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Application of the Dualist Model. Generation of Kekulé Structures and Resonant Sextets of Benzenoid Hydrocarbons

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The dualist model of Balaban is used for the enumeration and display of Kekulé structures K and resonant sextet numbers $r(G; k)$ of large cata-condensed benzenoid hydrocarbons.

The key steps are: (1) Transform the benzenoid graph into the corresponding dualist and associate with it a linear-angular, *L—A*, sequence, (2) Fragment the dualist into subgraphs after each *L—A* pair. The resulting subgraphs are called fragment graphs. (3) Colour each fragment graph, containing v vertices, $v + 1$ times such that each colouring contains at most on black vertex (the rest being white). (4) Re-assemble the coloured fragments into their initial geometry, preserved in the dualist, to produce a set of coloured dualists such that no coloured dualist has more than one black vertex in each linear segment. The number of such coloured dualists is *K*, the Kekulé count. By convention, each black dualist vertex corresponds to a proper resonant sextet. This, plus the fact that a linear segment can have at most one resonant sextet, completely defines all of the individual VB Kekulé structures and their resonant sextets. The method is an illustration of data reduction schemes and is quite suited for large benzenoid hydrocarbons.

A number of formulae for computing the number of Kekulé structures of various families of cata-condensed benzenoid hydrocarbons are derived. In addition, the above approach is applicable to large benzenoid systems consisting of cata-condensed fragments and thin peri-condensed fragments.

INTRODUCTION

In this work we wish to introduce the use of the dualist model[1] for the enumeration and display of Kekulé structures and the individual resonant sextet numbers[2] of large cata-condensed benzenoid hydrocarbons, BH's (cata-fusenes).[3]

The problem of enumeration (i.e. producing the total number) and display (i.e. constructing all the perfect matchings) of Kekulé structures is continously being discussed in the literature.[4–21] In addition, the recent interest in Kekulé structures is related to their role in structure--resonance theory[10,22] and in the conjugated circuits model.[23–26] Finally, Kekulé structures play one of the key roles in understanding the mathematical basis for the intimate connection between Pauling's VB model and Hückel's MO model.[27–29]

Some years ago Hosoya and Yamaguchi[2] introduced the concept of a resonant sextet number, $r(G;k)$, for a benzenoid graph (structure), G, as the number of ways in which k disconnected, but mutually resonant, sextets can be chosen from G. A sextet polynomial[2] is defined as,

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

where $r(G;0)$ is defined to be unity, and m is the maximum value of k. The sextet polynomial has been shown to possess many interesting properties[2,30–35] and reflects the main features of Clar's sextet theory.[36] Clar's sextet theory predicts that, of the set of isomeric BH's, the one with the largest number of sextets is the most stable isomer. Experimental evidence supports Clar's theory.[36]

There are at least three important properties of the sextet polynomial, viz.,

(i) The sum of its coefficients is equal to the number of Kekulé structures, $K(G)$, of cata-fusenes and thin peri-fusenes[2]

$$B(G;x=1) = \sum_{k=0}^{m} r(G;k) = K(G). \tag{2}$$

Thin peri-fusenes are defined as those peri-condensed BH's which do not contain the coronene skeleton as a substructure.[2,32]

(ii) The first derivative with respect to x (at $x=1$) is equal to the number of γ_1 permutations appearing in the structure-resonance theory of Herndon.[22] γ_1 represents the resonance between two Kekulé structures related by a permutation of three double bonds within a six-membered ring.

(iii) When a Kekulé structure is transformed into the subspace of its double bonds, a Kekulé factor graph $F(k)$, is obtained[37], (originally called a submolecule graph[38]), e.g.

Let $\overline{m}$ and $\underline{m}$ indicate respectively the maximum and minimum numbers of bivalent vertices in an $F(k)$. Furthermore, let a_θ indicate the population of $F(k)$'s containing θ number of bivalent vertices. It has recently been proved[33,34] that:

$$a_{\overline{m}-j} = r(G;j) ; \qquad j = 0, 1, \ldots, m \tag{3}$$

for a nonbranched-all-benzenoid hydrocarbon, and

$$a_{\underline{m}+j} = r(G;j) ; \qquad j = 0, 1, \ldots, m \tag{4}$$

for a nonbranched non-all-benzenoid hydrocarbon containing two linear acene fragments (e.g., pentaphene, etc.).

DEFINITIONS

(I) The Dualist, D(G)

The dualist (dualistic graph[1,39] charateristic graph[40]) is the inner (internal) dual graph which preserves information about the angles between the branches of a BH. The inner dual graph is the dual graph without the vertex representing the outer part of a plane.[41] A dualist is not a graph in the strict graph-theoretical sense, that is, a set of vertices and a set of edges. We understand the structure of the dualist as a weighted graph with two-valued weights (L = linear and A = angular) of vertices. Angular weights correspond to kink or branched points in the skeleton.

The dualist model has been developed to acknowledge the structural differences between the isomeric cata-condensed BH's for which the inner dual graphs are the same. The dualist and inner dual graphs of anthracene and phenanthrene are shown in Figure 1.

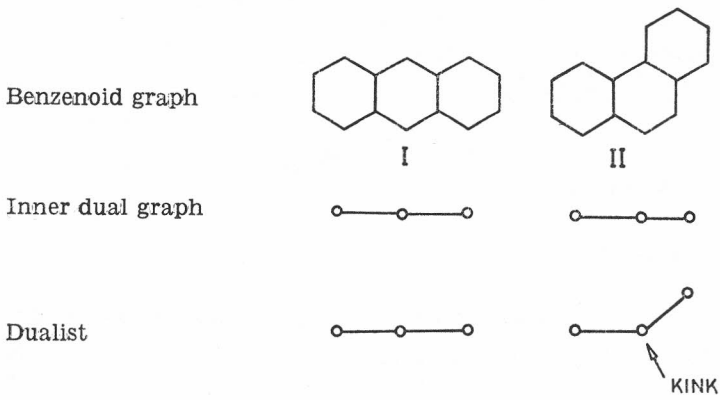


Figure 1
The dualists and inner dual graphs of anthracene (I) and phenanthrene (II)

The carbon skeletons of the BH's in Figure 1 are depicted by benzenoid graphs.[31,42] A benzenoid graph is a bipartite planar graph which can be constructed in the plane by assembling R regular hexagons in

such a way that two hexagons have exactly one common edge or are disjoint. The inner dual graph is obtained by linking the centers of the individual benzene rings of a BH through the bond that is common to two hexagons. The dualist preserves the geometric information of ring annelation. We denote a dualist by $D(G)$.

(II) Modes of Ring Annelation

We make use of the two modes of ring annelation, viz., linear mode, L, angular mode, A. These are shown below

(III) The L—A *Sequence,* S(G)

Every non-branched cata-fusene containing R hexagons generates a so called $L-A$ sequence[31] given by

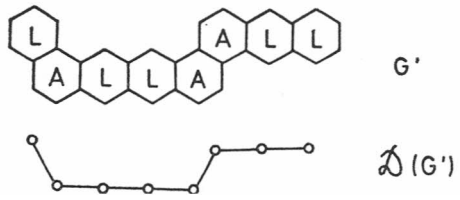
$$\{S_1\ S_2\ \ldots\ldots\ S_{R-1}S_R\} \tag{5}$$

where, by convention,

$$S_1 = S_R = L; \qquad S_i = A \text{ or } L; \qquad 1 < i < R \tag{6}$$

depending on the mode of ring annelation.

As an illustration we give a cata-condensed BH G' and its $L-A$ sequence



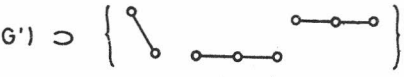
(IV) Fragment Graphs, f(G)

Each $L - A$ sequence is divided into several subsequences, the fragmentation of the sequence being after each LA pair (or after each AA pair, if there is a series of more than two A's). E.g. $S(G')$ is divided in subsequences as follows

$$S(G') = \{L\,A \mid L\,L\,A \mid A\,L\,L\} \tag{13}$$

The pictorial representations of the subsequences are fragment graphs, $f(G)$'s. Thus, the above sequence $S(G')$ is represented as

$$\mathcal{D}(G') \supset \left\{ \right\} \tag{14}$$

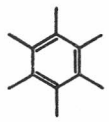


The branched systems are dissolved into a set of $f(G)$'s in several steps depending on the number of branched vertices in $D(G)$.

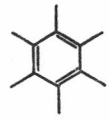
The most important property of these fragment graphs (subsequences) is that each f(G) contains at most one resonant sextet.[34]

(V) Proper and Improper Sextets[32]

These are schematically represented below



proper sextet



improper sextet

Clar's representation of a given Kekulé structure is defined as a simultaneous substitution of all proper sextets by circles and replacing all double bonds by single bonds.[32] The above concepts are illustrated in Figure 2.

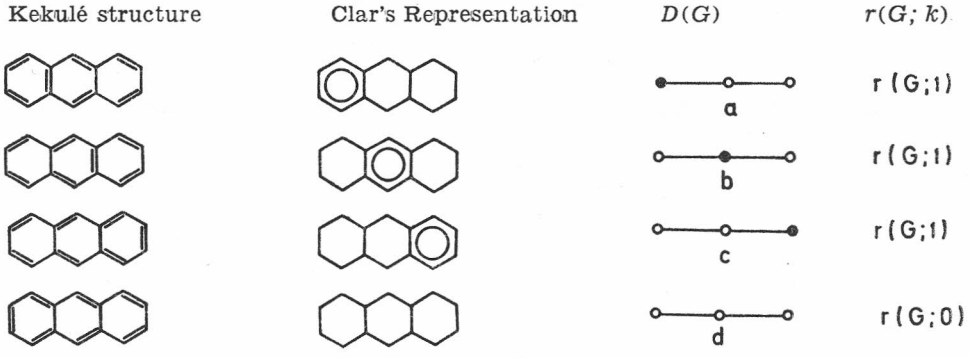


Figure 2
B (anthracene; x) $= 1 + 3x$
B' (anthracene; x = 1) $= n\gamma_1 = 3$

(VI) Colouring the Fragment Graphs

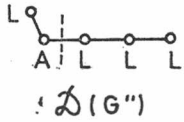
Each fragment graph is coloured by two colours, black and white, in such a way that at most one vertex is black. This produces $v + 1$ colourings (v is the number of vertices in $f(G)$). By convention, a black vertex corresponds to the hexagon containing the proper sextet, i.e. the hexagon with the circle in Clar's formalism.

(VII) Assembling the Coloured Fragment Graphs

The coloured $f(G)$'s are re-asembled in their initial L—A sequence such that none of the resulting coloured $D(G)$'s contain linear segments with more than one black vertex.

GENERATION OF KEKULÉ STRUCTURES AND RESONANT SEXTET NUMBERS OF CATA-FUSENES

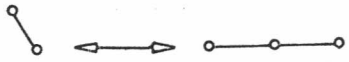
To obtain all allowed colourings of $D(G')$ we first obtain those of $D(G'')$ given below,



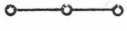
$D(G'')$

and then combine them with those of

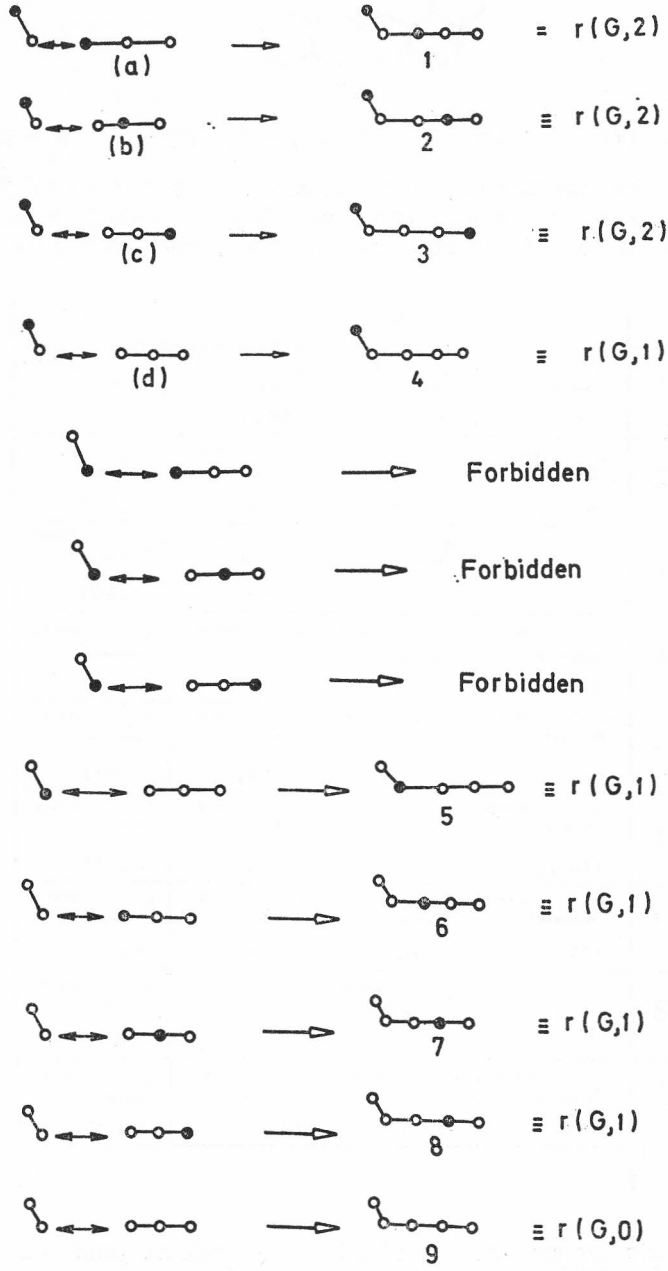
In order to obtain all possible colourings of $D(G'')$ we combine the following fragment graphs



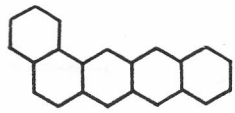
The fragment graph  has three colourings shown below.

The fragment graph  has four colourings and these are shown in Figure 2.

The colourings of $D(G'')$ are given below.



Dualists 1—9 correspond, of course, to benzo[a] tetracene, G'', for which we may now immediately write the sextet polynomial:



G"

$$B_{G''}(x) = 1 + 5x + 3x^2, \quad K(G'') = 9; \quad n\gamma_1 = 5 + 6 = 11 \qquad (11)$$

where $n\gamma_1$ is the number of γ_1 permutations $= B'_{G''}$ $(x = 1)$. Interaction between colourings 1 — 9 and those of O——O——O, i.e. a, b, c, d (in Figure 2), leads to a 4×9 counting matrix, shown in Figure 3.

	a	b	c	d
1	r(G;3)	r(G;3)	r(G;3)	r(G;2)
2	r(G;3)	r(G;3)	r(G;3)	r(G;2)
3	0	r(G;3)	r(G;3)	r(G;2)
4	r(G;2)	r(G;2)	r(G;2)	r(G;1)
5	r(G;2)	r(G;2)	r(G;2)	r(G;1)
6	r(G;2)	r(G;2)	r(G;2)	r(G;1)
7	r(G;2)	r(G;2)	r(G;2)	r(G;1)
8	0	r(G;2)	r(G;2)	r(G;1)
9	r(G;1)	r(G;1)	r(G;1)	r(G;0)

Figure 3
Counting matrix for construction of all allowed colours (and thus all Kekulé structures and individual resonant numbers) of G'.
B_G, (x) $= 1 + 8x + 17x^2 + 8x^3$; $K(G') = 34$
$B'_{G'}$ (x = 1) $= n\gamma_1 = 8 + 34 + 24 = 66$

Only two combinations are forbidden, viz., (3a) and (8a), so we have

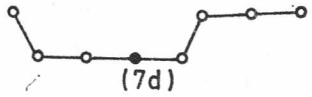
$$K(G') = 4 \times 9 - 2 = 34 \tag{16}$$

and

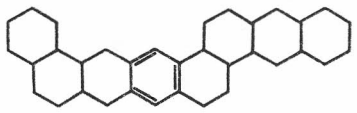
$$B(G';\ x) = 1 + 8x + 17x^2 + 8x^3 \tag{17}$$

$$n\gamma_1(G') = \mathrm{B}'\ (G';\ x = 1) = 8 + 2 \times 17 + 3 \times 8 = 66 \tag{18}$$

The individual Kekulé structures can easily be generated, because colouring one vertex per $< g_i >$ fixes the whole Kekulé structure. As an example we consider colouring (7d) from the counting matrix,

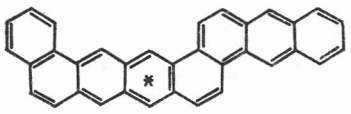


which transforms to



The remaining double bonds must be assigned in such a way that none of the remaining hexagons possess proper sextets.

This restriction results in only one perfect match, viz.,



$k_{7\text{-}d}$

To summarize the procedure consists of the following steps:

(1) Transform the cata-fusene graph into the corresponding dualist and associate with it on $L - A$ sequence.

(2) Divide the dualist into fragment graphs.

(3) Colour each fragment graph. $v + 1$ colourings should be obtained. Each colouring should contain at most one black vertex, the rest being white.

(4) Re-unite the coloured fragment graphs into their initial geometry, preserved in the dualist, to produce a set of coloured dualists. No coloured dualist should have more than one black vertex in each linear segment.

(5) Transform the coloured dualists into Kekulé structures of the initial cata-fusene. Note that by convention every black vertex in the dualist corresponds to a proper resonant sextet. This convention and the fact that each linear segment can have at most one resonant sextet, completely defines all of the individual Kekulé structures and their resonant sextets of a given cata-fusene.

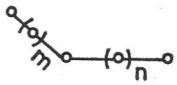
The method desribed is inferior to the Gordon-Davison procedure[6], or any other enumerative scheme,[8,9] if we are only after the enumeration of the Kekulé structures for cata-fusenes. However, if we need to display the Kekulés' structures then our procedure competes well with the Randić procedure[11] and the procedure based on the reduced graph model.[17,18] However, our procedure has one advantage over all these methods; it also generates resonant sextet numbers of cata-fusenes. Besides, it allows derivation of compact formulae for computation of the number of Kekulé structures for various sub-classes of cata-condensed benzenoid hydrocarbons. In addition it reveals the intimate relationship that exists between Kekulé structures and resonant sextet numbers of cata-fusenes.

SOME EXPERESSIONS FOR K(G) BASED ON THE DUALIST MODEL

We consider several general types of dualist graphs.

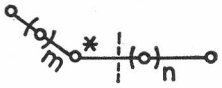
(a) Non-branched cata-fusenes

(I)



$\mathcal{D}(I)$

To calculate $K(G)_I$ we fragment $D(I)$ as follows:



Therefore, $K(G_I) = K(\text{m}) \cdot K(\text{n}) - D$ (19)

where **D** is the number of forbidden combinations between fragments

m and n

Since

$$K(\text{m}) = m+3 \qquad (20)$$

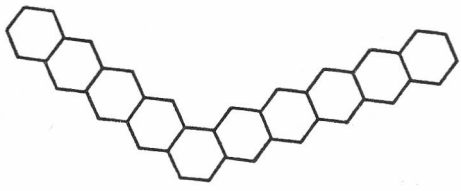
and

$$K(\text{n}) = n+2 \qquad (21)$$

and since **D** is simply the number of times the junction vertex (denoted by an asterisk) becomes black, that is $(n + 1)$ times, we may write:

$$K(G_I) = (m + 3) \cdot (n + 2) - (n + 1) \qquad (22)$$

E.g. $m = 3$, $n = 4$ corresponds to the following BH

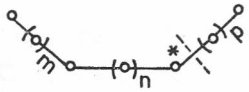


Thus

$$K = (3 + 3) \cdot (4 + 2) - (4 + 1) = 31$$

Of course, for $n = m = 0$ one is dealing with phenanthrene for which $K = (3) \cdot (2) - 1 = 5$.

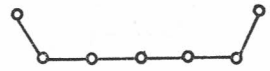
(II)

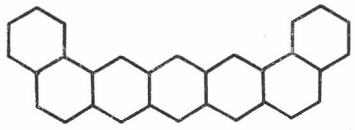


$\mathcal{D}$(II)

Using similar arguments and eq. (22), we arrive at the following expression for $K(G_{II})$:

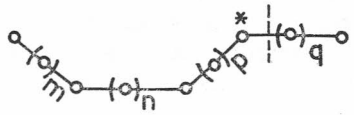
$$K(G_{II}) = [(m + 3)\ (n + 2) - (n + 1] \cdot (p + 2) - [(p + 1)\ (m + 2)] \qquad (23)$$

E.g. $m = p = 0$, $n = 3$ 

which corresponds to 

for which $K = [(3)\ (5) - (4)] \cdot (2) - 2 = 20$.

(III)



$\mathcal{D}$(III)

Using eq. (23) and the fact that the junction vertex becomes coloured black $(m + n + 3)$ times we write:

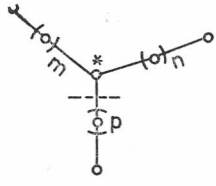
$$K(G_{III}) = [(m + 3)\ (n + 2) - (n + 1)] \cdot (p + 2) -$$
$$[(p + 1)\ (m + 2)] \cdot (q + 2) - [(q + 1)\ (m + n + 3)] \qquad (24)$$

It is evident that more complicated expressions can be derived from simpler ones, since eq. (24) is based on eq. (23), and the latter on eq. (22).

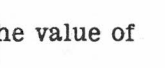
(b) Branched cata-fusenes

We can easily adapt the technique used for non-branched cata--fusenes to branched cata-fusenes. Instead of an L—A sequence we have an L—A tree. We can either choose one terminal vertex as the root and continue to make fragments according to IV (in previous section, see page 343), then carry out the colouring process and reassemble them, or take a path from one terminal point to another and calculate the other branches separately and then combine them as in the following cases:

(IV)



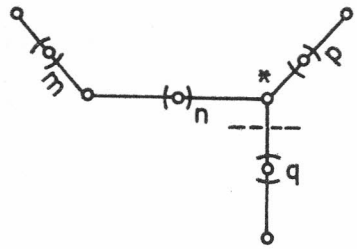
$\mathcal{D}$(IV)

From eq. (22) we know the value of $K\left(\text{  }\right)$ and knowing that the junction vertex becomes black only once we can immediately write:

$$K(G_{IV}) = [(m + 3) \cdot (n + 2) - (n + 1)] \cdot (p + 2) - (p + 1) \qquad (25)$$

Naturally for $m = n = p = 0$ *D(IV) is* D(triphenylene); for which $K = (6 - 1)\ (2 - 1 = 9$.

We now consider another type of branched dualist graph:

(V) 

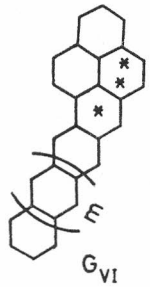
$\mathcal{D}$(V)

From eq. (23) and the fact that there are $(m + 3)$ colourings in which the junction vertex (denoted by an asterisk) is black (the dashed line indicates partitioning), we conclude that the number of forbidden combinations is $(m + 3)\ (q + 1)$ and thus we have:

$$K(G_V) = \{[(m + 3) \cdot (n + 2) - (n + 1)] \cdot (p + 2) - [(p + 1) \cdot (m + 2)]\} \cdot (q + 2) - (m + 3) \cdot (q + 1) \qquad (26)$$

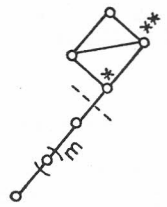
EXTENSION OF THE APPROACH TO LARGE BENZENOID HYDROCARBONS CONSISTING OF CATA-FUSENE AND THIN PERI-FUSENE PARTS

The above approach leads to a variety of expressions for (KG)'s of various general types, and in principle every cata-fusened benzenoid hydrocarbon can be assigned an appropriate $D(G)$. A corresponding value of $K(G)$ can thus be computed. The procedure can be extended to include large BH's consisting of cata-fusene fragments and thin-perifusene fragments. As an illustrative example we will demonstrate the extension of the above procedure for the composite benzenoid hydrocarbons possessing the general structure shown below.



G_{VI}

The corresponding dualist is the following structure.

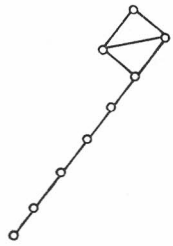


$\mathfrak{D}$(VI)

We know by investigating all Kekulé structures of pyrene that the hexagon denoted by * assumes a proper sextet twice while that denoted by ** assumes a proper sextet just once, and hence the expression for K is:

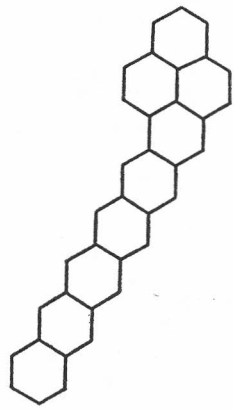
$$K(G_{VI}) = 6(m + 3) - 3(m + 2) \tag{27}$$

E.g. $m = 3$,



$\mathfrak{D}$(VII)

The corresponding BH is



G_{VII}

for which $K = 6(3 + 3) - 3(3 + 2) = 21$. This result agrees with independent computation from the graph spectrum of G_{VII}.[44]

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SAŽETAK

Primjena dualističnog modela. Generiranje Kekuléovih struktura i rezonancijskih seksteta benzenoidnih ugljikovodika

S. El-Basil, P. Křivka i N. Trinajstić

Balabanov dualistični model upotrijebljen je za prebrojavanje i prikazivanje Kekuléovih valentnih struktura i rezonancijskih seksteta velikih kata-kondenziranih benzenoidnih ugljikovodika. Izvedene su formule za izračunavanje broja Kekuléovih struktura nekih klasa kata-kondenziranih benzenoidnih ugljikovodika. Dualistični je model također upotrijebljen za prebrojavanje Kekuléovih struktura nekih benzenoidnih ugljikovodika koji su složeni od kata-kondenziranog fragmenta i »tankog« peri-kondenziranog fragmenta.