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ON THE ORDERING OF KEKULÉ STRUCTURES IN TWO-DIMENSIONAL SPACE,

SOME TOPOLOGICAL PROPERTIES OF SUBMOLECULES OF CATA-CONDENSED BENZENOID HYDROCARBONS

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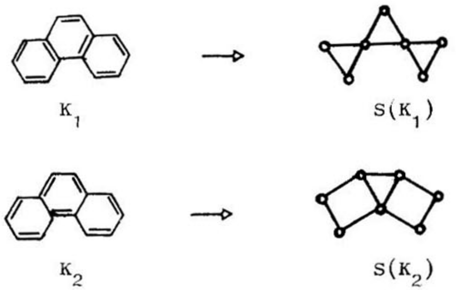
ABSTRACT

The potential of using vertex partitions of submolecules[1] to order the corresponding Kekulé structures in a two-dimensional space is explored. Nine graph-theoretical properties of submolecule graphs derived from catacondensed benzenoid hydrocarbons are given as functions of graph topology.

INTRODUCTION AND THE DEFINITION OF SUBMOLECULE GRAPH, S(K)

A submolecule is a graph which results when the Kekulé structure of a benzenoid hydrocarbon is transformed into the subspace of its double bonds. As an illustration we consider the "most" and "least" aromatic Kekulé structures of phenanthrene and their corresponding submolecules as shown below.



Joela seems to be the first to introduce the concept of the transformation of aromatic molecules into the subspace of their double bonds(1). Submolecules must be viewed as rewarding substrates useful for both developing graph-theoretical concepts as well as chemical concepts. This is because, while a Kekulé structure is no more than a particular permutation(2) of double bonds, its corresponding submolecule is the connected graph that represents that particular permutation. Naturally, since Kekulé introduced his valence-bond structures to represent aromatic molecules, many attempts were made to assign relative importance (weights), to the individual Kekulé structures belonging to some benzenoid hydrocarbon. Most recent of these attempts is a VB-MO index, called Kekulé index, K(L), developed some years ago by a group of graph-theorists(3) and is given by eqn. (1) in cases of alternant hydrocarbons:

$$K(L) = \frac{1}{2N} \sum_{(\mu,\nu)\in L} (2 + 2\, p_{\mu\nu})^{\frac{1}{2}} \qquad (1)$$

where 2N is number of pi electrons and p is a bond order. On the other hand, this author(4) postulated that a submolecule contains all information pertinent to the description of a Kekulé structure, and calculated a branching index(5), x_A of a set of submolecules corresponding to a set of Kekulé structures, as defined by eqn. (2) viz.,

$$x_A = \sum_{i,j} \left[(m_i \; m_j)^{\frac{1}{2}}\right]^{-1} \qquad (2)$$

where m_i is degree of i th vertex in the submolecule, taking the summation over all (i,j)-edge types in the S(K) graph.

As anticipated, the order resulting from x_A's parallels the order of the corresponding K(L) values of the Kekulé structures. Now, since K(L) is a VB-MO quantity, while x_A is a VB one, the result was taken as a substantiation and explicit illustration of the relation between the two main theories of organic chemistry, viz., MO and VB theories, proved recently by Cvetković, Gutman and Trinajstić(6).

The idea of relating VB characters of aromatic submolecules to their MO counterparts of the corresponding Kekulé structures was, then, extended to studying the non-adjacent numbers of Hosoya(7) of submolecules, and again the resulting orders of these numbers were found identical to orders generated from K(L) values(8). The success of the approach encouraged us to investigate other graph-theoretical properties of the S(K) graphs and how they can be related to known VB-MO indices, such as K(L), in two-dimensional space(9) (see below).

THE VERTEX CODE OF A SUBMOLECULE GRAPH

We define for every submolecule graph, S(K), of a particular Kekulé structure a vertex code (or partition) given by the sequence of numbers $\{v_i, v_j, v_k\}$ where, in general, v_m is the number of vertices of degree m. The entries of such codes might be viewed as coordinates of a point in a multi-dimensional space, or as defining a vector in such a space. There is, however, the difference that the sequences of our codes enumerate different quantities (i.e. vertices of different degrees), hence the transformation properties of vector spaces can no longer be legitimately considered, nevertheless, the language of vectors is convenient. Our original objective was to use a pair of v_m's (such as $\{v_i, v_j\}$, $\{v_i, v_k\}$, or $\{v_j, v_k\}$ as the coordinates of a two-dimensional space defining points represenging particular S(K) graphs, hoping that such a pictorial immage of a set of submolecules, will order them, as predicted from the Kekulé indices of their corresponding Kekulé structures. Naturally, ordering requires comparison and the latter implies certain criteria (in our case the various v_m's). The legitimacy of the use of sequences of numbers representing valencies (degrees) of graphs has been examined(10), and the concept of ordering is only a recent one in chemistry(11).

ORDERING SUBMOLECULES USING THEIR VERTEX CODES:

Figs. 1-3 show how one might use pairs of v_m's as coordinates through which individual submolecule graphs are

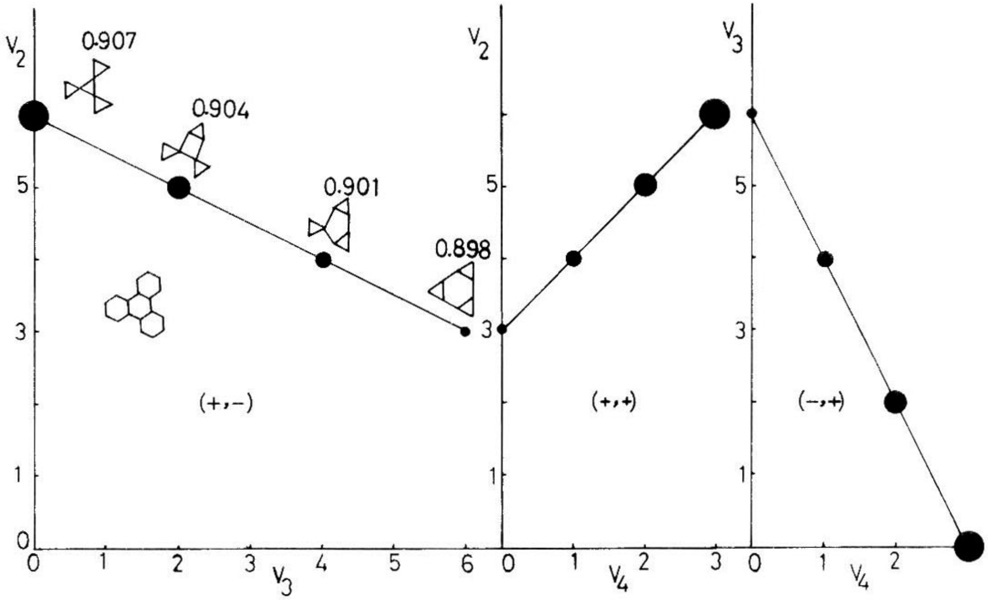


Fig. 1: Submolecules of triphenylene, numbers above S(K) graphs are K(L)values, eqn.1, V_m is number of vertices in S(K) of degree m.

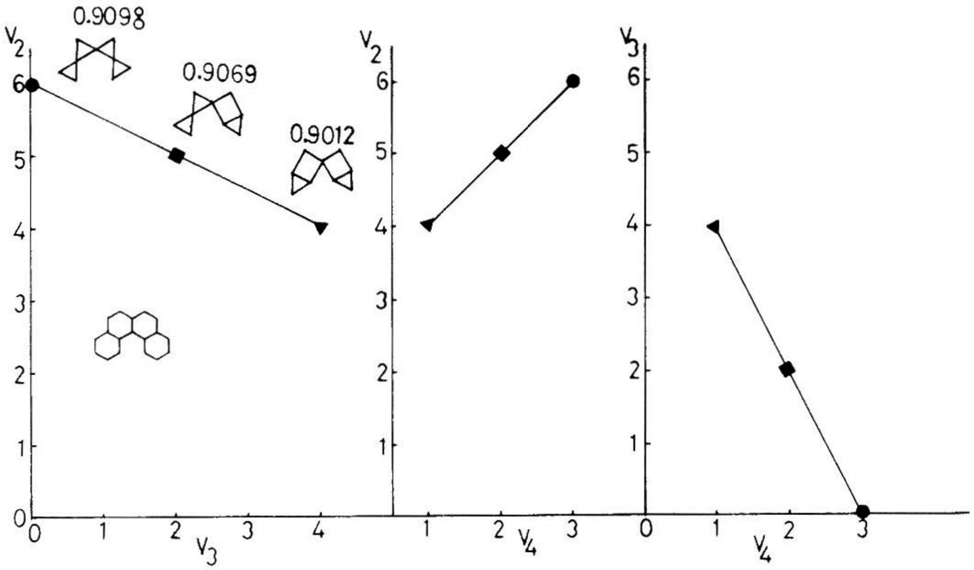


Fig. 2: Ordering of S(K) graphs of 3,4-benzphenanthrene accroding to their vertex partitions. Numbers above graphs are computed via eqn.1.

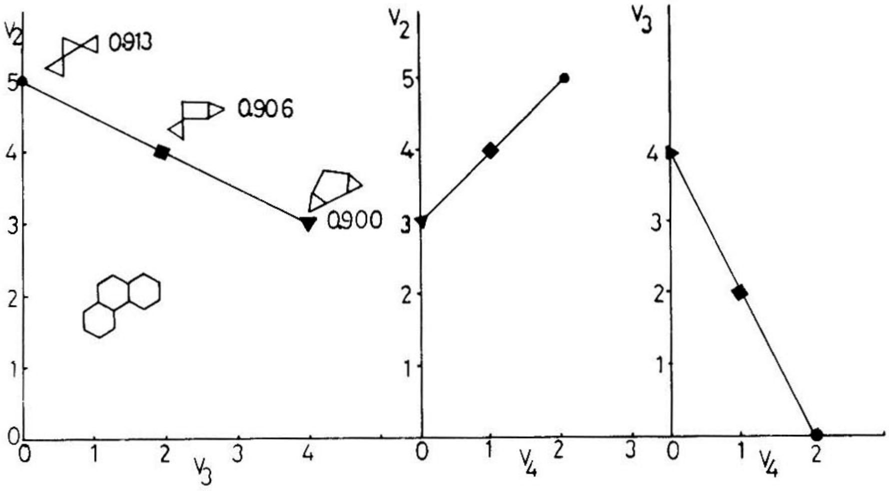


Fig. 3: Phenanthrene submolecules ordered according to their vertex partitions. Numbers above graphs are calculated using eqn. 1.

defined in two-dimensional space. The numbers written above each S(K) graph are Kekulé indices, K(L)'s, of the corresponding Kekulé structures(3). The signs used in parentheses indicate either an increase, (+), or a decrease, (-), in the numerical values of K(L)'s as one proceeds from a structure with a smaller number of v's to structures with larger v parameters(12). Thus, e.g. (+, -) means that K(L) increases as v_2 does, but decreases as v_3 increases, and so on. The "size" of the closed circle (identifying the location of a particular subgraph) is meant to be proportional (roughly) to the corresponding K(L) values in case of triphenylene, Fig. 1, as an illustration.

It turned out, however, upon studying large numbers and types of benzenoid hydrocarbons (including linear acenes, non-branched all-benzenoid, branched all-benzenoid, and non-all benzenoid catacondensed systems) that the results are actually <u>not</u> as encouraging as they might first appear to be. Fig. 4 shows all submolecules of benz [a] anthracene as an example of a non-branched, non-all benzenoid catacondensed hydrocarbon. Vertex codes and K(L) values are given below each graph. It becomes evident that more than one submolecule the Kekulé structures of which have <u>different</u> Kekulé indices might have <u>identical</u> vertex codes. Fig. 5 illustrates the situation with a non-branched all-benzenoid catacondensed hydrocarbon. Again a <u>complete</u> ordering of the S(K) graphs does not seem possible using their vertex partitions. A number of interesting questions, however, arose in connection with how these vertex codes partition themselves according to the topology of the hydrocarbon. Some of these questions are i) Given a set of m vertices, to be "combined" somehow, so that some become bivalent, others trivalent and/or tetravalent (i.e. possible degrees are only 2, 3 or 4), how many <u>allowed</u> partitions are there to correspond to the various <u>permutations</u> of double bonds in the corresponding Kekulé structures? i.e. if $m \longrightarrow \{v_2, v_3, v_4\}$ where v_x is number of vertices of degree x, can we find all allowed $\{v_2, v_3, v_4\}$'s consistent with a particular

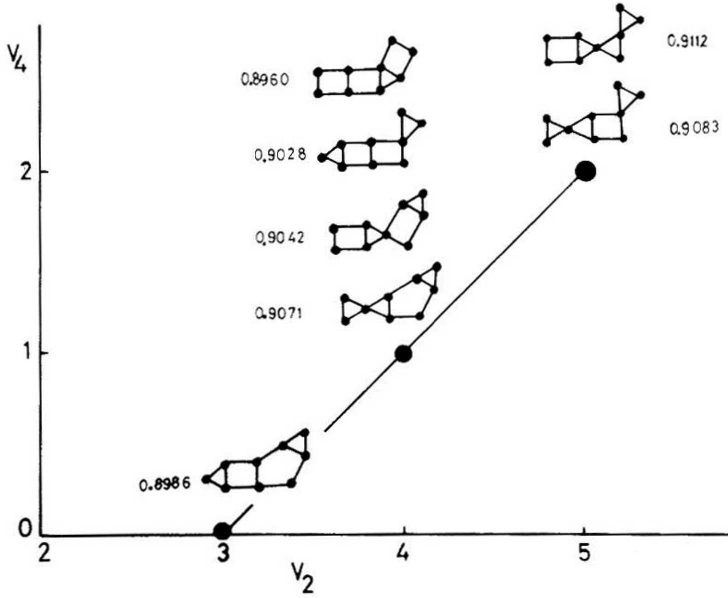


Fig. 4: Submolecules of benz[a] anthracene ordered according to their vertex distribution. The plot is intended to show failure of the vertex-codes to distinguish members of different K(L) values with BH's of high "linear acene" character.

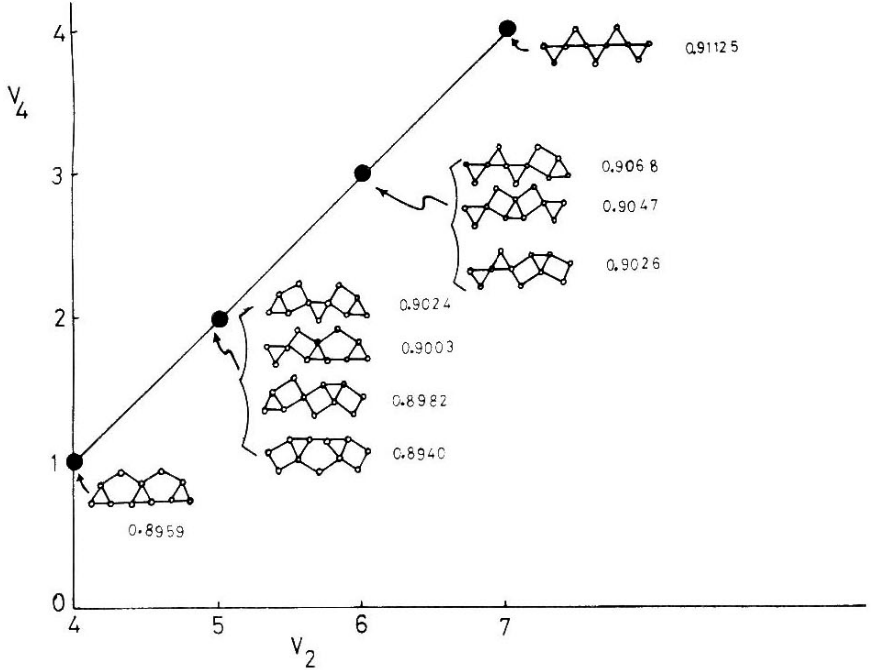


Fig.5: Ordering of S(K) graphs of picene using vertex partition. K(L) values, eqn. 1, are given beside graphs.

hydrocarbon topology? ii) Is it possible to deduce highest and lowest allowed values of v_2, given a particular topology? Obviously, doing so, defines boundaries of all possible vertex partitions of the hydrocarbon, iii) Let the number of benzene rings in the hydrocarbon be R, can we express $(v_2+v_3+v_4)$ as an f(R)? Doing so, would help answer i) at least partially. Obviously the total number of vertices in S(K) is given by: $v_2+v_3+v_4 = (4R+2)/2 = 2R+1$. iv) One observes from Figs 1-3 that dv_2/dv_4 is always unity: What is the impact of this observation, if real, on the partial sums resulting from the integers composing the vertex codes, considering inequalities of Muirhead(13)? The latter being essential for testing the legitimacy of comparison of a set of structures(14). Answers to the above, and such questions are of graph-theoretical interest and importance, and as such, the topic deserves consideration.

GRAPH-THEORETICAL PROPERTIES OF SUBMOLECULES OF CATACONDENSED BENZENOID HYDROCARBONS:

At the outset it is convenient to distinguish five types of the above category of hydrocarbons(15), viz., a) The linear acenes, b) Non-all benzenoids e.g. benz [a]-anthracene, pentaphene etc. c) All-benzenoid systems e.g. phenanthrene, chrysene etc. d) Branched non-all benzenoid and e) Branched all-benzenoid hydrocarbons.

The following properties are general to types a-e of benzenoid hydrocarbons(16)

1° The number of independent cycles in S(K) is equal to R, the number of hexagons in the hydrocarbon graph.

2^o The total number of vertices of S(K) is $m = b/2$, where b is the number of vertices in the graph of the benzenoid hydrocarbon. The total number of vertices in S(K) is related to R by eqn 3, viz. $m = \frac{b}{2} = 2R+1 = v_2+v_3+v_4$. (3)

3^o The size of the smallest cycle of S(K) is always three.

4^o S(K) possesses only vertices of degrees of 2, 3 and 4.

5^o As a result of the topology of benzenoid hydrocarbons a single tetravalent vertex generates four bivalent vertices, two tetravalent vertices lead to five bivalent ones and so on. This relation is expressed by eqn. 4:

$$v_2-v_4 = 3 \tag{4}$$

As a consequence of this, partitions of vertices which contain only three bivalent vertices shall have no tetravalent vertices. Such particular codes (partitions) might be expressed as $\left\{3,\ (2R-2),\ 0\right\}$. (c.f. relation 2^o).

6^o From 2^o and 5^o one concludes that the total number of bonds in a submolecule graph equals

$$2v_2 + 3v_3 + 4v_2 = 6R = b + 2(R-1) \tag{5}$$

7^o Relations 5^o and 6^o predict that a linear relation exists between v_i and v_j. However, the slope is unity only for dv_2/dv_4.

8^o On going from one partition to another v_3 increases (decreases) twice as much as either v_2 or v_4 decreases (increases). For example, phenanthrene partitions might be generated from one another as illustrated below

$$\left\{5 \xrightarrow{-1} 0 \xleftarrow{-1} 2\right\} \rightleftarrows \left\{4 \xrightarrow{-1} 2 \xleftarrow{-1} 1\right\}$$

$$\longrightarrow \left\{3 \xleftarrow{-1} 4 \xrightarrow{-1} 0\right\} \nwarrow \left\{4 \xleftarrow{-1} 2 \xrightarrow{-1} 1\right\}$$

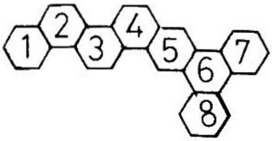
consequently the partial sums resulting from these codes violate inequalities of Muirhead(13). The above codes of phenanthrene e.g., lead to the following partial sums: 5,5,7; 4,6,7 and 3,7,7

9° THE NUMBER OF PARTITIONS, n

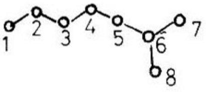
In order to compute all possible vertex partitions consistent with a given topology one should know the upper and lower limits on some v_j ($j = 2,3,4$) plus property 8°. It turns out that the boundaries on v_j is a specific function of the particular type of the catacondensed hydrocarbon (a-e, above). At this point we need to cite some rather uncommon definitions to facilitate writing this part of the manuscript.

It is convenient to represent benzenoid hydrocarbons using their dual subgraphs(17). These graphs are generated from the hydrocarbon graphs by replacing their hexagons by vertices and then connecting adjacent ones, thus, e.g.

$G(I) \longrightarrow D(I)$:



G(I)



D(I)

We define the following terms.

(a) Linear Subgraph(18), G_L (Straight Subgraph). It is defined as a subset of hexagons (or the corresponding dual vertices) fused (linked) in a straight line fasion. G_L containing p hexagons is said to be of order p. It is denoted by $G_L(p)$. The linear acenes, as a result of this definition, contain only such subgraphs. D(I), e.g., contains the following linear subgraphs

$G_L(2) = \{1,2\}$; $G_L(2) = \{2,3\}$, $G_L(2) = \{3,4\}$, $G_L(3) = \{4,5,6\}$, $G_L(2) = \{6,7\}$, and $G_L(2) = \{6,8\}$. The numbers in parentheses are indices of hexagons in G(I), i.e. indices of vertices in D(I).

(b) Terminal vertex

It is a dual vertex defining the terminus of the graph. For example D(I) contains three such vertices located at positions 1, 7 and 8.

(c) Kink vertex

We shall call a dual vertex a kink if it defines either the intersection of two linear subgraphs, one of which is terminal (normally, it contains a terminal vertex) or if it is located at the intersection of two G_L's, both of which have orders of 2. Thus D(I) has kink vertices at positions 2 and 3 only (observe that vertex at position 6 defines intersection of three G_L's, so it is outside the scope of our definition, so is vertex 4 since neither $\{3,4\}$ nor $\{4,5,6\}$ is terminal, while the latter has an order of 3). A vertex that defines the intersection of two non-terminal linear subgraphs, one of which has an order $\geqslant 3$ will be termed a bend. The vertex at position 4 in D(I) is such a vertex. We shall use the following symbol L = Number of independent G_L's(L),

D(I), e.g. has L = 6

Υ = Number of terminal vertices in dual

$\mathfrak{k}$ = Number of kink vertices in D

β = Number of bend vertices in D

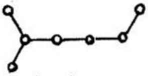
ϑ = Number of dual vertices which are not termini of linear subgraphs

D(I), e.g. has one such vertex, at position 5, thus

$$\vartheta_{D(I)} = 1$$

As a result of the above definitions we have the following facts 1) For a molecule of linear acene one has $\Upsilon = 2$, $\mathfrak{k} = \beta = 0$, $\vartheta = R-2$: (R = number of dual vertices), 2) A non branched, all-benzenoid catacondensed hydrocarbon is characterised by $\Upsilon = 2$, $\mathfrak{k} = L+1$, $\beta = \vartheta = 0$, 3) A non-branched, non-all benzenoid catacondensed hydrocarbon is characterised by $\Upsilon = 2$, $\mathfrak{k} = L+1$, $\vartheta \neq 0$, 4) A branched all-benzenoid catacondensed system has $\Upsilon \geqslant 3$, $\mathfrak{k} = L+1$, $\beta = \vartheta = 0$, and 5) A branched-non-all benzenoid catacondensed hydrocarbon will have $\Upsilon \geqslant 3$, $\mathfrak{k} = L+1$, $\vartheta \neq 0$.

Observe that a non-vanishing value of β would necessarily indicate a non-all benzenoid system, however, the reverse is not true, thus D(II), e.g. is non-all benzenoid, but has a vanishing value of β



D(II)

$$\Upsilon = 3, \quad \mathfrak{k} = 1, \quad \beta = 0, \quad \vartheta = 2$$

Now we are in a position to set boundaries on v_2 in S(K) graphs as a function of hydrocarbon topology

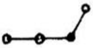
NON-BRANCHED NON-ALL BENZENOID CATACONDENSED SYSTEMS

Let v_2 (min.) = minimum number of v_2 in S(K), v_2 (max.) be maximum of that number. The following two equalities hold

$$v_2 \text{ (min.)} = 2 + \mathfrak{K} \tag{6}$$

$$v_2 \text{ (max.)} = 3 + L = 4 + \mathfrak{K} + \beta \tag{7}$$

Examples of this class of hydrocarbons are benz [a] anthracene, D(III), and pentaphene, D(iv), the duals of which are shown below:



D(III)

D(IV)

For both duals, $\mathfrak{K} = 1$ (closed vertex) and $L = 2$. Thus we can write for the two duals

$$v_2 \text{ (min)} = 3; \qquad v_2 \text{ (max)} = 5,$$

but we know that $v_2 - v_4 = 3$, therefore there must be two distributions defining the boundaries of the vertex partitions, for both hydrocarbons, viz.,

$$\{3,\ v_3,\ 0\} \quad \text{and} \quad \{5,\ v_3,\ 2\}$$

In order to compute v_3 we make use of relation 2°, viz.,

$(v_2 + v_3 + v_4) = 2R + 1$, which leads to the following upper and lower limits of vertex codes (partitions):

Benz [a] anthracene: $\{3,6,0\} \longleftrightarrow \{5,2,2\}$

Pentaphene : $\{3,8,0\} \longleftrightarrow \{5,4,2\}$

or, in general

$$\{v_2(\text{min}),\ v_3(\text{max}),\ v_4(\text{min})\} \longleftrightarrow \{v_2(\text{max}),\ v_3(\text{min}),\ v_4(\text{max})\}$$

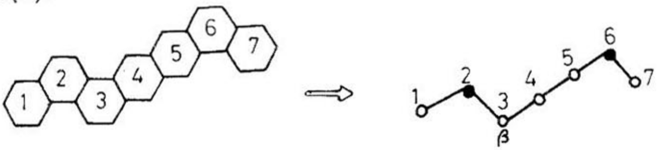
The number of different partitions, n, is then given by:

$$\begin{aligned} n &= v_2(\text{max}) - v_2(\text{min}) + 1 \\ &= L - \mathfrak{K} + 2 = \beta + 3 \end{aligned} \tag{8}$$

Corollary

Catacondensed non-branched non-all benzenoid hydrocarbons containing vanishing values of β have only three different partitions

We illustrate the application of the above finding with D(v):

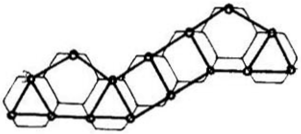


D(V)

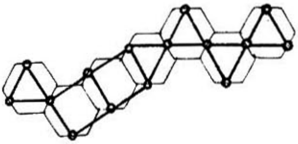
D(v) has the following values of the variables:
k = 2 (positions 2 and 6), β = 1 (position 3), L = 4.
Therefore v_2(min) 2 + k = 4, v_2(max) = 3 + L = 7, whence
n = 7 - 4 + 1 = 4.

We might easily construct the four different partitions, thus:
$\{4,10,1\} \longrightarrow \{5,8,2\} \longrightarrow \{6,6,3\} \longrightarrow \{7,4,4\}$.

Two of the S(K) graphs defining the boundaries of the partitions are drawn below:



S(K),v_2(min)
$\{4,10,1\}$



S(K),v_2(max)
$\{7,4,4\}$

Theorem

For a non-branched non-all benzenoid catacondensed hydrocarbon, its Kekulé count, K is $>$ n

Proof

$$v_2(\max) = L+3 \;; \quad \text{but} \quad L = R-1-\theta$$

Therefore, $v_2(\max) = R+2-\theta$ but $v_2(\min) = 2+\mathscr{k}$,

whence $n = v_2(\max) - v_2(\min) + 1 = R-(\theta+\mathscr{k})$. (9)

Now K (linear acene) = R+1 $\therefore$ $K > R$ (for non-linear acene).

Since both θ and $\mathscr{k}$ are non-negative parameters K must be $>$ n.

Equation (9) enables us to put limits on the potential of ordering a set of Kekulé structures in the two dimensional space via the vertex codes (vertex partitions) of their submolecule graphs. Obviously the linear acenes must be regarded as particularly discouraging in this respect:

Theorem

The vertices of a set of submolecules belonging to a linear acene might be partitioned in only two distinct ways

Proof

For any linear acene $\mathscr{k} = 0$ and $\theta = R-2$,

whence $n = R-(\theta+\mathscr{k}) = R-R+2 = 2$.

In the above context we might speak of a "linear-acene character"; the more such character gets, the less are the number of partitions of the corresponding S(K) graphs.

NON-BRANCHED-ALL BENZENOID CATACONDENSED HYDROCARBONS

The following relations hold:

$$\begin{aligned} \text{(a)}\ v_2(\min) &= L+1 = k+2 \quad \text{for} \quad R = 3,4 \\ &= L \quad = k+1 \qquad (R = 5,6) \\ &= L-1 = k \qquad\quad (R = 7,8) \\ &= L-2 = k-1 \qquad (R = 9,10) \\ &\text{etc.} \end{aligned} \tag{10}$$

$$\begin{aligned} \text{(b)}\ v_2(\max) &= L+3 \\ &= k+4 \end{aligned} \tag{11}$$

Observe that for this class of hydrocarbons we have

$$L = k+1 \tag{12}$$

Let $n(i,j)$ be the number of different partitions for an all-benzenoid non-branched catacondensed hydrocarbon. The following relations might easily be written:

$$\begin{aligned} n(3,4) &= 3, \\ n(5,6) &= 4, \\ n(7,8) &= 5 \quad \ldots\ldots \quad \text{etc.} \end{aligned} \tag{13}$$

An obvious conjecture for this class of hydrocarbons is that <u>K is larger than n</u>, but since K, in these cases, increases faster than n we conclude that as the size of the hydrocarbon increases its vertex codes become less efficient in assigning weights to its Kekulé structures.

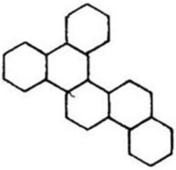
ALL-BENZENOID BRANCHED CATACONDENSED HYDROCARBONS

$$v_2(\min) = \Upsilon + k \tag{14}$$

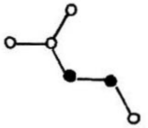
$$v_2(\max) = 2\Upsilon + k \tag{15}$$

$$\therefore \quad n = \Upsilon + 1 \tag{16}$$

As an illustration we consider D(vi), for



G(VI)



D(VI)

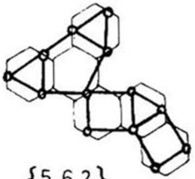
which $\mathfrak{k} = 2$, $\Upsilon = 3$; therefore

$v_2(\min) = 5$; $v_2(\max) = 8$ leading to the following partition boundaries:

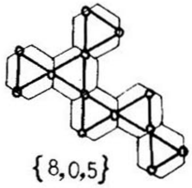
$$\{5,6,2\} \longleftrightarrow \{8,0,5\}$$

where we have made use of 2° and 5°.

Two S(K)'s representing the above partitions are outlined below



{5,6,2}



{8,0,5}

Other partitions in between these two limits might most easily be computed.

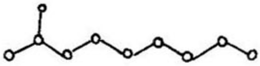
Eqn. (16) allows one to speak of "branching" of a graph in terms of its vertex partitions:

Conjecture

In a set of isomeric all-benzenoid catacondensed hydrocarbons a more branched system has more vertex partitions of its S(K) graphs than a less branched one has.

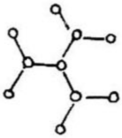
Naturally as the number of partitions goes up vertex codes become more efficient in distinguishing Kekulé structures.

We can tell that by inspection: Consider D(VII) and D(VIII):



D(VII)

$\tau = 3$



D(VIII)

$\tau = 6$

The dual on the left has only 3+1 = 4 partition while the more branched one to its right has 7. Using eqns. 14, 15 together with relations 2° and 5° allow constructing such partitions without actually drawing any graphs!

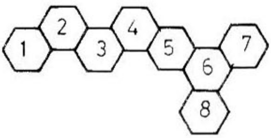
BRANCHED NON-ALL BENZENOID CATACONDENSED HYDROCARBONS

$$v_2(\min) = \tau + k \tag{17}$$

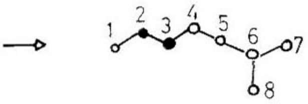
$$v_2(\max) = 2\tau + k + \beta \tag{18}$$

$$n = \tau + \beta + 1 \tag{19}$$

We illustrate the above relations with D(IX):



G(IX)



D(IX)

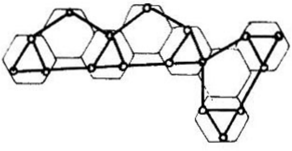
D(IX) has the following parameters

$\tau = 3$, $k = 2$ (positions 2 and 3),

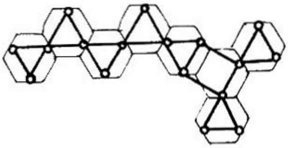
$\beta = 1$ (position 4).

$\therefore$ $v_2(\min) = 5$, $v_2(\max) = 9$

Two such limiting S(K)'s are shown below



$\{5,10,2\}$

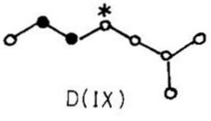


$\{9,2,6\}$

Conjecture

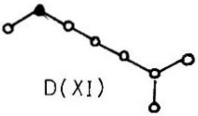
In a set of isomeric branched non-all benzenoid cata-condensed hydrocarbons, the number of vertex partitions goes up with the number of bend vertices.

Graphs (IX), (X) and (XI) are illuminating the point



D(IX)

D(X)



D(XI)

D(IX): $\beta = 1$, $k = 2$, $n=5$

D(X) : $\beta = 1$, $k = 1$, $n=5$

D(XI): $\beta = 0$, $k = 1$, $n=4$

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Professor Ivan Gutman kindly contributed some of the mathematical properties of the S(K) graphs of which relation 6° was unknown to the author.

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(4) S. El-Basil, Internat. J. Quantum Chem. 21, 771; 779; 793 (1982).

(5) Branching index given by eqn. (2) is actually the reciprocal of the connectivity index introduced by Randić, c.f. M. Randić, J. Am. Chem. Soc. 97, 6609 (1975).

(6) See Proof p. 2702 of ref. 2. An older proof is available; M.J.S. Dewar and H.C. Longuet-Higgins, Proc. R. Soc. A214, 482 (1952).

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(8) S. El-Basil and A.N. Osman, Work in progress.

(9) Ordering structures in two-dimensional space was first suggested by Randić and Wilkins, see, e.g., M. Randić and C.L. Wilkins, Chem. Phys. Letters, 63, 332 (1979); J. Phys. Chem., 83, 1525 (1979).

(10) W.K. Chen, The Matrix and Tensor Quarterly, June, 1974, p. 123, and Sep., 1974, p. 1.

(11) E. Ruch, Theoret. Chim. Acta, 38, 167 (1975); E. Ruch and A. Schonhofer, ibid., 19, 225 (1970).

(12) See, however relations 5° and 6°.

(13) See, e.g., G.H. Hardy, J.E. Littlewood and G. Polya, "Inequalities", Cambridge University Press, London (1934), p. 45.

(14) c.f. M. Randić, Internat. J. Quantum Chem. S5, 245 (1978).

(15) A molecular network which is composed entirely of regular hexagons is called benzenoid. If no three hexagons have a common atom, the system is called cata-condensed (in the opposite sense, the system is pericondensed). If every hexagon of a cata-condensed system has at most two neighbouring hexagons, it is said to be non-branched.

(16) I. Gutman, private communication.

(17) Professor Balaban used to call these graphs, the "characteristic graphs"; A.T. Balaban and F. Harary, Tetrahedron, 24, 2505 (1968). Later on, he called them "dualist graphs"; A.T. Balaban, Rev. Roum. Chim., 22, 45 (1977). This author (not knowing this part of Balaban's work) called them "generating graphs"; S. El-Basil, MATCH (Comm. Math. Chem.), 11, 97 (1981). We now prefer the term "dual graphs". (c.f. O.E. Polansky and D.H. Rouvray MATCH, 2, 63, 91 (1976), A.T. Balaban, Tetrahedron, 27, 6155 (1971).

(18) The term "linear" is used here in the chemical sense (to mean linear fusion of hexagons as in linear acenes, c.f. I. Gutman, Theoret. Chim. Acta, 45, 311 (1977). The term must not be confused with mathematical terminology of linear graphs as described in F. Harary, Graph theory (Addison-Wesley, Reading), pp. 150-152 (1969).