Journal of Mathematical Chemistry 4(1990)357–375

ON THE CONCEPT OF THE WEIGHTED SPANNING TREE OF DUALIST*

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Abstract

The concepts of dual, inner dual and dualist are reviewed. The application of these concepts to polyhexes is briefly described. The concepts of a spanning tree and a weighted spanning tree of dualist are introduced. The uses of the weighted spanning tree of dualist in coding and enumerating polyhex hydrocarbons are outlined.

1. Introduction

The concept of dualist was introduced in 1968 by Balaban and Harary [1]. The terms they used for dualist were characteristic graph and skeleton. However, Balaban [2] subsequently stated that a more suitable term for the characteristic graph is the dualist graph. Yet, the dualist graph (or the characteristic graph) is not a graph at all [3].

In the initial studies by Balaban and Harary [1] and by Balaban [4], the dualist was used as a basis for a systematic nomenclature of polyhex hydrocarbons and for the enumeration of cata-condensed polyhexes. It is interesting to note that Smith [5], seven years before Balaban and Harary, in his work on capacitive energy and the ionization potentials of benzenoid hydrocarbons very cleverly used dualists as a shorthand notation for these molecules. Apparently, Balaban and Harary were not at the time aware of the work by Smith and did not mention his paper in their contribution.

Since the pioneering work by Balaban and Harary, the concept of dualist was employed in various studies of polyhexes and benzenoids, especially in the last few years (e.g. [6–11]). Recently, this concept was extended to the notion of a weighted spanning tree of dualist and used as a basis for a novel computer-oriented code of polyhex hydrocarbons [12] and for a very fast enumeration of polyhexes [13].

In this article, we wish to review the concept of dualist and its evolution, to give one example of its use in the chemistry of polyhex hydrocarbons, and to present the concept of a weighted spanning tree of dualist. The article is structured as follows. Section 2 contains graph-theoretical concepts that will be used in this paper. The dual

*This article is dedicated to Frank Harary, the grandmaster of graph theory, and to Alexandru T. Balaban, the grandmaster of chemical graph theory.

and inner dual of a polyhex are presented in section 2, while the dualist of a polyhex is discussed in section 4. In section 5, the weighted spanning tree of dualist is described. Certain uses of this concept are given in section 6. The paper ends with concluding remarks.

2. Graph-theoretical concepts

In this paper, we will consider planar hexagonal hydrocarbon structures. These will be depicted graph-theoretically by a special kind of hydrogen-suppressed molecular graphs [14,15]. The carbon skeleton of benzene is represented by a regular hexagon. A single hexagon is called by Balaban [16] a hex; hence, a connected set of h hexagons is called a polyhex (denoted by P). Polyhexes are thus graphs which may be obtained by any combination of regular hexagons such that two hexagons have exactly one common edge or are disjoint [17]. Here, we are interested in planar polyhexes. A polyhex is planar if, and only if, it can be embedded in the plane. We will adopt the term polyhex hydrocarbons for hydrocarbons whose carbon skeletons can be depicted by polyhexes.

The two most studied kinds of polyhexes are cata-condensed polyhexes (cata-polyhexes, cata-hexes) and peri-condensed polyhexes (peri-polyhexes, peri-hexes). One way to distinguish them is as follows. A polyhex embedded in a plane divides it into one infinite region and a number of finite regions [8]. All vertices and edges of a polyhex which lie on the boundary of the infinite region form the perimeter of a polyhex. The internal (inner) vertices are those which do not belong to the perimeter. Cata-polyhexes do not contain internal vertices. Strict peri-polyhexes contain internal vertices which are all of the same degree, that is, 3. If internal vertices of degree 2 appear, then a given polyhex contains a hole. A hole in a polyhex is simply an n-membered ring, with $n \geq 8$. Planar polyhexes with holes have various names in the literature [19–21] such as, for example, corona-condensed polyhexes or coronoids [22].

An important subset of the polyhex family are benzenoid graphs [15]. A polyhex is a benzenoid graph if, and only if, it is a 1-factorable graph [17]. A benzenoid graph B is the graph-theoretical representation of the carbon skeleton of a benzenoid hydrocarbon. 1-factorization signifies that the benzenoid hydrocarbon in question possesses Kekulé structure(s) [23] because only such polyhex hydrocarbons are expected to show similarity in their chemical behaviour with benzene. For example, polyhex hydrocarbons without Kekulé structures are extremely unstable [24]. Thus, according to the above terminology, there are twenty-two members of the penta-hex hydrocarbon family and among them, fifteen benzenoid hydrocarbons.

A subgraph G' of a graph G is a graph for which all vertices and edges are contained in G [25]. Informally, a subgraph is any graph G' derived from G by deleting any number of vertices or edges, or both. We should note that a graph can be its own subgraph. A spanning subgraph is any subgraph G' of G containing all vertices of G. A spanning tree of G is an acyclic subgraph containing all vertices of G.

A path is a finite sequence of edges $e_1, e_2, \ldots, e_N$, where $e_i = (v_{i-1}, v_i)$, $i = 1, 2, \ldots, N$; that is, the terminal vertex v_i of e_i is the initial vertex of e_{i+1}. A graph G is a connected graph if there is at least one path between any two of its vertices. Otherwise, a graph G is considered disconnected. A cutset of a connected graph G is a collection of edges whose removal disconnects G and consequently produces a disconnected graph.

3. The dual and inner dual of a polyhex

Given a planar polyhex $P = P(V, E)$, its dual $P^* = P^*(V^*, E^*)$ can be constructed as follows [25–28]: Place one vertex in the center of each region of P and one vertex on the plane outside the perimeter of P and, if two regions have an edge e in common, join the corresponding vertices by an e^* crossing only e. As an example, in fig. 1 we show the construction of the dual for bihex (naphthalene graph). The number of vertices

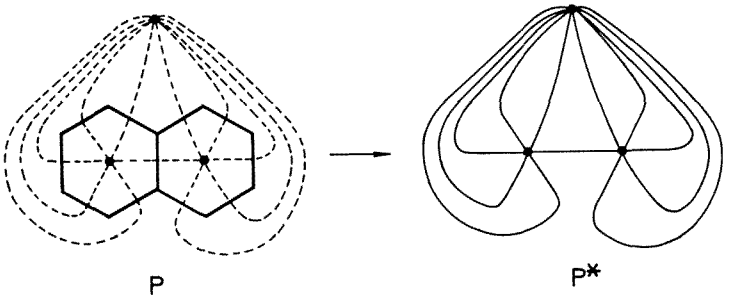


Fig. 1. The construction of the dual for the naphthalene graph.

in P^* is given by $V^* = h + 1$, where h is the number of finite regions in P, and the number of edges in P^* is equal to the number of edges in P, i.e. $E^* = E$. The above dual is also called the complete or geometric dual [7,25]. The complete dual of a planar polyhex is also a planar graph. It should be noted that the dual of the dual of P is a graph isomorphic to the original polyhex.

An abstract formulation of the geometric dual is a combinatorial definition of dual [25]. A graph P^* is a combinatorial dual of P if there is a one-to-one correspondence between their sets of edges such that a set of edges of P forms a cycle in P if and only if the corresponding set of edges of P^* forms a cutset in P^*.

The concept of dual has found application in the characterization of planar graphs. A connection between planarity of a polyhex (graph) and its combinatorial dual, which is known as the Whitney theorem [29], may be formulated as: A polyhex (graph) is planar if and only if it has a combinatorial dual.

The inner dual [30] (sometimes also called bual) is a special subgraph of the dual, because it does not contain the vertex corresponding to the infinite part of a plane. It is also a much simpler graph than the dual. The inner dual of a polyhex $\mathcal{P}^* = \mathcal{P}^*(\mathcal{V}^*, \mathcal{E}^*)$

can be obtained by connecting the centers of individual hexagons through the edge that is common to two rings [3,15]. The number of vertices in $\mathcal{P}^*$ is equal to the number of hexagons h in P, i.e. $\mathcal{V}^* = h$, while the number of edges in $\mathcal{P}^*$ is equal to the number of adjacent hexagons (the number of internal edges [31]) in P, i.e. $\mathcal{E}^* = h - 1 + v_i$, where v_i is the number of internal vertices. As examples, in fig. 2 we give the inner duals of

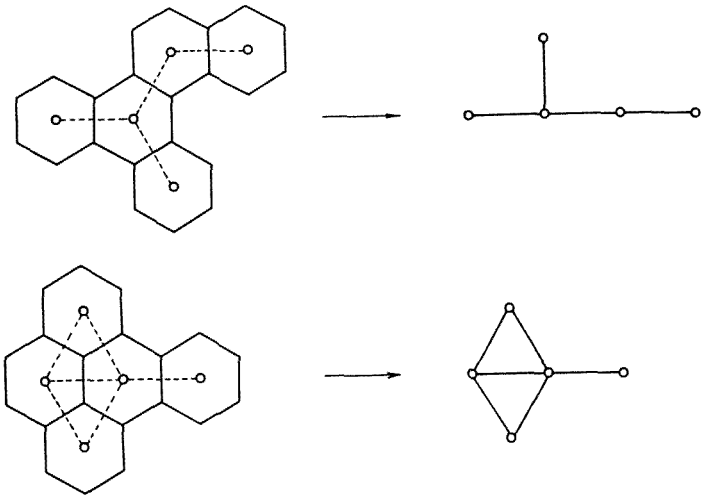


Fig. 2. The inner duals of the benzo[g]chrysene graph and the benzo[e]pyrene graph.

one cata-condensed penta-hex (benzo[g]chrysene graph) and one peri-condensed pentahex (benzo[e]pyrene graph). (The nomenclature system used for naming polyhex hydrocarbons is taken from Dias [32].)

In the case of cata-polyhexes, the corresponding inner dual always has the form of a tree, while in the case of peri-polyhexes, it contains cycles. This property of inner duals was used by Balaban and Harary [1] for differentiation between cata- and peri-condensed polyhex hydrocarbons. The other, less pleasing, property of inner duals – their non-uniqueness, i.e. that two or more polyhexes may possess the same inner dual, led Balaban and Harary to the concept of dualist.

The inner duals have found limited use in chemical graph theory, but one example of their use in chemistry is very elegant. The inner dual of P may be used for counting the spanning trees of a (labelled) polyhex [7,11]. The number of spanning trees in general graphs follows from the matrix-tree theorem [33,34]. In a (labelled) planar polycyclic graph, the problem can be approached via the generalised [35] characteristic polynomial of the corresponding inner dual [7]. The number of spanning trees is of interest in calculations of ring current magnetic properties of polycyclic π-systems [36–38].

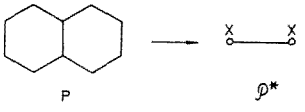
Let us consider an inner dual $\mathcal{P}^*$ of a polyhex P and its characteristic polynomial $\varphi(\mathcal{P}^*, x)$ defined as [7]:

$$\varphi(\mathcal{P}^*; x) = \det |\boldsymbol{D}^* - \boldsymbol{A}^*|, \tag{1}$$

where $\boldsymbol{A}^*$ is the adjacency matrix of $\mathcal{P}^*$ and $\boldsymbol{D}^*$ is a diagonal matrix with elements $d^*(k)$, $k = 1, 2, \ldots, h$, where $d^*(k)$ is the number of edges in the boundary of the ring k of P that is in a 1:1 correspondence with vertex k of $\mathcal{P}^*$. To obtain the count of spanning trees $t(P)$ of a polyhex, one inserts 6 for x in $\varphi(\mathcal{P}^*; x)$. The above procedure is illustrated for the naphthalene graph in table 1. If the azulene graph is, for example,

Table 1

The count of spanning trees for the naphthalene graph



$$\varphi(\mathcal{P}^*; x) = \begin{vmatrix} x & -1 \\ -1 & x \end{vmatrix} = x^2 - 1$$

$$t(P) = \varphi(\mathcal{P}^*; x = 6) = 35$$

considered instead of the naphthalene graph, then the polynomial has the following form: $\varphi(G^*; x, y) = xy - 1$, and the spanning tree count is given by: $t(G) = \varphi(G^*; x = 7, y = 5) = 34$.

4. The dualist of a polyhex

We have already mentioned that two or more isomeric polyhexes possess the same inner dual. For example, all four cata-condensed unbranched tetra-hexes have the same inner dual (see fig. 3). Balaban and Harary [1] introduced the concept of dualist in order to accommodate the structural differences between isomeric polyhexes with the isomorphic inner duals. The dualist $\mathcal{D}^*$ of a polyhex P can be simply constructed by placing a vertex in the center of each hexagon of P and then connecting those vertices which are in adjacent fused hexagons. To this point, the construction of the inner dual and dualist is identical. However, the dualist, unlike the inner dual, preserves the geometric information on the direction of ring annelation in P. The dualists corresponding to cata-condensed unbranched tetra-hexes are also given in fig. 3.

A dualist is not a graph in the strict graph-theoretical sense, that is, a set of vertices and a set of edges, because in the case of dualist, angles are also important. Therefore, we can define dualist as [39] $\mathcal{D}^* = \mathcal{D}^*(\mathcal{V}^*, \mathcal{E}^*, \theta)$, where the vertex set $\mathcal{V}^*$ is the set $\{h\}$, $\mathcal{E}^*$ is the edge set $\{h - 1 + v_i\}$, and θ is the set of angles between incident edges.

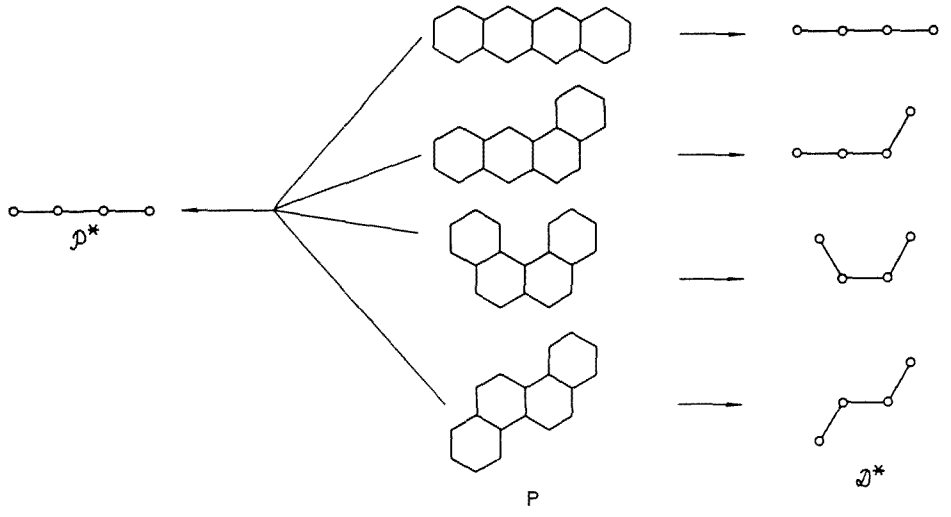


Fig. 3. The inner dual and dualists corresponding to cata-condensed unbranched tetra-hexes.

The dualist is a unique representation of a polyhex. In other words, two or more non-isomorphic polyhexes cannot possess the same dualists. This property of dualists is a basis for their use in the characterization and classification of polyhexes. The dualist has thus become an accepted tool for characterizing polyhexes, for nomenclature and coding purposes, and for the classification of polyhexes [1,2,4,16,40–43]. Planar polyhexes may be classified into the following three classes [43,44]:

(1) cata-hexes (cata-fusenes), when the dualists are trees;

(2) peri-hexes (peri-fusenes), when the dualists contain 3-membered rings;

(3) corona-hexes (corona-fusenes), when the dualists contain larger rings than 3-membered rings.

One example for each of these three classes of planar polyhexes and their dualists is shown in fig. 4.

A number of applications of the concept of dualist are described in the literature. Here, we will present one example: We wish to show that there is a simple connection between the dualist and the number of Kekulé structures and the number of sextets [8] of an unbranched cata-hex. Before we outline this relationship, we need to define the following concepts: The aromatic sextet, Clar's representation of a Kekulé structure of a benzenoid hydrocarbon, the sextet polynomial, and the L–A sequence of an unbranched cata-hex.

An aromatic sextet (abbreviated to sextet) is defined as a set of three double bonds circularly conjugated as in either of the two Kekulé structures of benzene and is represented by a cycle [45]. Two kinds of sextets are distinguished: proper (right) and

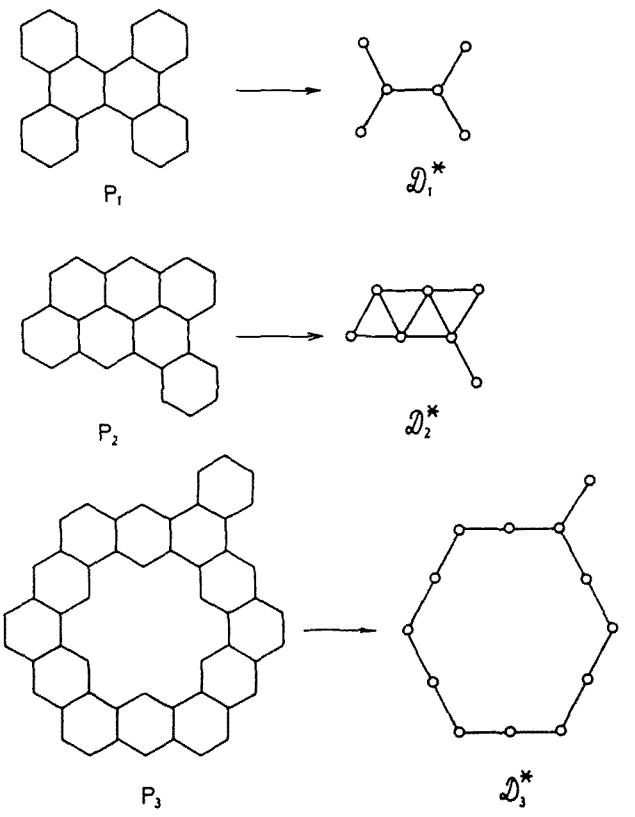


Fig. 4. Examples of cata-hexes (dibenzo[a,c]triphenylene, P_1), peri-hexes (benzo[e]anthanthrene, P_2), and corona-hexes (benzo[a]kekulene, P_3) and the corresponding dualists ($\mathcal{D}_1^*$, $\mathcal{D}_2^*$, $\mathcal{D}_3^*$).

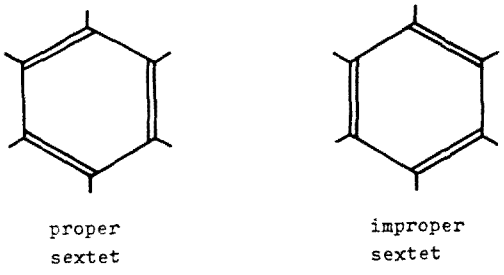


Fig. 5. Proper and improper sextets.

improper (left) sextets [46]. They are depicted in fig. 5. Clar's representation (i.e. the Clar graph [46a]) of a given Kekulé structure is defined as a simultaneous substitution of all proper sextets by cycles and replacement of all double bonds by single

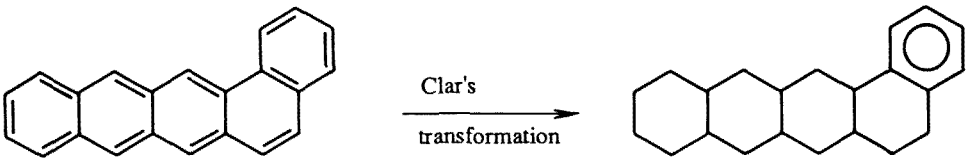


Fig. 6. Clar's representation of a Kekulé structure of benzo[a]tetracene.

bonds (see fig. 6). Two (or more) rings in a benzenoid hydrocarbon are mutually resonant if there exists a Kekulé structure such that all these rings possess an aromatic sextet, provided that no two sextets have common bonds.

The sextet polynomial of a benzenoid graph B, denoted $\beta(B;x)$, is defined as [45]:

$$\beta(B;x) = \sum_{k=0}^{m} r(B;k)x^k, \tag{2}$$

where $r(B;k)$ is the resonant sextet number of B which represents the number of ways in which k disconnected, but mutually resonant, proper sextets can be chosen from B. $r(B;0)$ is defined to be unity for all B, and m is the maximum value of k. The important property of coefficients of the sextet polynomial is as follows:

$$\beta(B;x = 1) = \sum_{k=0}^{m} r(B;k) = K(B), \tag{3}$$

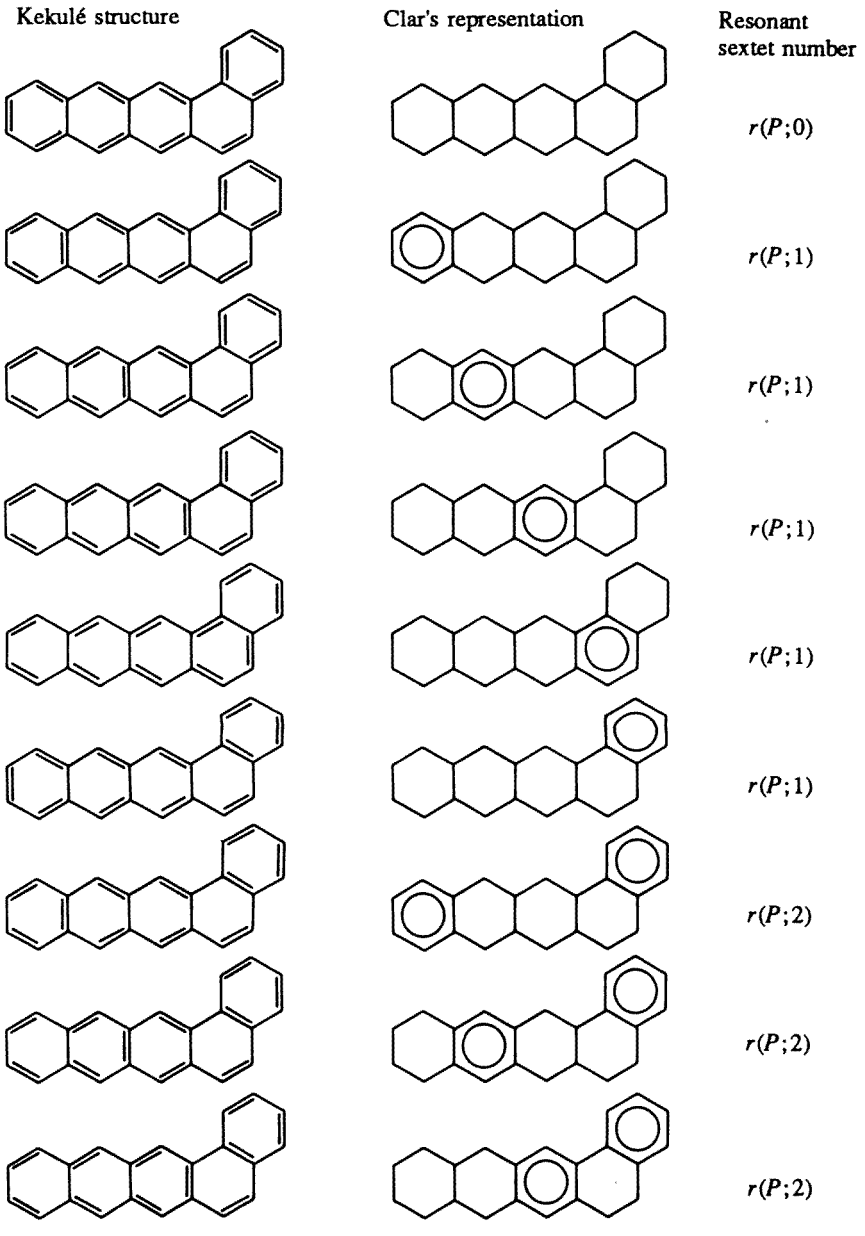
where $K(B)$ is the number of Kekulé structures of cata-fused benzenoids and thin peri-fused benzenoids. Thin peri-fused benzenoids are defined as those peri-condensed benzenoid hydrocarbons which do not contain the coronene skeleton as a sub-structure [45,46]. As an example, in fig. 7 we give the construction of the sextet polynomial for benzo[a]tetracene.

The sextet polynomial was introduced as a convenient device for the enumeration of Clar's sextets [47], a concept which originates from the early work of Armit and Robinson [48]. Clar's sextet theory predicts that, of the set of isomeric benzenoid hydrocarbons, the one with the largest number of resonant sextets is the most stable isomer. The experimental evidence supports Clar's theory [32,49].

There are two modes of ring annelation in unbranched cata-hexes, namely, the linear mode, denoted by L, and the angular mode, denoted by A. Every unbranched catahex P containing h hexagons generates an L–A sequence $S(P)$ given by [50]:

$$S(P) = \{s_1\, s_2 \ldots s_{h-1}\, s_h\}, \tag{4}$$

where, by convention:



$$\beta(B;x) = 1 + 5x + 3x^2$$

Fig. 7. The construction of the sextet polynomial for benzo[a]tetracene.

$$s_1 = s_h = \mathrm{L}, \tag{5}$$

$$s_i = \mathrm{A} \text{ or } \mathrm{L}, \qquad 1 < i < h. \tag{6}$$

As an example, the L–A sequence of the benzo[a]tetracene graph and the corresponding dualist are shown in fig. 8.

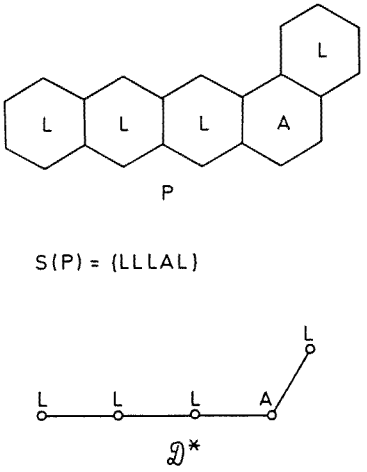


Fig. 8. The L–A sequence of the benzo[a]tetracene graph and the corresponding dualist.

Each L–A sequence may be divided into several subsequences, the fragmentation of the sequence being after each LA pair or before each AL pair (or after each AA pair, if there is a series of more than two A's). The pictorial representations of the subsequences are fragment graphs (subgraphs of dualist) denoted by $f(P)$. The subsequences and corresponding fragment graphs of the benzo[a]tetracene graph are given in fig. 9.

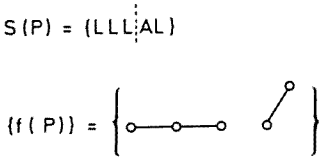
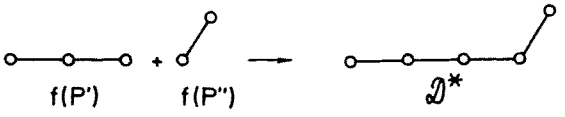


Fig. 9. The subsequences and the corresponding fragment graphs of the benzo[a]tetracene graph.

The most important property of fragment graphs is that each $f(P)$ is related at most to one proper sextet [51]. The vertex in $f(P)$ corresponding to a proper sextet may be coloured black. Thus, vertices in each fragment graph may be coloured either by two

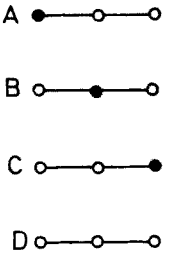
colours, black and white, in such a fashion that at most only one vertex is black, or by one colour, white. This produces $v + 1$ colourings, where v is the number of vertices in $f(P)$. The coloured $f(G)$'s can be re-assembled into their initial dualist such that none of the resulting coloured dualists contain linear segments with more than one vertex in black. The allowed coloured dualists represent the counts of the resonant sextets, and each allowed coloured dualist can be transformed into one Kekulé structure of a benzenoid hydrocarbon.

As an example, we will generate all (coloured) dualists belonging to benzo[a]tetracene by combining the corresponding (coloured) fragment graphs:

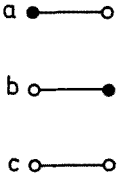


(7)

The fragment graph $f(P')$ gives rise to four coloured graphs:



The fragment graph $f(P'')$ gives rise to three coloured graphs:



The fragments A–D and a–c are combined via (7). In total, there are twelve possible combinations, but all of them are not allowed. These twelve combinations are given in matrix form in table 2. The number of black vertices in coloured dualists is equal to the count of resonant sextets. The quantities in table 2 immediately lead to the sextet polynomial. Each allowed coloured dualist can be easily converted into the corresponding Kekulé structure. In fig. 10, we give as an example the conversion of coloured dualist bC (taken from the matrix in table 2) into the corresponding Kekulé structure of benzo[a]tetracene.

Table 2

The counting matrix for coloured dualists

	A	B	C	D
a	0	0	0	r(P;1)
b	r(P;2)	r(P;2)	r(P;2)	r(P;1)
c	r(P;1)	r(P;1)	r(P;1)	r(P;0)

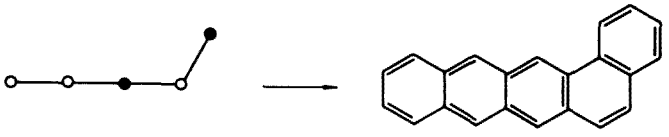


Fig. 10. The conversion of coloured dualist bC into the corresponding Kekulé structure of benzo[a]tetracene.

This approach, which is based on a rather simple combinatorial procedure, may be used to generate resonant sextet numbers of unbranched cata-fusenes according to the following protocol:

(1) represent an unbranched cata-fusene by the corresponding cata-hex;

(2) transform the unbranched cata-hex into the corresponding dualist;

(3) divide the dualist into fragment graphs;

(4) colour each fragment graph;

(5) re-assemble the coloured fragment graph into coloured dualists, retaining the shape of the initial dualist;

(6) evaluate the sextet number for each coloured dualist and construct the sextet polynomial;

(7) transform, if needed, each coloured dualist into the corresponding Kekulé structure of the initial unbranched cata-fusene.

5. The weighted spanning tree of dualist

The concept of the weighted spanning tree of dualist is introduced with the aim of providing a basis for a novel systematic code of polyhex hydrocarbons and for the enumeration of planar polyhexes. In this respect, it represents the natural extension of

the original work of Balaban and Harary [1] on the concept of dualist. The whole idea of introducing the weighted spanning tree of a dualist is akin to the idea of progressing from the concept of the inner dual (a graph-theoretical notion) to the concept of the dualist (a cross-linking of a graph-theoretical notion and a geometric notion).

A spanning tree of the dualist $\mathcal{D}^*$ is an acyclic connected subgraph of $\mathcal{D}^*$ containing all the vertices of the dualist. If the dualist is a tree, then such a dualist is its own spanning tree. If the dualist contains cycles, then such a dualist has several spanning trees. An example of a spanning tree (denoted by T^*) of the dualist corresponding to the tribenzo[a,e,i]phenalene graph is shown in fig. 11. The dualist corresponding to tribenzo[a,e,i]phenalene has three isomorphic spanning trees.

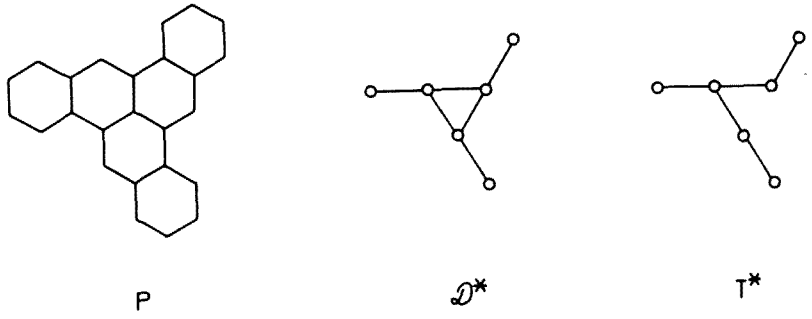


Fig. 11. Polyhex depicting tribenzo[a,e,i]phenalene, the related dualist, and a spanning tree of the dualist.

The weighted spanning tree (denoted by $\mathcal{T}^*$) of the dualist may be introduced in the following way. The weight of each vertex in $\mathcal{T}^*$ contains information about the absence or presence of neighbouring hexagons in specific directions relative to the direction of the starting hexagon. These weights are arbitrary because many different conventions may be chosen. In our work, we selected the following convention for the directions of the adjacent hexagons and their ordering relative to the entrance edge of the starting hexagon: 60° to the left, straightforward, 60° to the right, and a 1–1 mapping of them onto the three numbers: 4, 1 and 2. This is depicted in fig. 12.

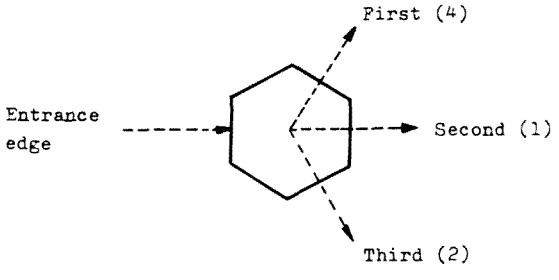


Fig. 12. Ordering of directions and their weights (in parentheses).

This idea was also exploited by Balaban [1,2,4,16,42,43]. However, this particular selection of directions and their weights was the result of our efforts to design a fast procedure for counting polyhexes. This choice led to the fastest counting algorithm that could be related to our earlier procedure based on the boundary code [52].

The step-by-step construction of the weighted spanning tree of the dualist corresponding to tribenzo[a,e,i]phenalene is given in fig. 13. Because of symmetry, the two other possible weighted spanning trees that can be obtained from the dualist correspond-

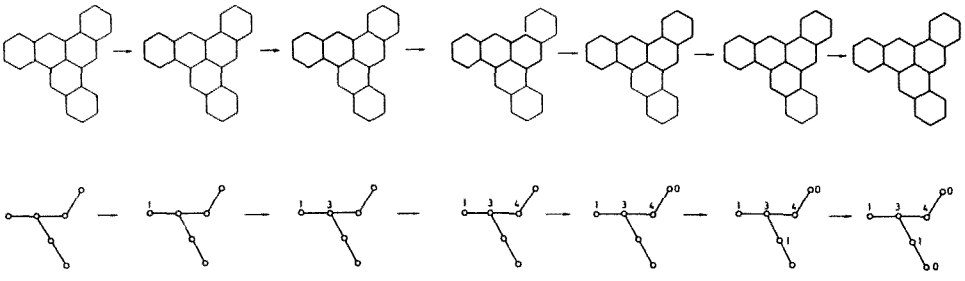


Fig. 13. The construction of the weighted spanning tree of the dualist corresponding to tribenzo[a,e,i]phenalene.

ing to tribenzo[a,e,i]phenalene are isomorphic to the weighted spanning tree in fig. 13. This is not always so. There are cases with the same spanning trees and different weights, and cases with different spanning trees and different weights. In such cases, we have to choose the representative weighted spanning tree according to a certain convention. This is elaborated below.

The weights of a spanning tree are used to build an N-tuple code [53] whose entries are the weights. We named this molecular code the DAST code [12]. DAST is an acronym for the *d*ualist *a*ngle-restricted *s*panning *t*ree. The DAST code for the weighted spanning tree of tribenzo[a,e,i]phenalene and consequently for the tribenzo[a,e,i]phenalene graph is 134010. The selection rule in the case of several DAST codes corresponding to several possible weighted spanning trees for the same polyhex is to choose lexicographically the smallest code.

As an example, let us consider the dibenzo[a,l]pyrene graph. Three orientations of this hexa-hex with the corresponding weighted spanning trees and DAST codes are given in fig. 14. Among the three possibilities, the code 132020 is lexicographically the smallest, and it is thus chosen according to the convention to be the DAST code for the molecule.

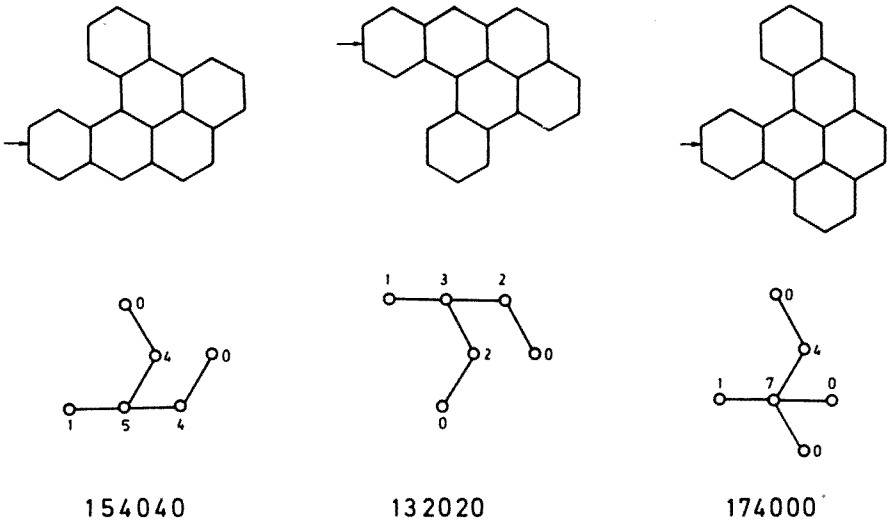


Fig. 14. The selection of the weighted spanning trees for the dibenzo[a,l]pyrene graph. Arrows indicate the starting hexagons.

6. The use of the weighted spanning tree of dualist

The weighted spanning tree of dualist has so far been used for deriving the DAST codes of polyhex hydrocarbons [12] and for a fast enumeration of planar polyhexes [13,54].

In the preceding section, we have shown how the weighted spanning tree and the corresponding DAST code can be generated. The DAST code is the unique polyhex code whose entries are digits from 0 to 7 describing the neighbourhood of each hexagon considered. If there are hexagons in all three directions, then the entry is maximum, i.e. 7. If there are no hexagons in any of the three directions, then the entry is minimum, i.e. 0. This code can never start with zero, except in one case only, that is, in the case of a benzene whose code consists of just a single digit: 0. To guarantee that every hexagon can be reached, the first hexagon of the polyhex to be considered must be a hexagon without neighbours in the "forbidden" directions, i.e. backward 60° to the left and backward 60° to the right. To achieve this, we must start the whole process by entering the first hexagon of the polyhex across an edge of the polyhex boundary between two vertices of valency 2 (then the "forbidden" directions are empty). Such an edge must always exist, since on the periphery of the polyhex there are six more vertices of valency 2 than of valency 3. Since no hexagon can be entered twice, the DAST code contains one digit for every hexagon.

Once the procedure for constructing the DAST code is established, one can directly label each hexagon in a conveniently oriented polyhex with the appropriate entry, which will give rise to the lexicographically smallest code. In fig. 15, we give DAST codes for several polyhexes.

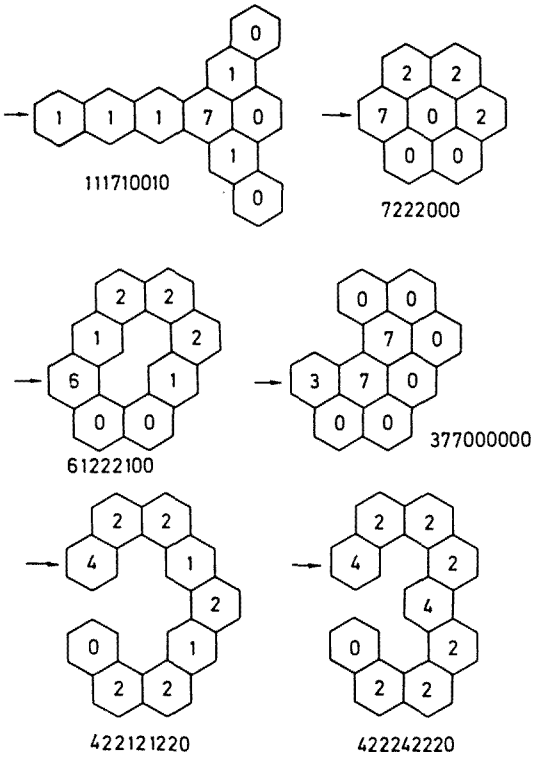


Fig. 15. The DAST code for several planar polyhexes. Arrows indicate the starting hexagons.

One can easily confirm that the selection of a different hexagon as a starting hexagon for each polyhex in fig. 15 in all cases results in lexicographically higher DAST codes, except in the case of coronene, all of whose six hexagons on the periphery are equivalent.

The polyhex is completely reconstructible from the DAST code. For example, the perylene graph may easily be recovered from the DAST code: 30300. However, there may be many possible starting edges, leading to different codes for the same polyhex. To make the code unique and to ease the problem of generating all the unique codes, we allow only those starting edges which, when drawn north to south, are most western, and among the most western, the most northern. This allows twelve cases (six rotational positions of the polyhex and mirroring), from which we choose the lexicographic minimum to be the unique DAST code (with respect to the chosen order and mapping of directions).

On the basis of the DAST code, a computer algorithm for generating and enumerating planar simply-connected polyhexes was developed [13,54]. In table 3, we give the number of planar simply-connected polyhexes with up to fifteen hexagons. The numbers for polyhexes with fourteen and fifteen hexagons are now available for the first

Table 3

The number of planar simply-connected polyhexes

Number of hexagons	Total number of planar simply-connected polyhexes
1	1
2	1
3	3
4	7
5	22
6	81
7	331
8	1435
9	6505
10	30086
11	141229
12	669584
13	3198256
14	15367577
15	74207910

time. For previous computations, the reader is advised to consult the consolidated report by Balaban et al. [55], supplemented by He et al. [56], and some of our earlier reports on the generation and enumeration of polyhexes [44,52,57]. The results in table 3 agree with all previous computations, while the results for polyhexes with thirteen hexagons were obtained only very recently [13,54].

7. Conclusions

The concept of the weighted spanning tree of dualist is introduced. The evolution of this concept starts with dual and passes through several stages. This can be schematized in the following way: dual → inner dual → dualist → spanning tree of dualist → weighted spanning tree of dualist. The starting concept of dual is purely a graph-theoretical notion, while the weighted spanning tree of dualist is an example of a pragmatic concept often encountered when the graph-theoretical ideas merge with ideas from physical or chemical reality. The concept of weight, for example, was introduced into the framework of graph theory to make it more usable in physics and chemistry (e.g. [15,58,59]). The net result of introducing the concept of the weighted spanning tree of dualist is in our case that we found in it a convenient basis for a novel compact code for polyhexes and for a powerful computational algorithm which, for the first time, allowed computer generation and enumeration of planar simply-connected polyhexes with up to fifteen hexagons.

Acknowledgements

This work was supported in part by the German–Yugoslav scientific cooperation program. Financial support from the Internationales Büro, Kernforschungsanlage-Jülich and from the Croatian Science Fund is gratefully acknowledged.

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