Note

ON THE CLASSIFICATION OF POLYHEXES*

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Abstract

An improved classification of polyhexes, a family of important chemical graphs, is proposed. This classification follows the hierarchy of criteria related to the graph-theoretical properties of polyhexes.

1. Introduction

A polyhex is one of the most important graphs in (organic) chemistry [1]. This is so because the carbon skeletons of polycyclic hydrocarbons, made up of fused benzene rings, may most conveniently be depicted by polyhexes [2]. The members of this particular family of polycyclic hydrocarbons are named polyhex hydro-carbons [2,3]. It is well-documented that the polyhex hydrocarbons are ubiquituous chemicals which sometimes cause a variety of harmful effects on the environment, plant and animal life, and people (e.g. [4-15]).

Since polyhexes represent significant elements of the symbolic language by which chemists communicate [16,17] and in the light of the recent developments in the theory of polyhexes and polyhex hydrocarbons [14,15,18-23], we decided to present an improved classification scheme for polyhexes. There are also available in the literature other classifications for both polyhex hydrocarbons and polyhexes (e.g. [14,15,18-24]).

2. Definitions

In this section, we will furnish the necessary (chemical) graph-theoretical definitions which represent the basis of our classification scheme. They will be given rather succinctly. For more details other sources, which are abundant indeed, should be consulted [1-3,14,18-33].

*The final version of this work was prepared whilst the author was in an air-raid shelter when the old part of air-raid defenceless Zagreb, the capital of Croatia, was bombed by Serbian fascists.

Hex	:	a single regular hexagon.
Polyhex	:	a network of regular hexagons such that any two hexagons have exactly one common edge or are disjoint.
Planar polyhex	:	a polyhex which can be embedded in the plane.
Non-planar polyhex	:	a polyhex which cannot be embedded in the plane.
1-factorization	:	a process of decomposing a polyhex into 1-factors.
1-factor	:	a set of disconnected edges into which a polyhex may be decomposed. It is isomorphic to the set of "double" bonds within a Kekulé structure of a polyhex hydrocarbon.
Hole	:	a finite region of a size greater than a hexagon.
Simply-connected polyhex	:	a polyhex without holes.
Multiply-connected polyhex	:	a polyhex with holes.
Kekuléan polyhex	:	a polyhex which is 1-factorable.
Non-Kekuléan polyhex	:	a polyhex which is non-1-factorable.
Benzenoid	:	a planar 1-factorable simply-connected polyhex.
Coronoid	:	a planar 1-factorable multiply-connected polyhex.
Coronahex	:	a planar non-1-factorable multiply-connected polyhex.
Helicene	:	a non-planar 1-factorable polyhex.
Quasi-coronoid	:	a coronoid containing non-planar part(s).
Quasi-coronahex	:	a coronahex containing non-planar part(s).
Inner vertex	:	a vertex shared by three hexagons.
Cata-polyhex	:	a polyhex which does not contain inner vertices.
Peri-polyhex	:	a polyhex containing inner vertices.
Unbranched polyhex	:	a polyhex without side chains of hexagons.
Branched polyhex	:	a polyhex with side chains of hexagons.

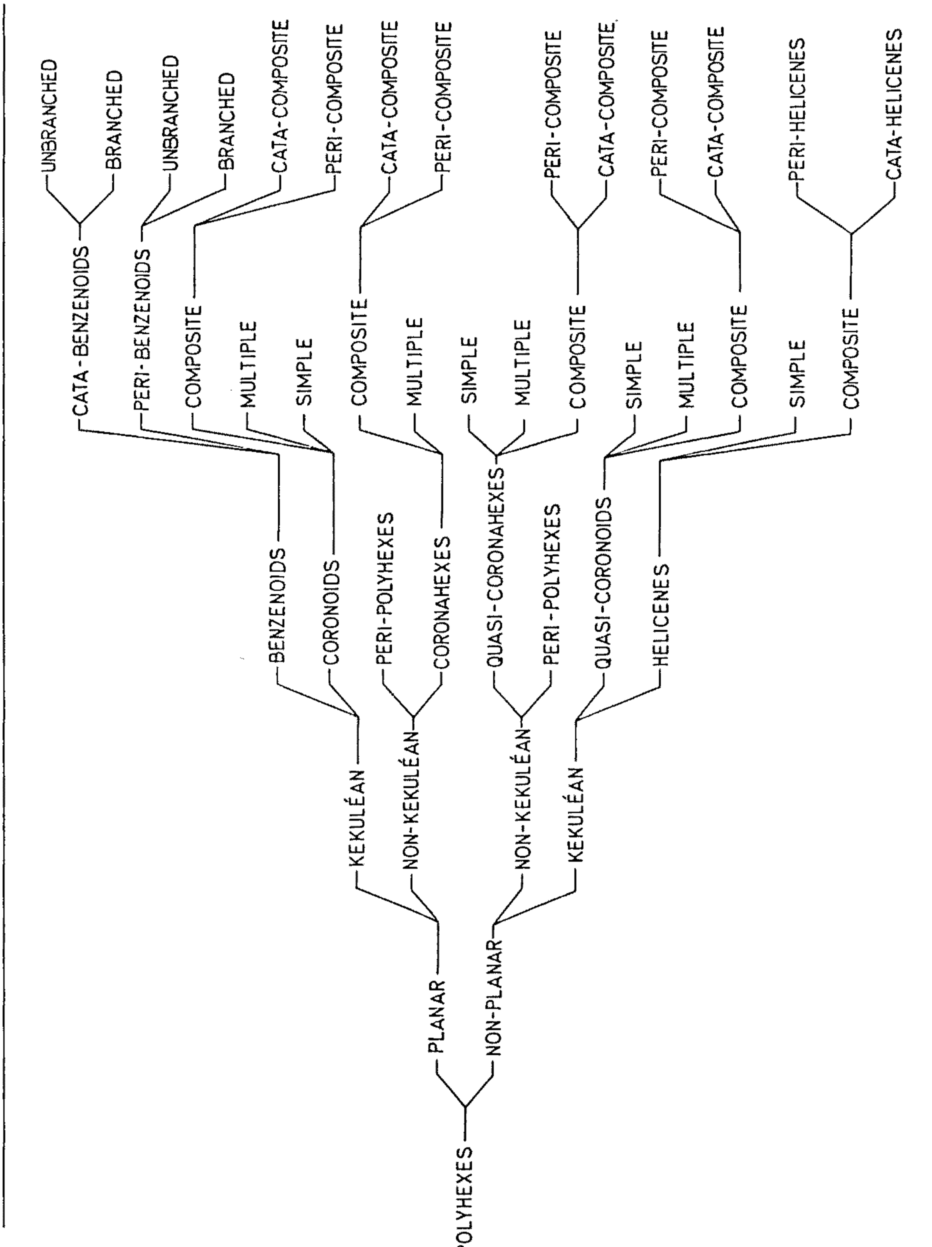
3. The classification scheme for polyhexes

Our classification scheme for polyhexes is given in table 1. This classification follows the hierarchy of criteria related to the graph-theoretical properties of polyhexes.

(1) The first criterion for the classification is the *planarity* of polyhexes. Polyhexes may be planar or non-planar, depending on whether they can or cannot be embedded in the plane. Hence, there are two classes of polyhexes according to the planarity criterion: planar polyhexes and non-planar polyhexes. In this note, we will consider only finite polyhexes. Infinite polyhexes may be classified much as finite polyhexes (e.g. [34]). Similarly, we will not consider classes of exotic polyhexes such as toroidal polyhexes [35,36] and fractal polyhexes [37].

Table 1

The classification scheme for polyhexes.



(2) The second criterion for the classification is the *1-factorization* of (planar and non-planar) polyhexes. Polyhexes may or may not be 1-factorable. Hence, there are two classes of planar polyhexes and two classes of non-planar polyhexes according to this criterion: Kekuléan (planar, non-planar) polyhexes and non-Kekuléan (planar, non-planar) polyhexes. It should be pointed out that it is not always possible to decide by a simple inspection whether a polyhex is Kekuléan or non-Kekuléan, especially in the case of large structures. However, there are many methods now available, some of which with a little practice can give the answer reasonably quickly even for very large polyhexes (e.g. [19,32,33]).

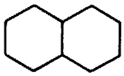
(3) The third criterion for the classification is the *simply-connectedness* of polyhexes. This criterion splits each group of Kekuléan polyhexes and non-Kekuléan polyhexes into simply-connected polyhexes and multiply-connected polyhexes, i.e. polyhexes with holes (coronoids, coronahexes, quasi-coronoids, quasi-coronahexes).

(4) The fourth criterion is the *cata–peri distinction* of polyhexes. This criterion partitions polyhexes into cata-condensed systems (cata-polyhexes) and peri-condensed systems (peri-polyhexes). Hence, for example there are two classes of benzenoids: cata-benzenoids and peri-benzenoids. It should be noted that non-Kekuléan (planar, non-planar) cata-polyhexes cannot exist and for this reason, we find in the scheme slots with only non-Kekuléan (planar, non-planar) peri-polyhexes.

(5) The fifth criterion used here is *branching*. Every class of (planar, non-planar, Kekuléan, non-Kekuléan) polyhexes may be separated into unbranched and branched structures.

Some additional explanations concerning the scheme in table 1 are perhaps needed. In our classification scheme, only planar Kekuléan simply-connected polyhexes are called benzenoids. There are some arguments against narrowing the term "benzenoid" to only the above class of polyhexes (e.g. [23]). The argument by Brunvoll et al. [23] is based, amongst other points, on the premise that the benzenoids should be immediately recognizable by sight. Another argument is that the definition of benzenoids which includes non-Kekuléan systems has been established "through long tradition". However, our definition is based on the premise that the term "benzenoid" is derived from the term "benzene". Therefore, the class of benzenoids should be identified by characteristic features that they carry over from benzene. These are in the first place the possession of the Kekulé structures and then the aromatic stability up to a certain degree. Neither of these two properties are present in the planar non-Kekuléan simply-connected polyhexes (peri-polyhexes in our scheme). In fact, Clar et al. [38] postulated that peri-polyhex hydrocarbons (non-Kekuléan peri-condensed polyhex hydrocarbons) cannot be isolated because of the instability due to their non-Kekuléan character.

Our proposal is also based on the premise that the polyhex can be immediately recognized by sight, and then by very little effort correctly classified into one of the classes given in the scheme.



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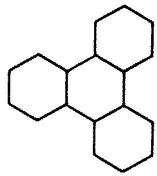

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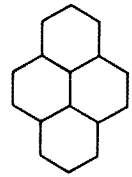

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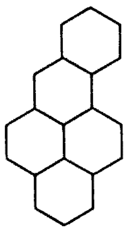

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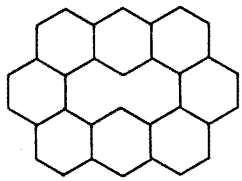

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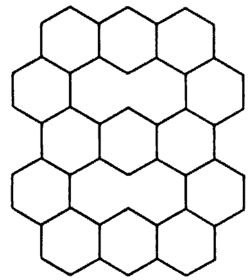

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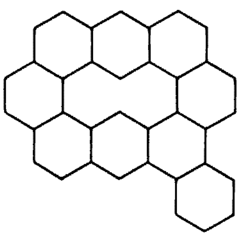

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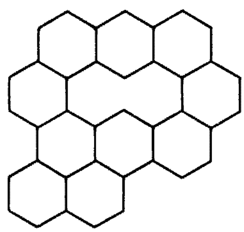

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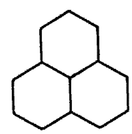

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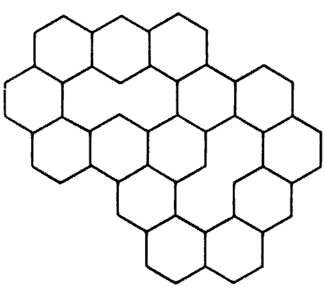

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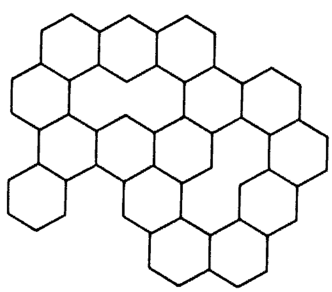

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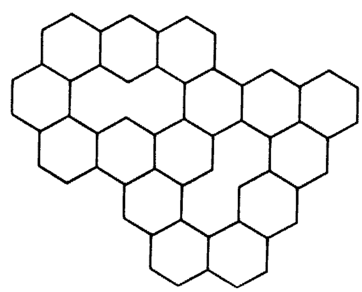

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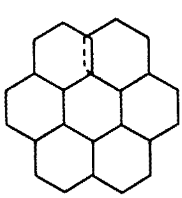

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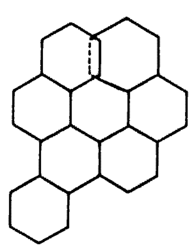

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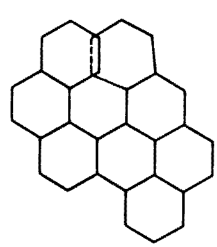

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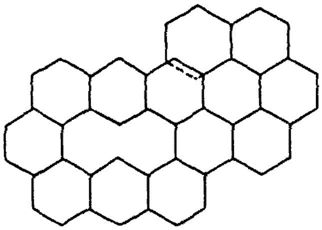
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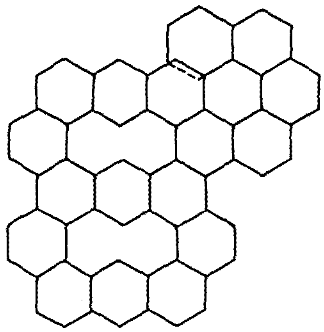
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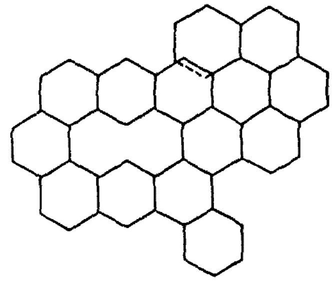
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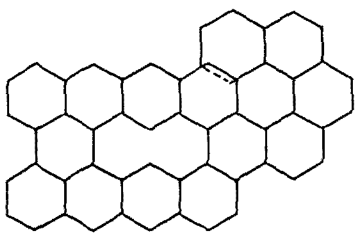
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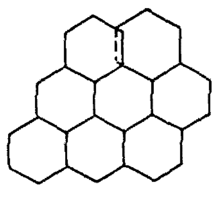
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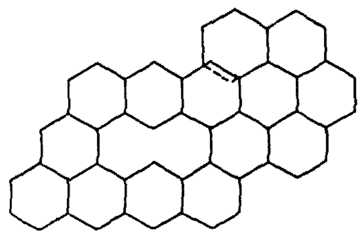
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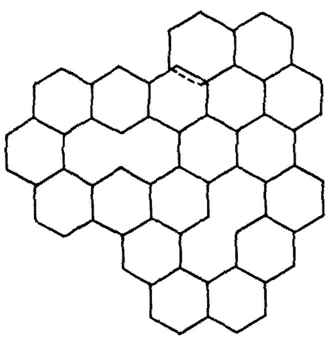
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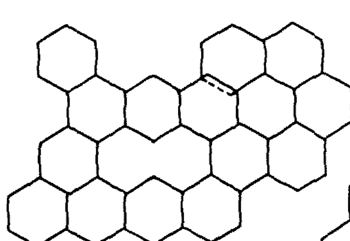
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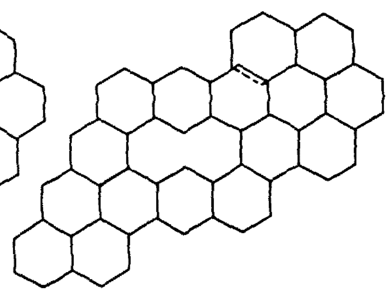
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Fig. 1. The smallest representatives of each class of polyhexes. They are given in the following order: unbranched (**1**) and branched (**2**) cata-benzenoids; unbranched (**3**) and branched (**4**) peri-benzenoids; simple (**5**), multiple (**6**), cata-composite (**7**) and peri-composite (**8**) coronoids; planar peri-polyhex (**9**), multiple (**10**), cata-composite (**11**) and peri-composite (**12**) coronahexes; simple helicene (**13**), cata-helicene (**14**), peri-helicene (**15**), simple (**16**, multiple (**17**), cata-composite (**18**) and peri-composite (**19**) quasi-coronoids; non-planar peri-polyhex (**20**), simple (**21**), multiple (**22**), cata-composite (**23**) and peri-composite (**24**) quasi-coronahexes.

Similarly, we have reserved the term "coronoid" for planar Kekuléan multi-connected polyhexes only. This class of coronoids may be partitioned into simple coronoids (called by Cyvin et al. [22] single coronoids), multiple coronoids and composite coronoids. Simple coronoids are polyhexes containing a single hole, whilst multiple coronoids contain two or more holes. Composite coronoids (earlier named complex coronoids [3,39]) contain one or more holes and cata- or peri-connected branches. Thus, the group of composite coronoids may further be divided into two subgroups: cata-composite coronoids and peri-composite coronoids.

The class of planar non-Kekuléan multiply-connected polyhexes was termed corona-condensed [40] polyhexes or coronahexes. This class was named by Cyvin et al. [22) non-Kekuléan coronoids. Arguments in favour of our proposal are much the same as before in the case of benzenoids and peri-polyhexes. This class of coronahexes may be split into two groups: multiple coronahexes and composite coronahexes. We should note that simple coronahexes are not possible because simple planar multiply-connected polyhexes necessarily possess Kekulé structures [19] and thus can belong only to a group of simple coronoids. Multiple coronahexes may be divided, in analogy with multiple coronoids, into cata-composite coronahexes and peri-composite coronahexes.

Non-planar coronoids and coronahexes cannot exist, but the related classes of quasi-coronoids and quasi-coronahexes are possible. Quasi-coronoids and quasi-coronahexes contain helicenic parts which are responsible for the non-planarity of these systems. Quasi-coronahexes are identified by Cyvin et al. [22] as non-Kekuléan quasi-coronoids.

In fig. 1, we give as an illustrative example the smallest representative, or one member in the set of smallest representatives, of each class of polyhexes discussed here.

Acknowledgements

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