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HAMILTONIAN PATHS IN POLYHEXES: THE USE OF BRANCHING SUBGRAPHS TO ASSIST DIAGNOSIS OF GRAPH TRACEABILITY

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Abstract

The traceability of some of the smaller polyhexes is examined. (A graph is said to be traceable or to have a Hamiltonian path if it has a path visiting every vertex just once.) Most polyhexes are traceable, and an attempt is made to develop some practical guidelines for finding those that are not. A subgraph consisting of the branching vertices of a polyhex, and of any edges which join pairs of such vertices, is a useful tool for this purpose. The "principal resonance structures" of such a graph suggest ways of finding simpler spannng subgraphs of the polyhex that will often make its traceability, or lack of it, more obvious.

1. Introduction

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. The problem of finding or enumerating such paths is closely related to that of finding or enumerating Hamiltonian circuits – closed walks connecting all the vertices of a graph. The name derives from William Rowan Hamilton, who was Astronomer Royal for Ireland for a period during the nineteenth century, and who formulated this problem as a game in which the object was to find these circuits on the dodecahedron graph [1].

On small graphs which are not too complicated, it is easy to see Hamiltonian circuits, and one might think that it would not be difficult to specify a non-empirical means of distinguishing graphs which have them from those that do not. However, despite a good deal of work (see, e.g. [1–19]) and the fact that the superficially similar problem of characterising graphs which are Eulerian (i.e. have a path which includes every edge just once) is more amenable, this has not been done. For many classes of graph, it is possible to define conditions for a graph to be Hamiltonian or path Hamiltonian, but necessary and sufficient conditions for an arbitrary graph have not been defined, and some think it unlikely that this will ever be achieved [20].

There are a number of reasons why one might wish to know which graphs are traceable. An example is the encryption of unweighted graphs for computer storage and manipulation; a convenient practical technique for entering the description at a key-board is to enter the number of vertices, followed by connections which, when made or broken, convert a consecutively numbered linear chain of the same size to the structure in question [21]. Simple examples are benzene: 6 1–6; octane: 8; and 3,4-dimethylhexane: 8 3–7 4–5. Ideally, but not necessarily, this corresponds to finding the minimum number of disjoint paths required to span the graph. Apart from the linear chains themselves, all trees must have at least one bond in the preliminary chain broken in order to arrive at the required structure. On the other hand, it was found in practice that many cyclic structures can be described in terms of new connections only, i.e. without any need to break the chain into smaller fragments. A minority do need a disconnection however, and it was curiosity about the proportions and distribution of such cyclic graphs that led to this study.

An additional reason is that traceability must be among the factors that determine what kinds of structure it is possible or impossible to form by intra-molecular cross-linking of a linear polymer.

The methods available for calculation of π-electron ring currents in conjugated systems depend upon whether or not they are traceable [22–25], and clearly Hamiltonian circuits are of some interest in the context of so-called "conjugated-circuit" theory [26–28], for they represent the largest of such possible circuits in a fully conjugated system.

Outside chemistry, the well-known "travelling salesman" problem – that of devising the most efficient route with which to visit a number of cities with no repetition and at minimum cost – first requires a search for graph traceability, and in many other fields there occur problems for which the properties of a network, including whether or not it is traceable, are important. Within graph theory itself, the enumeration of the spanning trees of a graph [8,29–32] is relevant; here, one seeks those graphs whose set of spanning trees includes a linear chain.

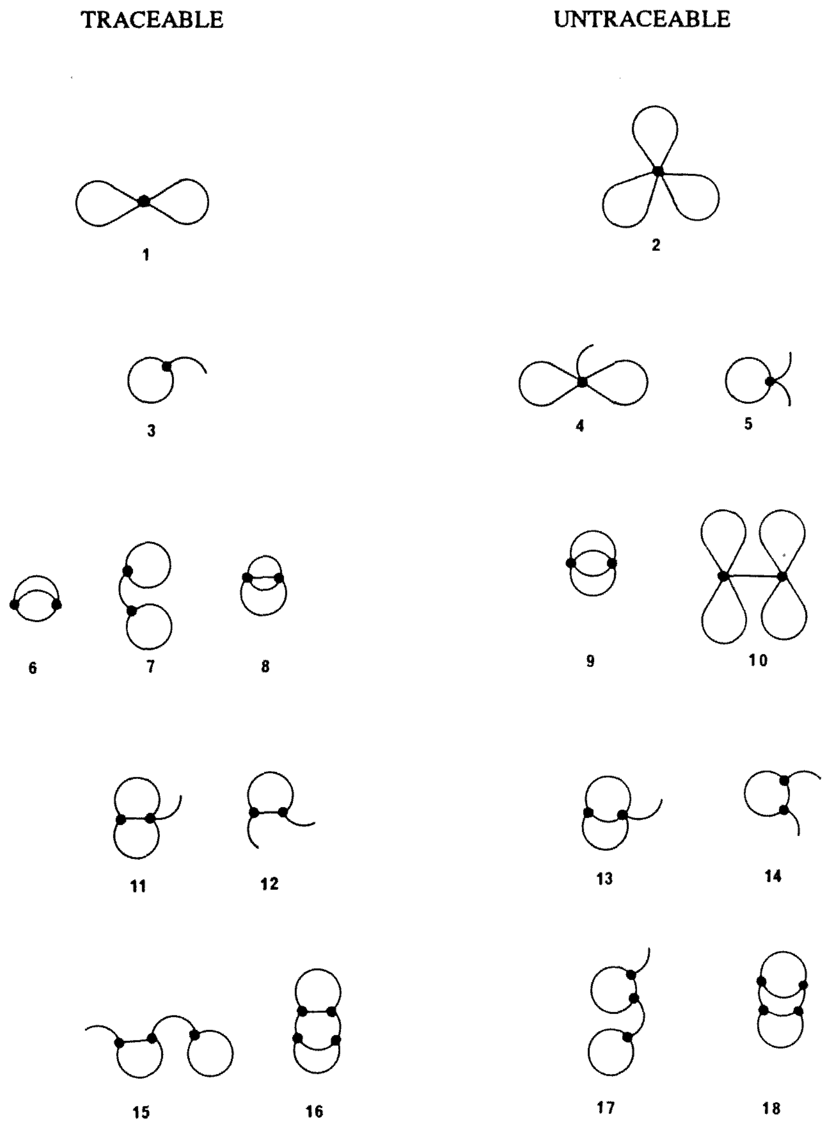
At the informal level of common sense, Hamiltonian paths are very like Hamiltonian circuits, but with obvious differences. More graphs are traceable than have Hamiltonian circuits, because for every Hamiltonian circuit there necessarily exist Hamiltonian paths, but the converse is not true.

The traceability of a graph depends upon the number, disposition and valency of vertices that are other than 2-valent. This paper approaches the matter from a practical point of view, and tries to devise some fairly simple rules and algorithms to aid recognition of traceable or non-traceable polyhexes.

2. Some general graphs whose traceability is easily seen

The nomenclature used in this paper generally follows that outlined by Wilson (see appendix). In the following illustrations, a line with curvature indicates a path through at least one 2-valent vertex, while a straight line denotes a single edge.

Structures (1)–(18) illustrate some of the graphs with disjoint branching vertices whose traceability is obvious. In these, it can be seen that if there are b branching vertices, and these are excised, then the number of components left reflects the traceability of the original graph ($b + 1$ = traceable; $b + 2$ = untraceable). For this discussion of polyhexes, particular interest attaches to (6) and (18).



3. Polyhexes

3.1. INTRODUCTION

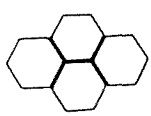
A polyhex is a network of regular hexagons such that any two hexagons are either disjoint or have a common edge. These are sometimes referred to as hexagonal animals or hexagonal polyominoes in mathematical literature, and the names benzenoid, arene or polyarene are used for 1-factorable polyhexes (e.g. [33,34]), although usage is not always consistent. Here, the term honeycomb-fragment is used for a structure that can be obtained by copying part of a hexagon grid; it may or may not have hexagons or terminal vertices (cf. [35]).

These polyhexes form a perennially interesting and a relatively uncomplicated class of chemical graph, and it is of interest to examine the distribution of traceable graphs within it, even though this is not especially useful for coding purposes (for there are faster ways of encoding this class of graph [21,34]). Each vertex has a valency of two or three.

Structure (6) is traceable, so if it can be recognised as a spanning subgraph of a polyhex, then that polyhex too must be traceable. A spanning subgraph with only 2-valent vertices is a 2-factor (a Hamiltonian circuit is one kind of 2-factor). The result of 2-factoring is to erase edges in such a way as to eliminate branching without introducing any terminal vertices. It is therefore appropriate to *extend* the concept of 2-factoring to an analogous process in which any spanning subgraph with a *minimum number* of disjoint branching vertices, but *no terminal vertices*, is accepted as a valid factor. If the result is a graph of type (6), then it is traceable, whereas if it resembles (18), it is untraceable.

3.2. DEFINITION AND SOME PROPERTIES OF THE BRANCHING GRAPH

For this study, it is useful to define a special subgraph of a polyhex called a "branching graph". Each vertex of the polyhex (G) appears in the branching graph (B) if and only if it has a valency greater than two. Each edge of G appears in B if and only if it joins two branching vertices in G. The structures (19) and (20) show an example of a polyhex/branching-graph pair. This subgraph should not be confused with other derived graphs such as the dualist, originating from Balaban and Harary's work [36–38].



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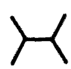

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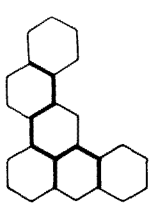
Any polyhex has only one branching graph but, as examples (21)–(23) show, more than one distinct polyhex may share the same branching graph. For the purpose



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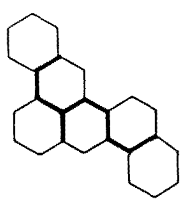

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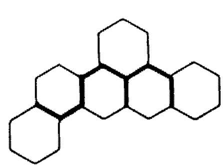
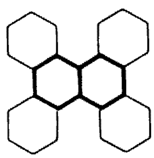


23

of investigating traceability this does not matter, and indeed is irrelevant, but for the reconstruction of a polyhex from a branching graph, it is necessary to consider the possible configurations that the latter can assume when superimposed upon a hexagon grid [36]. Even then, it is occasionally possible to draw two distinct polyhexes around a specific honeycomb fragment, e.g. (24) and (25).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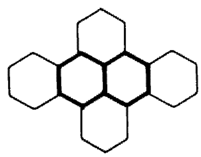
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It is interesting to note that Gutman has stated [33] that the theory of benzenoid systems suffers a fundamental problem, in that their definition is of a geometric rather than a topological nature.

It is conjectured here that it is only possible to draw two polyhexes around a given honeycomb fragment when it has no terminal vertices, and that this is a necessary but not a sufficient condition.

Not every honeycomb fragment represents the branching graph of some polyhex. A given graph with a maximum valency of three has one or more possible representations as a honeycomb fragment, and all, some or none of these may be valid branching graphs.

A branching graph may be disconnected (in the linear polyacenes, for example). However, a graph that is valid as a branching graph is not necessarily valid as a disconnected branching graph component. For example, (26) is a valid branching graph but, unlike (27), it cannot appear as an isolated component. This is because in (28), the polyhex of (26), there are no peripheral edges that are more than one edge distant from a branching vertex, so that any kind of condensation always extends (26).


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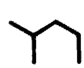
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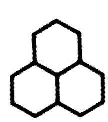
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The branching graphs of polyhexes with few internal vertices are usually acyclic. Larger polyhexes with more internal vertices will have smaller polyhexes, usually with acyclic attachments, as their branching graphs.

The number of vertices in the branching graph is even and, since they are mapped from the 3-valent vertices of the polyhex, the total is known to be $2(h-1)$, where h is the number of hexagons [33].

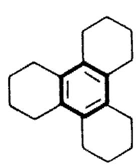
3.3. THE USE OF BRANCHING GRAPHS

A polyhex G can be 2-factored to a cycle graph if edges that connect two branching vertices can be chosen and deleted until no branching vertices remain. This means deleting as many disjoint edges of G as possible from those that appear in the branching graph B. This problem of selecting maximal sets of disjoint edges is equivalent to the problem of 1-factoring or of finding non-equivalent Kekulé structures or edge colourings [39–49]. A Kekulé structure of B will, by its double bonds, show a set of edges in G whose erasure will eliminate all branching vertices without introducing terminal vertices. If B does not have Kekulé structures, then edge erasure corresponding to the principal resonance structures will reveal ways in which the number of branching vertices in G can be minimised, while avoiding leaf formation.

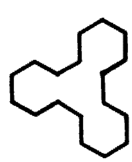
3.4. THE CLASSIFICATION OF POLYHEXES

When polyhex branching graphs and the corresponding polyhex factors are examined, the parent polyhexes fall into a number of categories which are described here. In each example shown, the double bonds of the embedded branching graph together represent one possible principal resonance structure. Such an example has *no* significance in the conventional sense of conjugation theory, but indicates that the polyhex is factorable, in the general sense described, by erasure of the set of double bonds shown.

It can be seen by inspection and introspection that if the branching graph B is 1-factorable, then the parent graph G is 2-factorable. If each 1-factor of the branching graph is taken in turn, and its edges are erased from a fresh copy of the parent graph, then this procedure will yield all the 2-factors of G. If at least one of these 2-factors is a connected graph, then G is traceable and also has a Hamiltonian circuit, e.g. (29a and b).

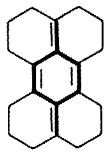


29a

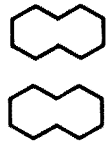


29b

If, on the other hand, B is 1-factorable, but G is 2-factorable only to a disconnected graph (i.e. all 2-factors have more than one component), then there is no Hamiltonian circuit, although usually G is traceable (e.g. 30a, b and c), depending upon the connectedness of the branching graph (see below).



30a



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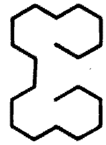
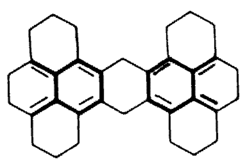


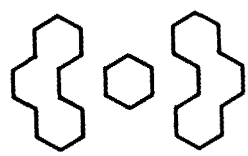
30c

It is conjectured that if the minimum number of components of the 2-factor is two, then the polyhex is always traceable (but has no Hamiltonian circuits). The reason for this is that one disconnection of the factored graph (to two components) must arise from edge erasure in accordance with the double bonds of a Kekulé structure of a single branching graph component (whether or not there are other components present). Such a Kekulé structure can always be converted to a diradical with one less double bond. The corresponding polyhex factor will have two branching vertices, and the conjecture is that there will always be a factor of this type that is connected and therefore traceable.

If the 2-factor must have more than two components, then it may be the case that more than one component of the branching graph causes disconnection in the 2-factor. If this is so, then a modified principal resonance structure that avoids disconnection of the polyhex 2-factor must be more than 2-valent, and it is clear that the polyhex must be untraceable, e.g. (31a and b).

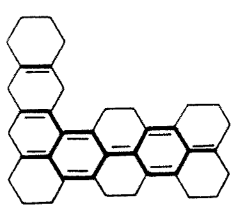


31a

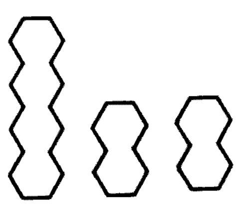


31b

If, however, the multiplicity of 2-factor components arises from a single branching graph component then, it is conjectured, a doubly branched but connected factor can be found, and the polyhex is traceable with no Hamiltonian circuits, e.g. (32a, b and c). This is perhaps the most tentative conclusion in this scheme, and it may prove to be invalid for more complicated systems, but a counter-example has not yet been found.



32a



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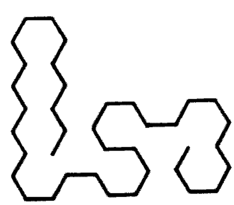
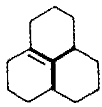
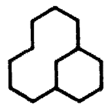


32c

If the branching graph is not 1-factorable but can have a diradical structure, then a factor can be found with just two branching vertices, and by comparison with (6) it can be seen that if this is *connected*, the polyhex is traceable, e.g. (28a, b and c).



28a



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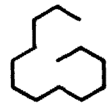
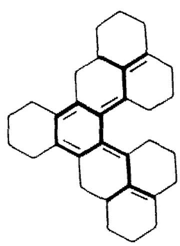
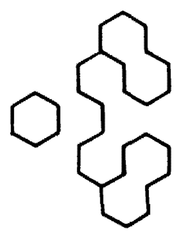


28c

If, on the other hand, it and all possible factors are *disconnected*, then it is conjectured that the polyhex is untraceable, e.g. (33a and b).

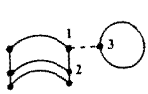


33a



33b

This may be seen by examining (34) as an example; on a graph with two disjoint branching vertices and no leaves, a Hamiltonian path must begin or end on a vertex adjacent to one branching vertex and end or begin on a vertex (labelled 1) that is adjacent to the other branching vertex, 2. To extend the path through another ring, a connection from vertex 3 on the other ring must be to vertex 1. However, if this is so then, in the original graph, 1–2 and 1–3 are two adjacent edges with a vertex in common. Since in a factoring every possible disjoint erasure of such edges is valid, 1–2 rather than 1–3 could be erased, giving (35), which is *connected*. Therefore, if all possible erasures give *disconnection* (or are not maximal), then the branching vertex connecting the cycle must be at some other vertex, 4, more than one edge distant from 2, as shown in (36), and such a graph is immediately seen to be untraceable.



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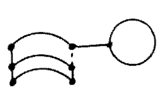

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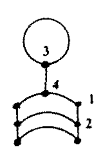

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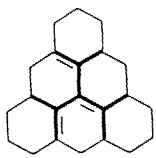
If the branching graph cannot have a principal resonance structure that is less than quadrivalent, then its parent graph cannot be reduced to a graph with less than four disjoint branching vertices (cf. 18), and is not traceable, e.g. (37a and b).



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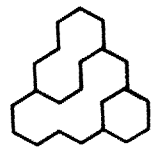


37b

It follows from these remarks, and it can be seen by inspection, that every catacondensed polyhex (one with no internal vertex) has both Hamiltonian paths and a Hamiltonian circuit. Catacondensation of a catacondensed polyhex (P) upon the edge $\upsilon_x - \upsilon_y$ of another graph (G) merely extends the path section $\upsilon_x - \upsilon_y$ to include the periphery of P, and does not change the traceability of G. So every polyhex with just one internal vertex, which is a catacondensation product of the 3-ring system (28), is traceable, but has no Hamiltonian circuit.

3.5. THE INCIDENCE OF TRACEABILITY AMONG POLYHEXES

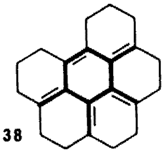
In addition to some trial and error work, a list of known polyhexes [34] with up to eight hexagons was used for some preliminary testing of the method. They were examined with the aid of a simple computer program and by visual inspection. The results are summarised in table 1.

Referring to the 81 six-hexagon systems [34] in more detail, the 36 catacondensed members (not shown) together with one other (38) form a group whose branching graphs all have Kekulé structures that do not lead to disconnection of the parent polyhex, and so all are (path- and circuit-) Hamiltonian.

Seven members (25 and 39–44) also have branching graphs with Kekulé structures, but in this case application to bond erasure always causes disconnection of the parent graph. The polyhexes therefore have multi-component 2-factors, but in every case they arise from one branching graph component, and they are path-Hamiltonian but not circuit-Hamiltonian.

There are 24 polyhexes (not shown) with one internal vertex. These have no Hamiltonian circuits, but are traceable. Another group of eleven (45–55) are more complicated, but they too have branching graphs whose principal resonance structures are diradicals that do not involve disconnection, and are therefore traceable.

Finally, there are two polyhexes (37 and 56) that, because their branching graphs have quadrivalent principal resonance structures, are untraceable. Examples of untraceability arising from disconnection, such as (31) and (34) mentioned in section 3.4, are encountered only in larger systems.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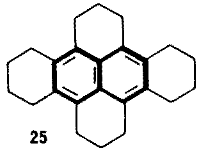
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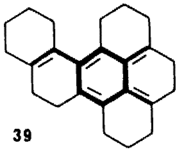
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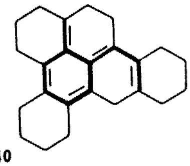
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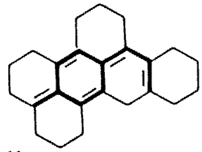
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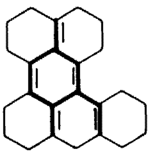
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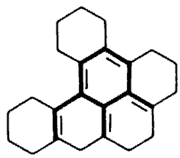
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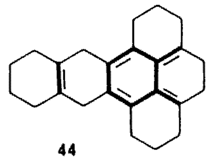
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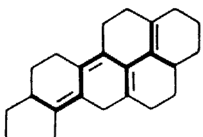
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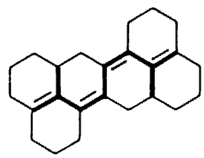
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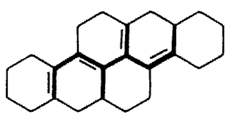
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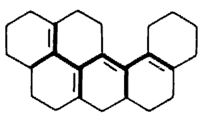
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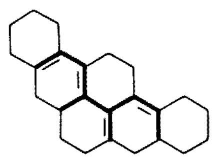
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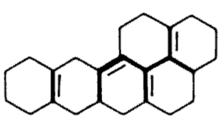
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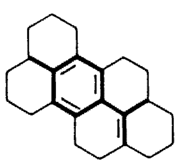
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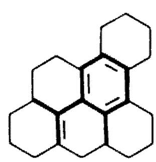
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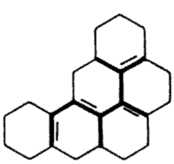
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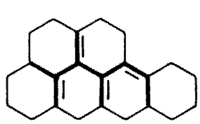
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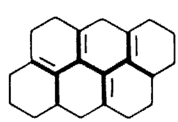
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Table 1

Analysis of polyhexes with up to eight hexagons

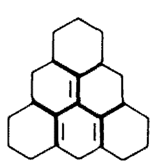
Number of hexagons:	2	3		4			5				6				
Number of internal vertices:	0	0	1	0	1	2	0	1	2	3	0	1	2	3	4
Number of structures:	1	2	1	5	1	1	12	6	3	1	36	24	14	4	3
$\upsilon = 0$:*	1	2		5			12		2		36		7		1
$\upsilon = 2$ (a):			1		1	1		6	1	1		24	6	4	1
$\upsilon = 2$ (b):															
$\upsilon = 4$:													1		1
Total untraceable:	0	0		0			0				2				
Total polyhexes:	1	3		7			22				81				
Number of hexagons:	7							8							
Number of internal vertices:	0	1	2	3	4	5	6	0	1	2	3	4	5	6	7
Number of structures:	118	106	68	25	10	3	1	411	453	329	144	67	21	9	1
$\upsilon = 0$:	118		39		4			411		175		25		5	
$\upsilon = 2$ (a):		106	21	24	5	3	1		453	99	127	32	20	3	1
$\upsilon = 2$ (b):										1	6	10	1		
$\upsilon = 4$:			8	1	1					54	11			1	
Total untraceable:	10							85							
Total polyhexes:	331							1435							

* $\upsilon = 0$: Each branching graph has a Kekulé structure; polyhexes with no internal vertices (catacondensed) were counted from the published list [34] without further examination. Every parent polyhex is traceable.

$\upsilon = 2$ (a): The branching graph has a divalent principal resonance structure, and application of this to the polyhex (see text) gave a connected graph with two disjoint branching vertices. Those polyhexes with one internal vertex were counted from the published list [34]. All are traceable.

$\upsilon = 2$ (b): The polyhex has the same kind of branching graph as above, but one that yielded a disconnected graph, so that this class is untraceable.

$\upsilon = 4$: The branching graph has a quadrivalent principal resonance structure, and the parent polyhexes are untraceable.



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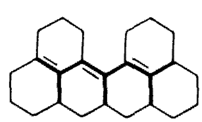

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Hence, it can be seen that the vast majority of polyhexes are traceable, including all those with five or fewer hexagons. This finding is in accordance with Mallion's observation, based on trial and error work [9], that conjugated systems that are not semi-

Hamiltonian seem to be rather uncommon. Within the range tested, the proportion of untraceable polyhexes increases with the number of hexagons (see table 1), and rises from 2.5% (six hexagons) to 5.9% of total numbers for eight hexagons, but it remains much smaller than the proportion lacking Kekulé structures, 2-factors or Hamiltonian 2-factors [50]. Few other statistics are available, but one study [51,52] showed that what might be called "near-Hamiltonian" paths and circuits on large polyhexes increase exponentially in number with size.

3.6. THE CONSTUCTION OF UNTRACEABLE POLYHEXES

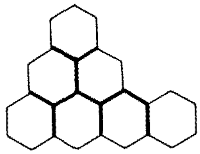
If one has the full set of polyhexes available, then each can be examined and those few that are untraceable picked out. However, how does one enumerate or count them directly? In general, this is done by constructing every possible branching graph whose minimally-valent principal resonance structures (the minimum valency that avoids disconnection of the polyhex when applied as described) is more than 2-valent.

A recursive construction process is easy in principle although very tedious in practice; each known untraceable polyhex is extended by one ring while preserving the branching graph type. It is easily seen how six (57–62) of the ten untraceable 7-ring polyhexes (57–66) can be derived in this way from the two 6-ring untraceable polyhexes (37) and (56). This is equivalent to expanding the branching graph by two edges. A second stage is to expand the branching graph in as many ways as possible by splitting it along one edge, duplicating that edge, and then setting the fragments into as many valid singly bridged or disconnected configurations as possible. This amounts to the insertion of polyhex systems between smaller polyhexes that are traceable but have no Hamiltonian circuit. For the 7-ring polyhexes, this gives (63–66).

Thus, the generation of a large selection of untraceable polyhexes is straightforward, but full counting or enumeration soon becomes unwieldy because of the variety of possible structures that must be considered. It is therefore not recommended for this latter purpose, it being safer to rely upon the testing of previously enumerated polyhexes insofar as they are available.

4. Concluding remarks

In this paper, the detection of, and to a lesser extent the enumeration of, Hamiltonian paths and circuits in polyhexes has been considered. No attempt was made to "solve" the general Hamiltonian problem in the formal sense of finding necessary and sufficient conditions [20]. Rather, the standpoint taken was that of the chemist armed with pencil and paper (and possibly a small computer), faced with an arbitrary polyhex structure; how is one to set about establishing whether the structure is traceable and, if it is, what paths there are? In fact, because most polyhexes *are* traceable, the first question is better posed in the negative: how does one establish that a given graph is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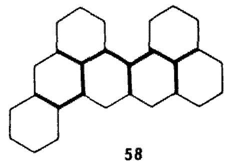
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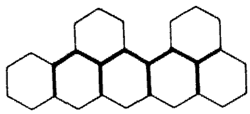
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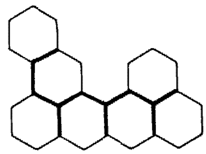
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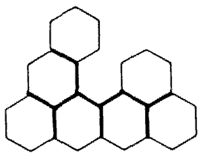
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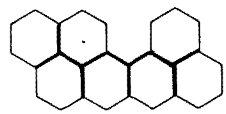
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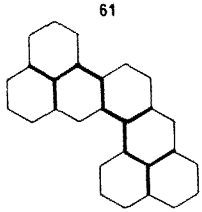
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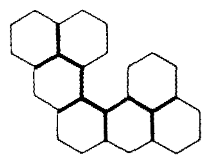
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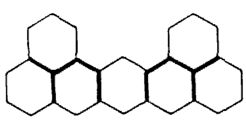
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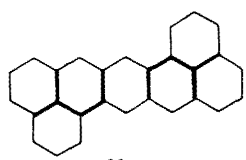
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untraceable? Verification of such a negative by inspection can be surprisingly laborious and error-prone, even for systems of moderate size.

With this in mind, a special subgraph has been introduced and used in conjunction with its principal resonance structure(s) as an exploratory device. Its properties – some obvious and easily demonstrated, and some conjectured – enable one (often immediately, sometimes after further tests) to establish traceability. The device can also be used as a guide for Hamiltonian path enumeration when the structure is traceable, because different resonance structures of this special subgraph reveal different paths.

Whether, overall, this scheme does save labour in answering such questions when compared with trial and error methods or computer searches, is to some extent a matter of judgement and experience.

Appendix

Glossary of graph theory terms used

See also refs. [53,54].

Chain: a structure consisting of a connected sequence of unbranched vertices.

Circuit: a (closed) walk visiting the sequence of N vertices $v_0, v_1, \ldots, v_N$ which are all distinct except that v_0 coincides with v_N.

1-factor: an independent set of edges which includes every vertex; a spanning subgraph where all vertices are 1-valent (equivalent to the set of "double" bonds of a Kekulé structure).

2-factor: a spanning subgraph where all the vertices are 2-valent; it consists of a ring or rings.

Hamiltonian circuit or path: a circuit or path including all the vertices of the graph; in the case of a circuit, it is a spanning 2-factor.

Leaf: a terminal vertex, of valency 1.

Path: a walk traversing distinct edges and vertices.

Walk: a sequence of edges connecting vertices v_0v_1, v_1v_2, $v_2v_3, \ldots$.

Practical methods

The method described is quite straightforward to apply by hand, but some computer assistance can be useful. A polyhex can easily be coded for computer manipulation. A convenient method is to superimpose it (in an arbitrary orientation) upon a triangular hexagon grid, read off coordinates for each hexagon, and allow a program to use this information to number the vertices and construct a connection table. A simple extension of this program then creates a connection table for the branching graph of the given polyhex.

A semi-random search method for finding principal resonance structures from an adjacency matrix was developed earlier [45]. This bears a partial resemblance to human trial and error methods, and is a useful technique to apply. What is first required here is to know whether there is at least one principal resonance structure of valency zero, two, or more. This is soon determined by allowing the program to automatically test the structure a number of times for each valency (50 is ample for the modestly sized systems mentioned here). The program terminates as soon as a principal resonance structure is found, and its valency is reported. If this is greater than two, then the test is complete, for the polyhex is untraceable. Otherwise, further tests must be conducted along the lines indicated in section 3.4.

The checks on disconnection were performed here by observation, but could be programmed. The fact that branching graphs frequently have several terminal vertices means that the number of principal resonance structures to be checked is not always as large as might be feared.

Acknowledgements

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