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THREE THEOREMS ON BRANCHING GRAPHS.

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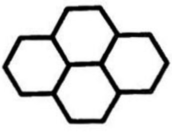
ABSTRACT

The branching graph is a recently introduced object associated with a polycyclic structure. A few results relating the structure of a polyhex to that of the corresponding branching graph are pointed out. The 2-factors of a polyhex are closely related to the 1-factors of its branching graph.

INTRODUCTION

The branching graph of a polycyclic graph is a special subgraph. Each vertex of the polycyclic graph (G) appears in its branching graph B(G) if and only if it is of at least degree three. Each edge of G appears in B(G) if and only if it connects two such branching vertices. For example:



The pyrene graph, G.

The branching graph of pyrene, B(G).

This abstract object was introduced[1] as a practical aid to diagnosing whether a graph does or does not have a Hamiltonian path (i.e. a path that visits every vertex just once). In a further study[2] it was found to afford some insight into why there are so few Clar sextet 2-factorable polyhexes among all the polyhexes that are theoretically possible. As the branching graph appears to have some use in chemical graph theory, it is desirable to characterize its structure and to understand its relationship to other objects. Here we present three results.

DEFINITIONS USED

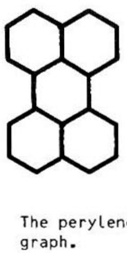
Polyhex: A polyhex is a network of regular hexagons such that any two hexagons are either disjoint or have a common edge. For a recent review see reference.[3]

1-Factor: If a graph has one, it is a set of disjoint edges that can be drawn to include every vertex, so that all vertices are of degree one. It is equivalent to the set of 'double' bonds within a Kekulé structure.

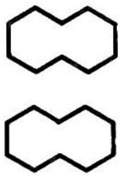
Kekulé structures
of benzene.

1-Factors of the
benzene graph.

2-Factor: If a graph has one, this is a set of disjoint rings that can be drawn to include every vertex. So, every vertex in this factor is of degree two. If the 2-factor consists of only one ring it is called a Hamiltonian circuit.



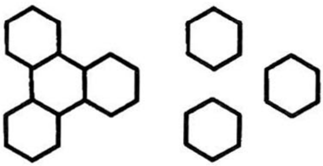
The perylene
graph.



A 2-factor of the
perylene graph.

A polyhex graph with a 2-factor that is also a Hamiltonian circuit.

Sextet 2-factor: This is a particular 2-factor in which all the rings are hexagons, i.e. it is a set of hexagons that accounts for all the vertices. These factors are of great interest to chemists because it is thought, with some empirical justification, that benzenoid hydrocarbons that can be fully drawn as an assembly of aromatic sextets connected by single bonds are particularly stable.[4,5]



The triphenylene graph and its corresponding sextet 2-factor.

The triphenylene graph drawn with inscribed circles to indicate the aromatic sextets and its sextet 2-factorability.

Traceability: A graph is said to be traceable or semi-Hamiltonian, or to have a Hamiltonian path, if one can trace a path along a connected sequence of vertices and visit every vertex just once. A Hamiltonian circuit is a path that visits every vertex just once and then returns to the starting vertex.

A THEOREM ON THE NUMBER OF 2-FACTORS OF A POLYHEX

In this section we demonstrate the existence of a one-to-one correspondence between the 2-factors of a polyhex and the 1-factors of its branching graph. This result provides the foundation for using branching graphs in the study of 2-factorability, traceability etc. of polyhexes. The result, which we now formulate as Theorem 1, was anticipated in previous papers[1,2] but a formal proof was not given.

<u>Theorem 1</u>: The number of 2-factors of a polyhex is equal to the number of 1-factors of the respective branching graph.

Instead of Theorem 1 we prove a somewhat more general result, namely Theorem 1a. Results similar to Theorem 1a have been known for a long time in graph theory, and are mainly due to Petersen (see for example[6]).

Let G be a graph possessing only vertices of degree two and degree three. Let $V_3(G)$ be the set of vertices of degree three within G. Denote by B(G) the subgraph of G induced by the vertices from $V_3(G)$.

<u>Theorem 1a</u>: The number of 2-factors of G is equal to the number of 1-factors of B(G).

It is well known[3] that all the vertices of a polyhex are of degree two or degree three. This means that G in Theorem 1a may be a polyhex. Then B(G) is just its branching graph. Therefore it is evident that Theorem 1 is an immediate special case of Theorem 1a.

<u>Proof</u>. Denote the number of 2-factors of G by f_2 and the number of 1-factors of B(G) by f_1.

(a) Let F_2 be a 2-factor of G. Then F_2 contains all the edges of G which (in G) are incident to all vertices of degree two. However, exactly one edge incident to each vertex of degree 3 of G is not contained in F_2. These edges both start and finish at vertices from $V_3(G)$. Hence the edges of G not contained in F_2 form a 1-factor of B(G). This 1-factor is uniquely determined by F_2, and to distinct 2-factors of G there correspond distinct 1-factors of B(G). Therefore $f_1 \geqslant f_2$.

(b) Let F_1 be a 1-factor of B(G). Delete from G the edges of F_1. In the graph which is obtained in this manner all vertices are of degree two. Hence this graph is a 2-factor of G. This 2-factor is uniquely determined by F_1, and to distinct 1-factors of B(G) there correspond distinct 2-factors of G. Therefore $f_2 \geqslant f_1$.

From $f_1 \geqslant f_2$ and $f_2 \geqslant f_1$ it follows that $f_1 = f_2$. ◻

Corollary 1.1. In the proof of Theorem 1a a one-to-one correspondence between the 2-factors of G and the 1-factors of B(G) was established. Thus the study of the 2-factors of G is reduced to a task which is much more familiar to organic chemists, namely to the examination of 1-factors (equivalent to Kekulé structures) of the smaller graph B(G).

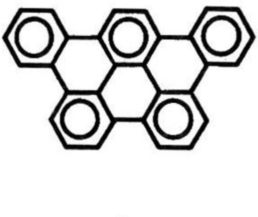
TOWARDS THE CHARACTERIZATION OF BRANCHING GRAPHS

An obvious question arising from the concept of branching graphs is: which graphs can be branching graphs ? At present we do not know the complete solution of this problem, but can offer only a few partial results. In the first place, it is remarkable that sometimes the branching graph of a polyhex is a polyhex itself.

Theorem 2. If P is a sextet 2-factorable polyhex, then each component of its branching graph B(P) is either a polyhex or is composed of several disjoint polyhex units where each edge connecting these units corresponds to an essentially single bond, i.e. a bond that is single in all Kekulé structures. The examples 1^o, 2^o and 3^o illustrate the cases which may occur. In the respective polyhexes the sextet 2-factor is indicated by circles symbolizing Clar-type aromatic sextets.

Proof. This follows by induction on the number of hexagons of P. The smallest sextet 2-factorable polyhexes are the benzene graph (one hexagon) and the triphenylene graph (four hexagons). Theorem 2 holds in a trivial manner for the benzene graph. Its validity for the triphenylene graph (whose branching graph is benzene) is also immediate. Hence Theorem 2 holds for the first two members of the sextet 2-factorable polyhex family.

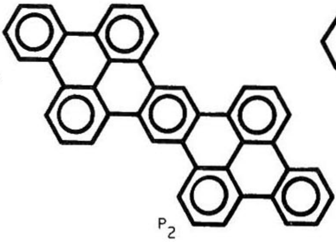
1^o



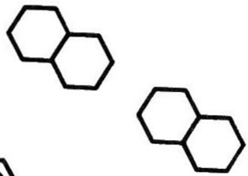
P_1

$B(P_1)$

2°

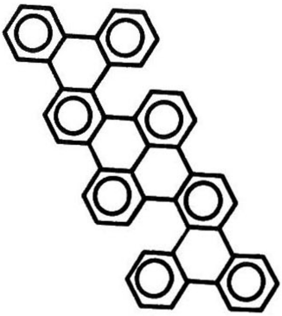


P_2

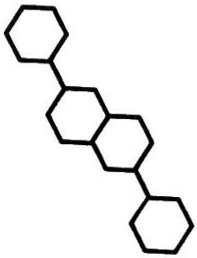


$B(P_2)$

3°



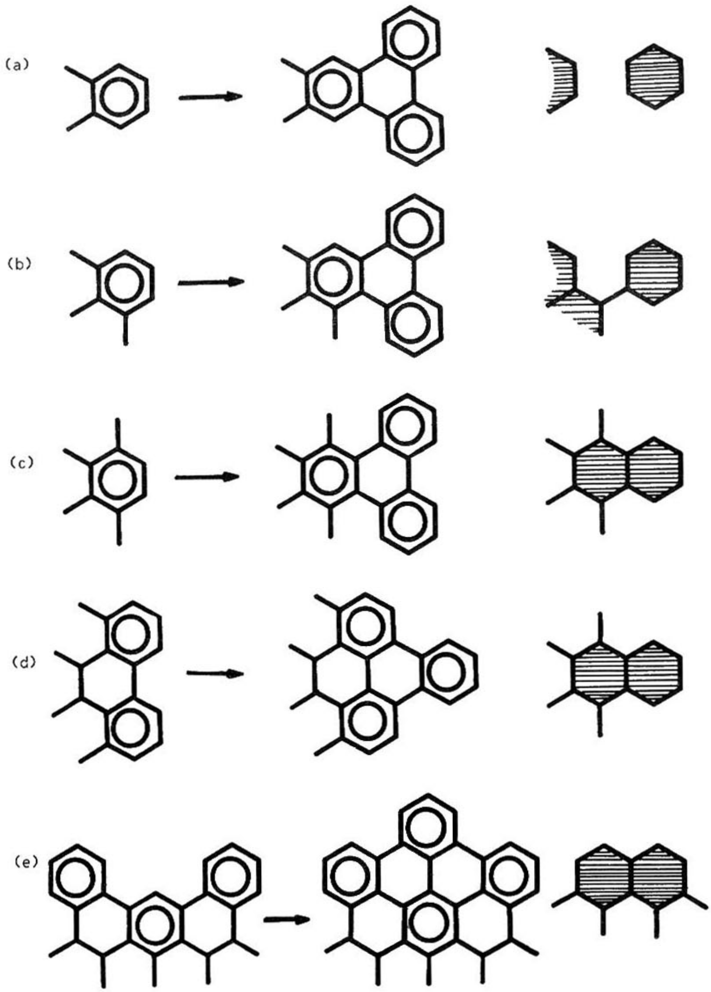
P_3



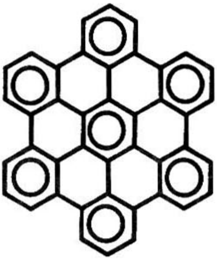
$B(P_3)$

All other sextet 2-factorable polyhexes can be obtained by means of one or more of the following construction modes (for details see reference[3], Chapter 4.9; and reference[7]). Examining the five cases one by one we can easily check that if the branching graph in the starting polyhex has the form described in Theorem 2, then the branching graph of the resulting polyhex also has the same form. These latter branching graphs are indicated below by the hatched diagrams. We see that 1° results from the construction modes (c), (d) and (e); case 2° from the mode (a); whereas case 3° is obtained when the construction mode (b) is applied.

Since the modes (a)-(e) suffice for the construction of all sextet 2-factorable polyhexes, the proof by induction is complete. ▱

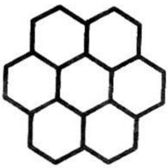


The reverse of Theorem 2 is not true, namely if the branching graph is a polyhex, then the original polyhex need not be sextet 2-factorable. Moreover, the sextet 2-factorability of a polyhex cannot in general be deduced from the respective branching graph. This is illustrated by the polyhexes P_4 and P_5 which have the same branching graph (= the coronene graph); P_4 is sextet 2-factorable whereas P_5 is not.



P_4

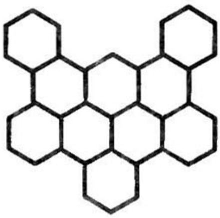
P_5



$B(P_4) = B(P_5)$

These examples show that a polyhex may be the branching graph of more than one polyhex. In fact if P is a polyhex then P can be the branching graph of two different polyhexes or of a single polyhex or of no polyhex at all. For instance, P_6 is the branching graph of a unique polyhex, namely P_7. On the other hand P_8 is not a branching graph.

P_6



P_7

P_8

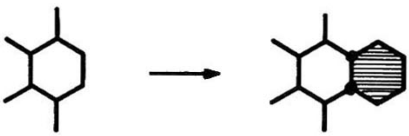
It was conjectured[1] that two is the maximum number of polyhexes compatible with the same branching graph when the branching graph is a polyhex. We now show that this conjecture is true. However, it should be noted that if the branching graph is <u>not</u> a polyhex, then it can be the 'child' of more than two polyhexes, because several geometric configurations of the branching graph may be possible, and each may be associated with a different polyhex.

<u>Theorem 3.</u> A polyhex P cannot be the branching graph of more than two distinct polyhexes.

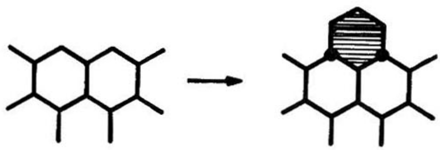
<u>Proof.</u> Suppose that we want to construct a polyhex P^* such that P is its branching graph. Then we have to add hexagons to the perimeter of P so that each vertex of degree two in P becomes a vertex of degree three in P^*. The newly added hexagons must possess at least one vertex of degree two. Such an addition can be realised in four distinct ways, viz. (a)-(d).

The newly added hexagon is indicated by hatching. The vertices which are of degree two in P and of degree three in P^* are indicated by heavy dots.

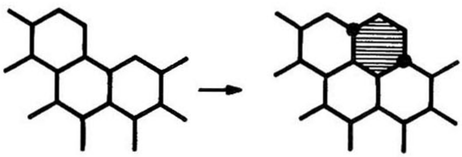
(a)



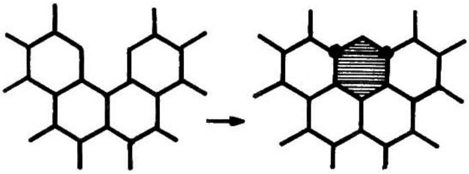
(b)



(c)



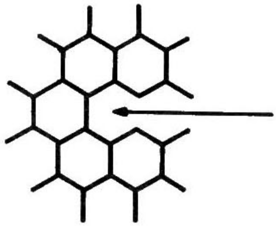
(d)



Theorem 3 follows now from the observation that each new hexagon transforms exactly two vertices of degree two into vertices of degree three. Hence the transformation $P \rightarrow P^*$ requires that, following the perimeter of P, the vertices of degree two of P be grouped into pairs. Such a grouping can be done in at most two ways. Consequently there will be at most two distinct polyhexes whose branching graph is P. □

<u>Corollary</u> <u>3.1</u>. If a polyhex P is a branching graph then the vertices of degree two on its perimeter are separated by at most 3 vertices of degree three.

<u>Proof</u>. If two vertices of degree two are separated by more than three vertices of degree three, then P possesses a fjord.

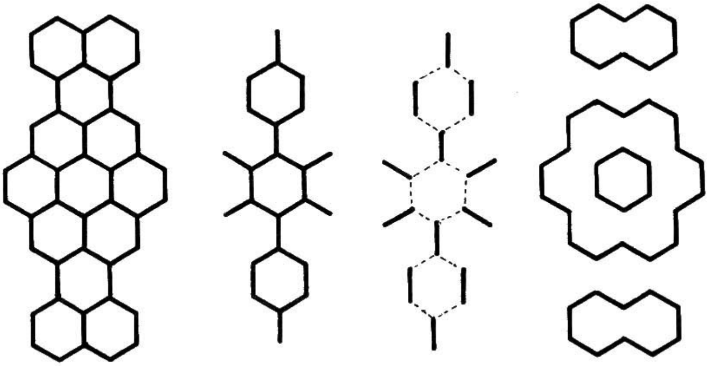


It is clearly impossible to construct P^* in such a case. □

A COUNTER-EXAMPLE FOR A CONJECTURE ON BRANCHING GRAPHS

Denote the minimum number of components of a 2-factor of P by C(P). A polyhex having a connected 2-factor (i.e. C(P)=1) is traceable. Kirby[1] showed that a polyhex P with C(P)=2 is traceable, and conjectured that it is also traceable if $C(P) > 2$ provided that the disconnections giving $C(P) > 2$ do not arise from more than one branching graph component.

This conjecture is false however, as can be seen from the counter-example P_9.



P_9 $B(P_9)$ $B(P_9)'$ $(P_9)_{2F}$

The polyhex P_9 is chosen so that its branching graph, $B(P_9)$, is connected and has a unique 1-factor, $B(P_9)'$. According to Theorem 1, P_9 has a unique 2-factor. Deleting from P_9 the edges of $B(P_9)'$, the 2-factor $(P_9)_{2F}$ is immediately obtained. For this example $C(P_9)=4$ and $B(P)$ is connected, yet P_9 is untraceable. It is difficult to demonstrate conclusively by trial and error that a graph is untraceable. In order to increase confidence in this conclusion, it is necessary to consider the basis upon which the original conjecture was founded[1]. This implicitly introduced another graph theoretical entity which we will here call a 'k-branch-factor'. This is defined by analogy with the familiar concept of 'principal resonance structures' (of which Kekulé structures form one class) used in organic chemistry. Thus a 2-Branch-factor, if a graph has one, is a set of disjoint edges that can be drawn to account for all but two of the vertices. For example -

and so on...

The naphthalene graph and some of its 2-branch-factors.

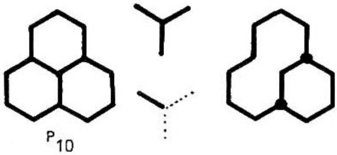
This concept can be generalised in an obvious manner to k-branch-factors where k is even. For any given branching graph $B(P)$ of a polyhex P, there will exist a minimum value for k. For example, if $B(P)$ has no 1-factors, then $k \geqslant 2$. Let the edges in a (minimal k) k-branch-factor of $B(P)$

be deleted from P. Provided that the resultant graph is connected, then

1° If k=0, B(P) has 1-factors; P has a Hamiltonian path and is traceable.

2° If k=2; P has no Hamiltonian circuit, but is traceable.

The branching graph of P_{10}, has no 1-factors (equivalent to 0-branch-factors), but it does have 2-branch-factors. Deleting such an edge set from P_{10} gives a connected spanning subgraph with just two branching vertices, and immediately indicates some of the Hamiltonian paths in P_{10}.



P_{10}

3° If k > 2 then any similarly derived spanning subgraph will have at least four branches, and it is easily shown that this makes P untraceable.

The conjecture being examined, rested upon the supposition that, because when a 0-branch-factor exists it is always possible to generate a k-branch-factor for k=2 (non minimal), then P would be traceable. This was mistaken, because edge deletion may still give rise to disconnection. Examination of $B(P_9)$ shows that 2-branch-factors also all give rise to disconnection. This is strong confirmatory evidence that P_9 is untraceable.

CONCLUSION

This study has revealed some properties of the branching graphs of polyhexes. Theorem 1 concerns the relationship between the 2-factors of a polyhex and the 1-factors of its branching graph. This is followed by the results (Theorems 2 and 3) of structural investigations for the case where the branching graph is itself a polyhex. We have not fully characterized these objects and, although more results may emerge, the conditions which must be fulfilled may be graph theoretical or geometrical, and are complicated. Characterization of branching graphs that are not polyhexes seems to be even more difficult, but further examination of these novel objects in the topological theory of benzenoid molecules, and other polycyclic structures, is desirable.

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