. Then each vertex of H of degree 2 is of degree 0 in H' if it is not an end vertex of P, and each vertex of H of degree 3 is of degree 1 in H' if it is not an end vertex of P. An end vertex of P is of degree 2 or 1 in H' if it is of degree 3 or 2 respectively in H. Let G' be the graph obtained by deleting all vertices of degree 0 from H'. Then all vertices of G belong to G'. Furthermore, there are at most two vertices of G' (possibly the end vertices of P) which do not belong to G. There are three cases.

(a) The end vertices v and v' of P are of degree 2 in H. Then v and v' are of degree 1 in G', and all other vertices of G' are also of degree 1 (because they are of degree

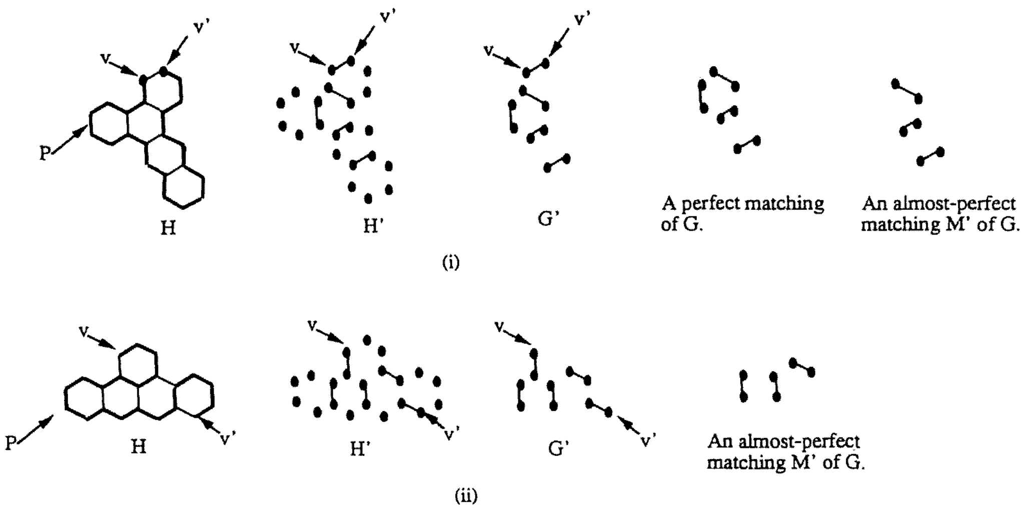


Fig. 5. The end vertices v and v' of P are of degree 2. In (i), v and v' are adjacent in M; in (ii), v and v' are not adjacent in M.

3 in H and internal vertices of P). Thus all bonds of G' are disjoint and form a perfect matching M of G'. If v is adjacent to v' in M, then deleting the bond between v and v' from M we obtain a perfect matching of G. Thus G has an almost-perfect matching M' contained in M. If it is not the case, deleting the two bonds of M which are incident with v and v' gives an almost-perfect matching M' of G. These cases are illustrated in fig. 5.

(b) Both v and v' are of degree 3 in H. Then G' and G have the same vertex set. v and v' are of degree 2 in G'. All other vertices of G' are of degree 1. So there is a vertex u (u') of degree 1 which is adjacent to v (v') in G'. Let e (e') be the bond between v and u (v' and u'). Then all the bonds of G' but e and e' form an almost-perfect matching M' of G. This case is illustrated in fig. 6.

(c) One of v and v' is of degree 2 and the other is of degree 3 in H. Without loss of generality, let v be of degree 2. Then v is of degree 1 and v' is of degree 2 in G' and all other vertices of G' are of degree 1. If v is adjacent to v', then all bonds of G' but the bond between v and v' form a perfect matching of G. Thus G has an almost-perfect matching M' contained in G'. If it is not this case, let e and e' be two bonds

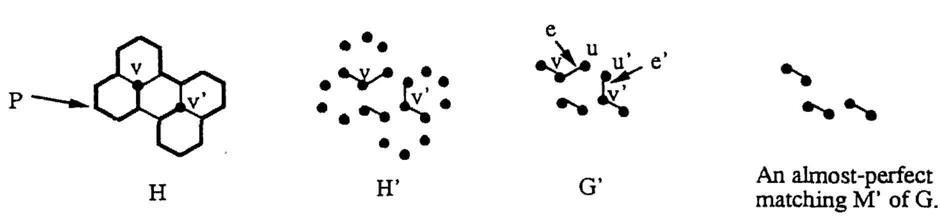


Fig. 6. The end vertices v and v' of P are of degree 3.

of G' which are incident with v and v' respectively. Then all bonds of G' but e and e' form an almost-perfect matching M' of G. Figure 7 illustrates the above cases.

In the cases (a), (b) and (c), the deletion from H of the bonds of M' but not their end vertices results in a graph which contains P. Thus this graph is connected.

Conversely if G has an almost-perfect matching M' such that the removal of the bonds of M' from H (but not of their end vertices) results in a connected graph H', then H' has all vertices of degree 2 except two of degree 3. Let P be a path of H' connecting the two vertices x and y of degree 3. After removal of all bonds of P together with their end vertices except x and y, a graph H'' is obtained. All the vertices of H'' are of degree 2. Thus H'' is the union of disjoint circuits. Since H' is connected and all the deleted vertices are of degree 2 in H', H'' contains at most two circuits. If H'' contains two circuits, then P connects the two circuits of H''. One can check that H' has a Hamiltonian path (see fig. 8(a)). Suppose H'' contains only one circuit. If P is a bond, then H'' is a Hamiltonian circuit of H. If P contains more than one bond, then delete from H' the bond which is incident with x and in P and the bond which is incident with y and but not in P. A Hamiltonian path of H is obtained (see fig. 8(b)). □

As above for theorem 2 and Hamiltonian circuits, an algorithm based on theorem 3 can be devised to find a Hamiltonian path in a benzenoid system H if there is one: generate sequentially all almost-perfect matchings in the branching graph of H and check each time if the deletion from H of the bonds in the current almost-perfect matching results in a connected graph. If this is the case, as in the proof of theorem 3, a Hamiltonian path can be determined. This algorithm also does not have a polynomial complexity. Algorithm to generate all perfect matchings can be

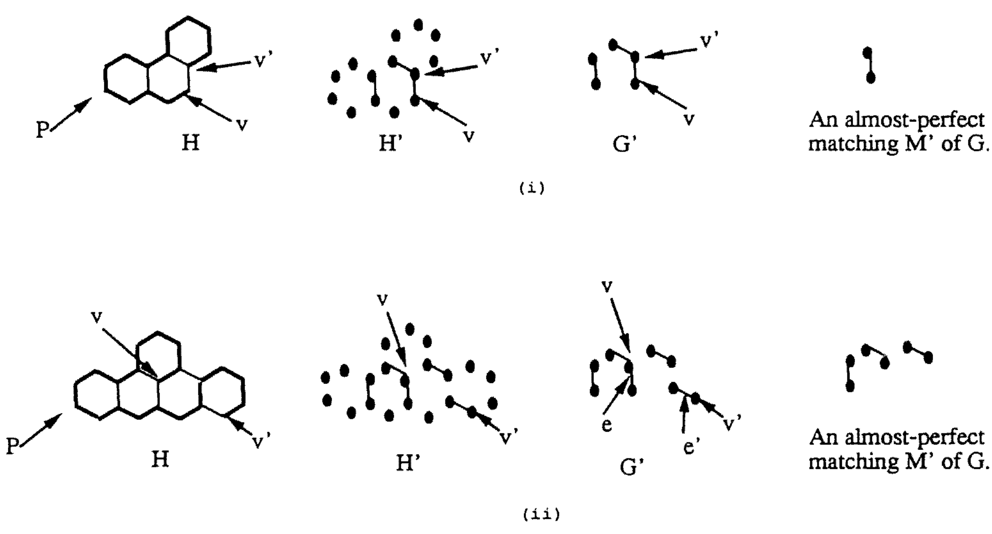


Fig. 7. One of the end vertices v and v' of P is of degree 2, the other of degree 3. In (i), v and v' are adjacent; in (ii), v and v' are not adjacent.

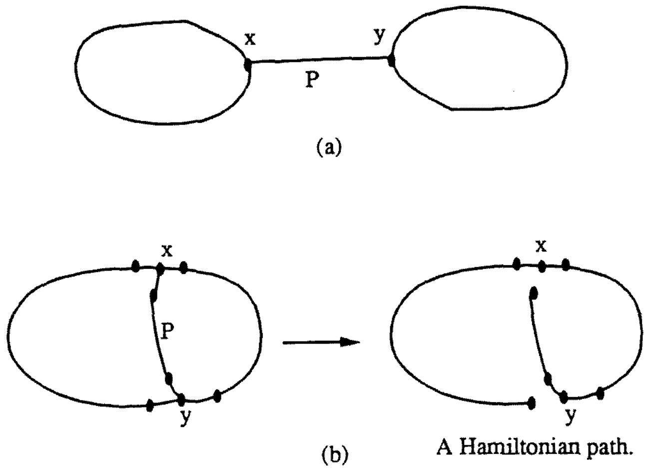


Fig. 8. Illustration of the proof of the second part of theorem 3.

used to find all almost-perfect matchings by excluding all possible pairs of vertices in sequence and then applying them.

3. Connected branching graphs

All branching graphs mentioned in this section are connected. Clearly, a branching graph of a benzenoid system has no interior faces larger than a hexagon. So we introduce the following definition: a *generalized-benzenoid system* is a connected finite subgraph of the infinite hexagonal lattice without interior non-hexagonal faces.

In this section, we present a necessary and sufficient condition for a generalized-benzenoid system to be the branching graph of a benzenoid system. As a consequence, we show that for any generalized-benzenoid system G there are at most two benzenoid systems whose branching graphs are G. We also give a necessary and sufficient condition for a generalized-benzenoid system to be the branching graph of a unique benzenoid system.

Let G be a generalized-benzenoid system. A *cut bond* of G is a bond such that the removal from G of this bond but not of its end vertices disconnects G. The *boundary* of G is defined to be the subgraph consisting of all bonds of G which belong to at most one hexagon of G. Traveling the boundary of G once, we obtain a walk $b(G)$ in which each cut bond of G is traversed twice (a *walk* is a sequence whose terms are bonds such that two consecutive bonds are adjacent). From now on we regard $b(G)$ as G's boundary and the two appearances of a cut bond as different bonds in $b(G)$. This convention plays an important role when we introduce some further definitions. Each bond e of $b(G)$ is contained in a unique hexagon $e(h)$ which is on the left hand side when one travels clockwise along the boundary $b(G)$

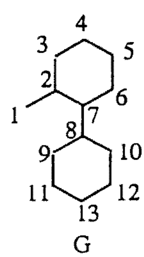
of G. Moreover $e(h)$ does not belong to G. Figure 9 shows a generalized-benzenoid system G and its boundary $b(G)$.

A *vertex-fjord* of G is a pair of vertices, $\{v, v'\}$, of G such that v and v' are adjacent in the infinite hexagonal lattice but not in G (this definition is based on a generalization of the concept of "fjord" [22]). See fig. 10(a) for an illustration. A *cove* is a path in $b(G)$ of length 4 (i.e., containing 4 bonds) which belongs to a hexagon of the infinite hexagonal lattice but not to a hexagon of G (see also fig. 10(a)).

A *leaf* of $b(G)$ is a bond which is an appearance in $b(G)$ of a pendant bond of G. Note that a pendant bond of G corresponds to two leaves of $b(G)$.

Let $LC(G)$ be the set of leaves and coves of $b(G)$ (see figure 10(b)). Let x and y be two elements of $LC(G)$. Then x and y are *clockwise-consecutive* if one can travel $b(G)$ clockwise from x to y without going through any other element of $LC(G)$. Let $P(x, y)$ be the subsequence of $b(G)$ in clockwise order around the boundary of G with x as its beginning and y as its end. The *hexagon-separation* $s(x, y)$ of two elements x and y of $LC(G)$ which do not correspond to the same pendant bond of G is the number of hexagons in the set $\{e(h) : e \in P(x, y)\}$. See fig. 10(b) for an illustration. By this definition, usually $s(x, y) \neq s(y, x)$. The hexagon-separation between two bonds of $b(G)$ which do not correspond to the same pendant bond of G is defined similarly. If x and y are different in $b(G)$ but correspond to the same pendant bond of G, then define $s(x, y) = s(y, x) = 0$. If $LC(G)$ is empty, then define $s(G)$ to be the number of hexagons in the set $\{e(h) : e \in b(G)\}$. The *hexagon-separation* $s(e)$ between a bond e of $b(G)$ and $LC(G)$ is defined as the number of hexagons which are on one's left hand side and are necessarily passed if one travels $b(G)$ clockwise from e to the first element of $LC(G)$ to be reached (the hexagon containing this element is also included). See fig. 10(c) for illustration. By convention, if e is contained in an element of $LC(G)$, then $s(e)$ is defined as 1. An *odd-bond* is a bond of $b(G)$ whose hexagon-separation $s(e)$ to $LC(G)$ is odd. An *edge-fjord* is a pair (e, e') of two odd-bonds e and e' of $b(G)$ such that the graph $G \cup e(h) \cup e'(h)$ has an interior face which does not belong to G and is not $e(h)$ or $e'(h)$ (see fig. 10(c)). An *even-cut-bond* is a cut bond e of G such that $s(e_1)$ and $s(e_2)$ are even for the two appearances e_1 and e_2 of e in $b(G)$ (see fig. 10(d)).

If $LC(G)$ is empty and $s(G)$ is even, then a cut bond e of G is *singular* if the hexagon-separations between its two appearances in $b(G)$ are odd. Two singular bonds



b(G)=(1,2)(2,3)(3,4)(4,5)(5,6)(6,7)(7,8)(8,10)
(10,12)(12,13)(13,11)(11,9)(9,8)(8,7)(7,2)
(2,1).

Fig. 9. Illustration of a generalized-benzenoid system G and its boundary walk $b(G)$.

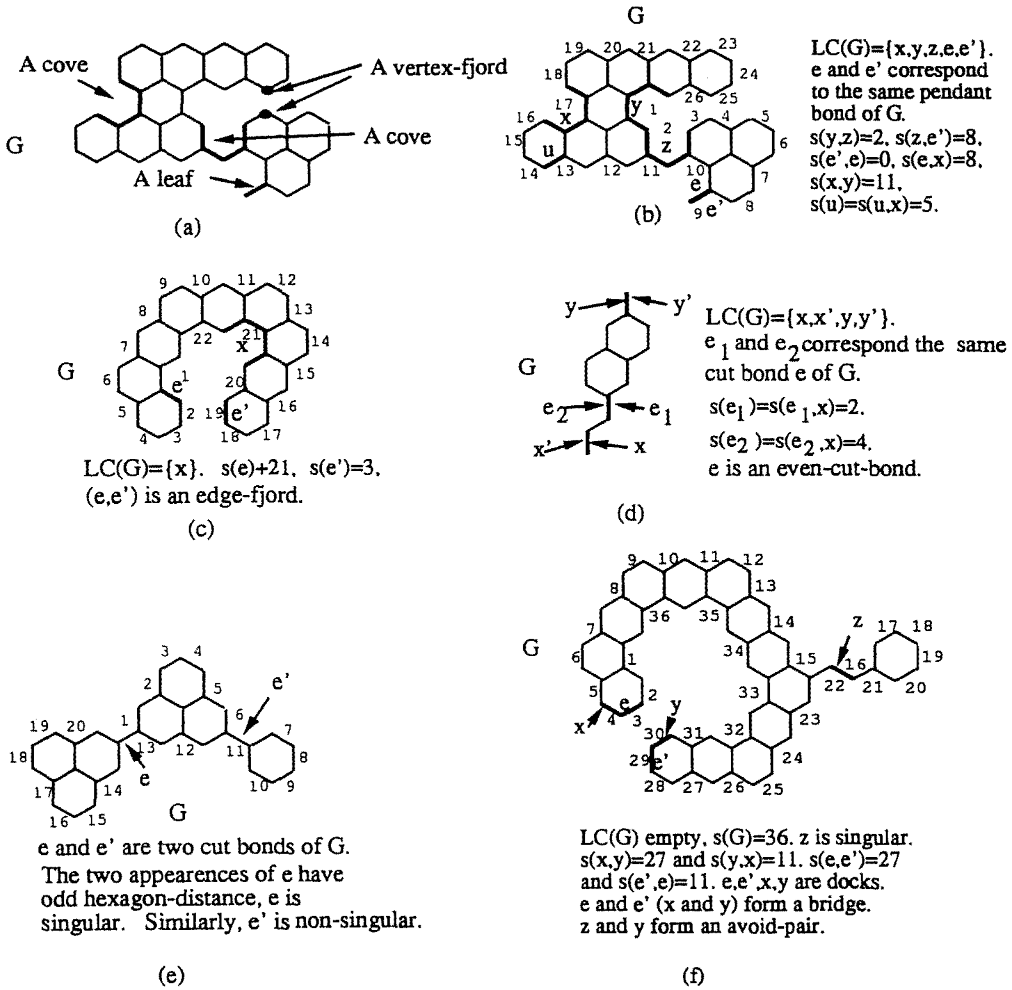


Fig. 10. Illustration of various definitions.

e and e' form a *singular pair* if one of the hexagon-separations between one of the appearances of e and one of the appearances of e' in $b(G)$ is even. A bond e of $b(G)$ is a *dock* if there is a bond e' of $b(G)$ such that $s(e, e')$ is odd and $e(h) \cup e'(h) \cup G$ contains an interior face which is not contained in G and is different from $e(h)$ and $e'(h)$. Two docks form a *bridge* if the hexagon-separation between them is even. A dock e and a singular bond e' form an *avoid-pair* if the hexagon-separation between e and an appearance of e' in $b(G)$ is odd. See fig. 10(f) for an illustration.

THEOREM 4

Let G be a generalized-benzenoid system. Then G is the branching graph of a benzenoid system if and only if the following conditions hold:

(1) G has no vertex-fjords, edge-fjords or even-cut-bonds.

(2) For any two clockwise-consecutive elements x and y of $LC(G)$, $s(x, y)$ is odd.
(3) If $LC(G)$ is empty, then $s(G)$ is even and G has no singular pairs, avoid-pairs or bridges.

By applying theorem 4 to the generalized-benzenoid system G shown in fig. 11, we conclude that G is not a branching graph.

Before proving this theorem, we need several lemmas.

Let x be an element of $LC(G)$; denote by $x(h)$ the hexagon which contains x and is one the left hand side when one travels clockwise along $b(G)$. Clearly, $x(h)$ does not belong to G.

LEMMA 1

Let G be the branching graph of a benzenoid system H. Then for each element x of $LC(G)$, the hexagon $x(h)$ must belong to H.

Proof

If x is a leaf of $b(G)$, by the definition of branching graph $x(h)$ belongs to H. Suppose that x is a cove. If $x(h)$ does not belong to H, then all hexagons adjacent to $x(h)$ must belong to H. This contradicts that x is a cove. □

LEMMA 2

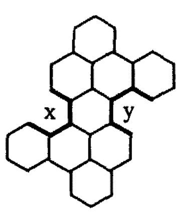
Let G be the branching graph of a benzenoid system H. Let h be a hexagon of H such that h does not belong to G and does not contain any element of $LC(G)$. Then the two bonds e and e' of H which are in the boundary of H and adjacent to h but do not belong to h are contained in G (see fig. 12).

Proof

If the lemma is not true, say e does not belong to G. Then the common vertex of e and h is the end vertex of a pendant bond of G. Thus h contains an element of $LC(G)$. This contradicts the assumption of the lemma. □

COROLLARY 1

Let G be the branching graph of H. If h and h' are two hexagons of H which do not belong to G and are adjacent, then both h and h' contain an element of $LC(G)$. Furthermore, the common bond of h and h' is a leaf of G.



LC(G)={x,y}.
s(x,y)=10.
G is not a branching graph.

G

Fig. 11. Application of theorem 4.

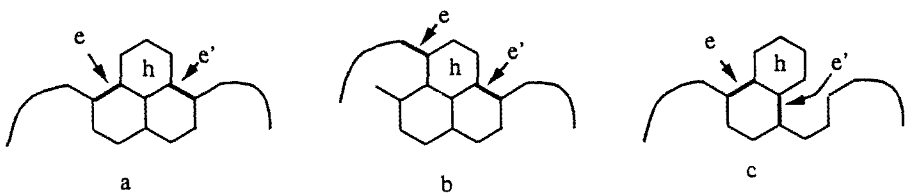


Fig. 12. All possible cases for the positions of e and e'.

LEMMA 3

Let G be the branching graph of a benzenoid system H. Let h and h' be two non-adjacent hexagons of H which do not belong to G; and let L be a subpath of the boundary of H with one end vertex in h, the other in h' and no other intersections with h and h'. If L is contained in $b(G)$, then L belongs to a hexagon of the infinite hexagonal lattice which is adjacent to both h and h'.

Proof

By the assumptions of the lemma, the vertices in L are of degree 3 in H. The number of such vertices is at most 4. Since L is contained in the boundary of H, it belongs to a hexagon of the infinite hexagonal lattice which does not belong to H and is adjacent to h and h'. □

LEMMA 4

Let G be the branching graph of a benzenoid system H. Let $LC(G)$ not be empty. Then for a bond e in $b(G)$, $e(h)$ belongs to H if and only if $s(e)$ is odd.

Proof

Let e be a bond of $b(G)$ and $s(e)$ be odd. If e is contained in an element of $LC(G)$, then by lemma 1 $e(h)$ belongs to H. If e does not belong to any element of $LC(G)$, then by repeatedly applying lemma 3 we can also show that $e(h)$ belongs to H. Conversely, let $e(h)$ belong to H. If e is contained in an element of $LC(G)$ then $s(e)$ by definition is 1. If e is not contained in $LC(G)$, let x be the first reached element of $LC(G)$ if one travels $b(G)$ clockwise from e. By lemma 1 $x(h)$ belongs to H. All the hexagons of H which do not belong to G and are passed when one travels $b(G)$ clockwise from e to x are disjoint by lemma 2 (see fig. 13). By repeatedly applying lemma 3, $s(e)$ is odd. □

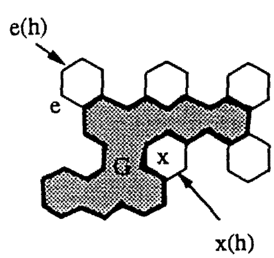


Fig. 13. Illustration of lemma 4.

LEMMA 5

Let G be the branching graph of a benzenoid system H and $LC(G)$ not be empty. Then G has no vertex-fjords, edge-fjords or even-cut-bonds.

Proof

If there is a vertex-fjord (v, v'), let e be the bond which joins v and v'. Note that e does not belong to G. Then the two hexagons of the infinite hexagonal lattice which share e do not belong to H. Therefore at least one of v and v' is not of degree 3. This is a contradiction. If there is an edge-fjord (e, e'), then by lemma 4 $e(h)$ and $e'(h)$ belong to H. But $G \cup e(h) \cup e'(h)$ has an interior face which is not contained in $G, e(h)$ or $e'(h)$. Then all vertices in this face are of degree 3 and thus belong to G. This is a contradiction again. If G has an even-cut-bond then by lemma 4, this bond is also a cut bond of H. But as H is a benzenoid system it has no cut bonds. □

LEMMA 6

Let G be the branching graph of a benzenoid system H. Let x and y be two clockwise-consecutive elements of $LC(G)$. Then $s(x, y)$ is odd. If $LC(G)$ is empty, then $s(G)$ is even.

Proof

By lemma 1, $x(h)$ and $y(h)$ belong to H. Similarly to the proof of lemma 4 (by repeatedly applying lemmas 2 and 3), we can show that $s(x, y)$ is odd. Also by lemmas 2 and 3, if $LC(G)$ is empty, $s(G)$ must be even. □

LEMMA 7

Let G be the branching graph of a benzenoid system H and $LC(G)$ be empty. Let e be a dock and e' be an appearance of a singular bond of G in $b(G)$. Then $e(h)$ does not belong to H and $e'(h)$ belongs to H.

Proof

Since e is a dock, there is a bond e' of $b(G)$ such that $s(e, e')$ is odd. By repeatedly applying lemmas 2 and 3, if $e(h)$ belongs to H then $e'(h)$ belongs to H. By the definition of dock, H has an internal vertex which does not belong to G. This is a contradiction. Since e' is an appearance of a singular bond e'' of G, then e' and the other appearance e''' of e'' in $b(G)$ have an odd hexagon-separation. By applying lemmas 2 and 3 repeatedly, we conclude that either $e'(h)$ and $e'''(h)$ or none of them belong to H. Since e'' is a cut bond of G, $e'(h)$ and $e'''(h)$ belong to H at the same time. □

LEMMA 8

Let G be the branching graph of a benzenoid system H. If $LC(G)$ is empty, then G has no singular pairs, avoid-pairs or bridges.

Proof

By lemma 6, $s(G)$ is even. Let e be a singular bond. Let e_1 and e_2 be the two appearances of e in $b(G)$. Then if $e_1(h)$ belongs (does not belong) to H, by repeatedly applying lemmas 2 and 3, we can show that $e_2(h)$ belongs (does not belong) to H also. Since G is a branching graph of H, both $e_1(h)$ and $e_2(h)$ belong to H. Suppose that there is a singular pair e' and e''. Let x and y be the appearances of e' and e'' in $b(G)$ respectively such that $s(x, y)$ is even. Then by repeatedly applying lemmas 2 and 3, one of $x(h)$ and $y(h)$ does not belong to H. This means one of e' and e'' will be a cut bond of H. This is a contradiction. If there is an avoid-pair, then there are two bonds of $b(G)$, e and e', such that e is a dock, e' is an appearance of a singular bond of G, and $s(e, e')$ is odd. By applying lemmas 2 and 3 repeatedly, we have either both $e(h)$ and $e'(h)$ or none of them belong to H. By lemma 7, $e(h)$ does not belong to H and $e'(h)$ belongs to H. This is a contradiction. Similarly we can show that G has no bridges. □

LEMMA 9

Let G be a generalized-benzenoid system and $LC(G)$ not be empty. Let h be a hexagon which does not belong to G and $b(G) \cap h$ be a path. Then either all the bonds of $b(G) \cap h$ are odd-bonds or none of them are odd-bonds.

Proof

Since $b(G) \cap h$ is a path which belongs to h, by the definition of odd-bonds, the lemma is true. □

Proof of theorem 4

By lemmas 1–6 and 8, the conditions (1)–(3) are necessary. Now we prove that they are also sufficient.

There are two cases:

Case 1. $LC(G)$ is not empty. Let H be the graph obtained by adding all hexagons of the infinite hexagonal lattice which are not in G but contain an element of $LC(G)$ or an odd-bond of $b(G)$.

Then each vertex of G in H has degree 3. Now we prove that all the vertices of H of degree 3 also belong to G. There are three subcases:

Subcase 1. If H has a vertex y of degree 3 which does not belong to G, then there are two hexagons h and h' of H such that y is one of the end vertices of the common bond e of h and h'. Let x be the other end vertex of e. Clearly h and h' do not belong to G. Thus each of h and h' contains an odd-bond of G (this is because if h and h' contain an element of $LC(G)$ then they contain an odd-bond; if they do not contain an element of $LC(G)$, then by the definition of H, they also contain an odd-bond). Let e_1 and e_2 be two such odd-bonds of h and h' respectively. Let P be the path in $h \cup h'$ with e_1 and e_2 as its end bonds which does not contain y (see fig. 14). By the choice of P, x belongs to it. Let P have a vertex z not in G (clearly z is not an end vertex of e_1 or e_2). One of z and y is an internal vertex of $G \cup h \cup h'$, otherwise the deletion of z and y from $G \cup h \cup h'$ results in a disconnected graph. Thus e_1 and e_2 belong to different connected components of G. This contradicts that G is con-

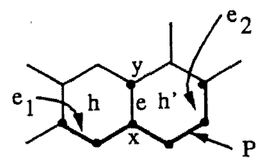


Fig. 14. Illustration of subcase 1 in the proof of theorem 4.

nected. Without loss of generality, let z be an internal vertex. Then z belongs to an interior face of $G \cup h \cup h'$ which is not in G, h or h'. Therefore (e_1, e_2) is an edge-fjord, a contradiction again. Hence all the vertices of P belong to G. We can regard P as a subpath of $b(G)$. Since $P \cap h$ and $P \cap h'$ are contained in $h \cap b(G)$ and $h' \cap b(G)$ respectively, and e_1 and e_2 are odd-bonds, by lemma 9 all bonds of P are odd-bonds. By this we can assume that e_1 and e_2 are adjacent to x. If each of e_1 and e_2 belongs to an element of $LC(G)$, then the hexagon-separation of the two elements of $LC(G)$ is 2. This contradicts the condition (2) of the theorem. If neither e_1 nor e_2 belong to an element of $LC(G)$, then by considering the relative positions of e_1 and e_2, we have that $|s(e_1) - s(e_2)| = 1$. Thus only one of e_1 and e_2 is an odd-bond. This is a contradiction again. The left case is that one of e_1 and e_2 belongs to an element of $LC(G)$ and the other does not. If e_2 belongs to an element B of $LC(G)$, then $s(e_1) = s(e_1, B) = 2$, i.e., e_1 is not an odd-bond. A contradiction. If e_1 belongs to an element B' of $LC(G)$, then there is an element B'' of $LC(G)$ such that $s(e_2, B'') = s(e_2)$. Since $s(B', B'') = 1 + s(e_2), B'$ and B'' have an even hexagon-separation, again a contradiction.

Subcase 2. If there is a bond e of H such that its two end vertices have degree 3 but e does not belong to G, then G has a vertex-fjord. A contradiction.

Subcase 3. If H has a cut bond e, then e belongs to G. By the definition of H, e is an even-cut-bond. A contradiction.

So by subcases 1–3, all the vertices of degree 3 together with the bonds between them belong to G. If H is not a benzenoid system, then it has an interior face which is larger than a hexagon. Thus H has some internal vertices of degree 2. We claim that there is a hexagon of H which contains an external vertex of degree 2 as well as an internal vertex of degree 2. If this is not true, then after deleting all external vertices of degree 2 from H a graph G' is obtained in which each internal vertex of degree 2 of H is also an internal vertex. Then after removing all the internal vertices of degree 2 from G', G is obtained. Thus G has an circuit which is larger than a hexagon. This is a contradiction. Let h be such a hexagon. Let v_1 and v_2 be two vertices of h such that v_1 is an external vertex of degree 2 and v_2 is an internal vertex of degree 2 in $H.v_1$ and v_2 are not adjacent otherwise both of them are either internal vertices or external vertices at the same time. If both of them are adjacent to a vertex v, then v is of degree 3; otherwise v_1 and v_2 are either internal vertices or external vertices at the same time. Thus v is the end vertex of a leaf of $b(G)$. By the definition of H, v_1 and v_2 are of degree 3 in H. This is a contradiction. For the same reason, none of the vertices of h are leaves of $b(G)$. The only possible positions of v_1 and v_2

are indicated in fig. 15. Let e and e' be the two bonds of h as shown in fig. 15. Since h does not belong to G, one of e and e', say e, is an odd-bond or an element of $LC(G)$. The end vertices of e' are not leaves of $b(G)$, and they are also not of degree 2 in H otherwise v_1 and v_2 are external or internal vertices of H. Thus e' belongs to G. If e' is an odd-bond, then clearly (e, e') is an edge-fjord. If e' is not odd, then the bonds of $b(G)$ which are adjacent to e' are odd-bonds. By the definition of H, one of v_1 and v_2 is not of degree 2 in H. There is a contradiction in both cases.

By the above discussion, we show that H is a benzenoid system and G is its branching graph.

Case 2. $LC(G)$ is empty. Let $S = \{e(h) : e \in b(G)\}$. The cardinality of S is $s(G)$. We rank the hexagons of S in an order $h_1, h_2, \ldots, h_{s(G)}$ such that when travelling $b(G)$ clockwise one passes h_i before passing h_{i+1}. Let $G(H)$ and $G(H)'$ be the two graphs obtained by adding hexagons h_i with odd subindices and even subindices to G respectively. If G has a singular bond e, without loss of generality, let e be in h_1. Then $G(H)$ has no cut bonds for G has no singular pairs. Similarly to case 1, we can show that each vertex of G is of degree 3 in $G(H)$. Moreover, each vertex of degree 3 in $G(H)$ belongs to G. The remaining case is to show that $G(H)$ has no interior faces larger than a hexagon. This is true because G has no avoid-pairs and bridges. Thus $G(H)$ is a benzenoid system with G as its branching graph. If G has no singular bonds, by noting that G has no bridges, we can also show that one of $G(H)$ and $G(H)'$ is a benzenoid system with G as its branching graph.

The proof is completed. □

COROLLARY 2

Let G be a branching graph. Then there are two benzenoid systems with G as their branching graph if and only if $LC(G)$ is empty and G has no singular bonds or docks.

Proof

By lemmas 1 and 4, if $LC(G)$ is not empty, then there is a unique benzenoid system with G as its branching graph. If $LC(G)$ is empty, then by lemmas 2 and 3, the only candidates with G as their branching graph are $G(H)$ and $G(H)'$ as in the proof of case 2 of theorem 4. If G has no singular bonds or docks, then both of them are benzenoid systems. □

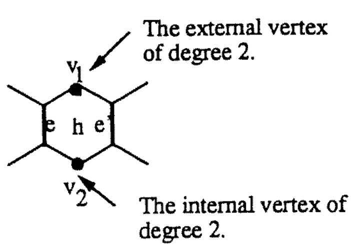


Fig. 15. Illustration of subcase 3 in the proof of theorem 4.

The following corollary is theorem 3 in [15]:

COROLLARY 3 (GUTMAN AND KIRBY)

Let G be a generalized-benzenoid system. Then G is the branching graph of two different benzenoid systems at most.

4. Disconnected branching graphs

A *hex-diagram* is a subgraph of the infinite hexagonal lattice without nonhexagonal interior faces and together with its exact position in the infinite hexagonal lattice. A *connected component* of a hex-diagram is a maximal subgraph of it in which any two vertices are joined by a path. A hex-diagram is a geometric diagram. When a hex-diagram is given, then all the positions of its vertices and bonds are known. For example, the two hex-diagrams shown in fig. 16 are different despite the fact that they have the same connected components.

In this section, we show that if a hex-diagram has more than one connected component, then it is the branching graph of at most one benzenoid system.

Let G be the branching graph of a benzenoid system H and have more than one connected component. Let C be a connected component of G. Let $H(C)$ be the subgraph of H formed by all hexagons of H which contain at least one vertex of C.

LEMMA 10

Let G be the branching graph of a benzenoid system H and C be a connected component of G. Then C is the branching graph of $H(C)$.

Proof

Every vertex of C in $H(C)$ is of degree 3. If $H(C)$ has a vertex v of degree 3 which is not in C, then there are two hexagons h_1 and h_2 of $H(C)$ which contain v. Let e be the common bond of h_1 and h_2. Then v is one of the end vertices of e. Let v' be the other end vertex of e. Clearly, v' and all the neighbors of v and v' do not belong to C, otherwise v belongs to C. By the choice of h_1 and h_2, $h_1 \cap C$ and $h_2 \cap C$ are nonempty. If either $h_1 \cap C$ or $h_2 \cap C$, say $h_1 \cap C$, contains only a single vertex, then the neighbors of this vertex in h_1 are of degree 2 in H. Since H is a benzenoid system, this is impossible. Thus each of $h_1 \cap C$ and $h_2 \cap C$ contains a single bond. Let

Fig. 16. Illustration of the definition of hex- diagram.

$h_1 \cap C$ be e_1 and $h_2 \cap C$ be e_2. Note that the end vertices of e_1 and e_2 are not neighbors of v and v'. The only possible positions of e_1, e_2, v and v' are shown in fig. 17. If both of v and v' are external vertices of H, then the deletion of v and v' from H results in a disconnected graph. Thus C is not connected. This is a contradiction. Without loss of generality, let v be an internal vertex of H. Then all neighbors of v are of degree 3. Moreover, v and its neighbors belong to the same connected component of G as e_1 and e_2. Thus v belongs to C, a contradiction again. Every vertex of degree 3 of $H(C)$ belongs to C. Clearly $H(C)$ has no cut bonds. We can also show that $H(C)$ has no interior faces larger than a hexagon. Thus $H(C)$ is a benzenoid system and C is its branching graph. □

LEMMA 11

Let G be the branching graph of a benzenoid system H. Then each hexagon of H contains at least one bond of G.

Proof

By the definition of G.

LEMMA 12

Let G be the branching graph of a benzenoid system H which is not connected, and C be a connected component of G. Then there is a connected component C' of G different from C and a hexagon h of H such that $h \cap C$ and $h \cap C'$ are two parallel bonds.

Proof

By lemma 10, C is the branching graph of $H(C)$. Since G is not connected, $H(C)$ is not equal to H. Thus there are a hexagon h of $H(C)$ and a hexagon h' of H such that h' is not in $H(C)$ and is adjacent to h. The common bond e of h and h' belongs to a connected component C' of G. Because h' is not in $H(C)$, C' is different from C. By lemma 11, h contains a bond of C. Every bond of $h \cap C$ is parallel to e, otherwise e is in C. Thus $h \cap C$ contains a single bond. Similarly, we can show that $h \cap C'$ contains a single bond which is e. The bonds of $h \cap C$ and $h \cap C'$ are parallel. □

The *boundary* $b(G)$ of G is defined to be the union of the boundaries of its connected components. For a bond e in $b(G)$, we define $e(h)$ to be the unique hexagon which contains e and is on the left hand side when one travels along the boundary of

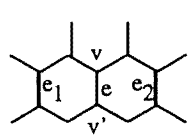


Fig. 17. Illustration of the proof of theorem 5.

G clockwise (here travelling along the boundary of G means to travel the boundaries of the connected components one by one). A *connected-band* e of $b(G)$ is a bond of $b(G)$ which is parallel to another bond e' of $b(G)$ such that they belong to different connected components of G and are contained in the same hexagon of the infinite hexagonal lattice. Such a pair (e, e') is called a *gulf* of G.

For each connected component C of G, let $A(C)$ be the set of coves and leaves and connected-bonds of $b(G)$ contained in $b(C)$. All the concepts (such as hexagon-separation, even-cut-bonds and so on) defined in the previous section can be extended to each component of G in a straightforward way. If G has more than one connected component, then by lemma 12 for each connected component C of G, $A(C)$ is not empty.

LEMMA 13

Let G be a hex-diagram and (e, e') be a gulf. If G is the branching graph of a benzenoid system H, then the hexagon containing e and e' belongs to H.

Proof

If the lemma is not true, then one can check very easily that e and e' belong to the same connected component of G. □

COROLLARY 4

Let G be a hex-diagram and e be a connected-bond of $b(G)$. Then $e(h)$ belongs to H.

THEOREM 5

Let G be a hex-diagram with more than one connected component. Let $C_1, C_2, \ldots, C_k$ be its connected components. If G is the branching graph of a benzenoid system H, then H is unique.

Proof

Let G be the branching graph of a benzenoid system H. By Lemma 10, C_i is the branching graph of $H(C_i)$. By lemma 12, C_i contains at least one connected-bond. By corollary 4 and following the proof of corollary 2, $H(C_i)$ is unique. Thus $\cup_i H(C_i) = H$ is unique. □

Acknowledgements

The first author has been supported by FCAR (Fonds pour la Formation de Chercheurs et l'Aide à la Recherche) grant 92EQ1048, NSERC (Natural Science and Engineering Research Council of Canada) grant to H.E.C. and grant GP105574, and AFOSR grants 89-0512B and F49620-93-1-0041 to Rutgers University. The second author has been supported by the International Fellowships Program of NSERC. The authors thank Catherine Lebatteux for useful discussions.

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