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LOCAL AROMATIC PROPERTIES OF BENZENOID HYDROCARBONS *

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Abstract - Individual benzene rings in polycyclic benzenoid hydrocarbons are examined from a graph theoretical position in an effort to characterize structural features responsible for variations in local molecular properties. The basis for the present study is the concept of conjugated circuits (M. Randić, Chem. Phys. Lett. 38, 68 (1976)). By enumeration of conjugated circuits that encompass individual rings, local diversities in conjugation can be studied quantitatively. The approach defines for each ring in polycyclic conjugated hydrocarbons a code, a sequence of integers which indicate the occurrence of conjugated circuits of size (4n + 2) for a ring. Ring codes thus derived offer an alternative partitioning of the molecular resonance energies. The average ring resonance energy appears to be a good index of the aromatic character for benzenoid systems. The use of the ring codes is further illustrated on a re-examination of ring currents, where regularities in the relative magnitudes, not previously recognized, are indicated.

INTRODUCTION

Some differentiation of individual rings in fused benzenoid systems had already been suggested by Robertson (1). The problem remained dormant for many years until Clar (2), lead by chemical intuition, was able to interpret some spectroscopic data in terms of local aromatic properties of benzenoid systems. Clar suggested for benzenoid hydrocarbons a novel type of valence structures in which some rings are viewed as fully aromatic, others are combined in partially aromatic rings, and finally some rings may even completely lack the aromatic content. Such rings were differentiated by inscribed circles, presence of formal CC double bonds, or simply left empty. Clar's concepts, it appears, have not induced commensurable interest among theoretical chemists. Nevertheless, some efforts were made to quantify the insights of Clar. Thus Polansky and Derflinger (3) initiated theoretical studies of Clar's valence structures by considering suitable MO indices for a characterization of the individual rings. Alternative ring indices, based on MO or VB calculations or some empirical grounds, followed (4). Here we will develop a graph theoretical, rather than quantum mechanical characterization for the individual rings in polycyclic benzenoid systems. In graph theory one is primarily interested in binary relations, and when graphs are pictorially represented this translates into the connectivity of the system. Applications of graph theory to molecules focuses on consequences of the given pattern of bonding. Usually the analysis consists in enumeration of selected graph invariants. Since in this work we are interested in the individual rings our analysis will be concerned with enumerations of subgraphs that can be associated with rings. We will first describe a particular encoding of the rings in benzenoid systems based on the concept of conjugated circuits (5). We will then see that the derived ring codes represent partitioning of the molecular resonance energy. We will continue with a discussion of ring currents and will see how ring codes lead to recognition of regularities in the relative magnitudes for the ring currents. It is noteworthy that no significant insight followed quantum chemical calculations on ring currents, which were reported for a decade and more. It is remarkable then that the new concept of ring codes offers novel important leads.

OUTLINE OF THE APPROACH

Conjugated circuits are defined as those circuits in individual Kekulé valence structures of a molecule in which there is a regular alternation of formally single and double CC bonds (5). In Fig. 1 we show one of the 13 Kekulé valence structures of 1,2:3,4-dibenz-

* Dedicated to Professor Eric Clar, doyen of benzenoid chemistry, whose work inspired much of the recent graph theoretical interest in aromaticity

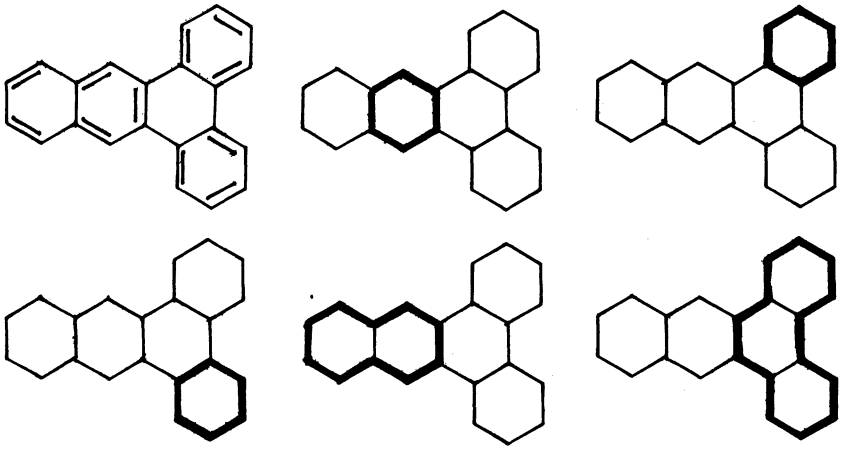
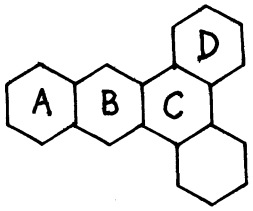


Fig. 1. Decomposition of one of Kekulé structures of dibenzanthracene into circuits with an alternation of the single and the double CC bond

anthracene and all conjugated circuits present in this valence structure. In benzenoid systems conjugated circuits are necessarily of size (4n + 2), i.e., involve 6, 10, 14, 18, etc carbon atoms. The smallest conjugated circuit is the benzene ring itself. Importance of formal benzene rings in larger valence structures was recognized in 1927 by Fries (6) even before the advent of MO and VB methods. Fries formulated an empirical rule prescribing among various Kekulé valence structures of a molecule one with the largest number of formal benzene rings as the dominant structure. Interestingly, the improvements in MO calculations when going from Hückel MO approximation to SCF MO approximations can be interpreted as supporting the empirical rule of Fries (7). Enumeration of benzene formal rings in a large structure represents a simple graph theoretical analysis of ring character (8). In Fig. 2 we show all 13 Kekulé valence structures of dibenzanthracene. The benzene character of a ring can be characterized by a fraction of structures in which the selected ring appears formally as a benzene ring. The results for dibenzanthracene are as follows:



ring	benzene character
A	8/13
B	8/13
C	2/13
D	12/13

Ring index for isolated benzene is clearly one. Of all rings in dibenzanthracene ring D approaches mostly that of benzene. Rings B and C show significant deviations from idealized benzene fragment, however, together they approach naphthalene core (8/13 = 0.6154, is not numerically very different from 2/3 which signifies naphthalene rings). The central ring exibits the least conjugation content, and is the ring which Clar correctly recognized as an "empty" ring (i.e., empty of conjugation). It is remarkable that already such a simple approach offers useful discrimination of fused rings. This suggests that the main assumptions of the approach are correct and justify further examination of related graph invariants in an effort to arrive at a comprehensive characterization of molecular local features. The discussion of aromaticity, conjugation, and the resonance energies in terms of conjugated circuits suggests that besides benzene fragments contributions from other conjugated circuits will provide important ingredients for a more complete structural characterization of ring environments in fused ring compounds. The work outlined here presents an extension and logical conclusion of the simple characterization of the benzenoid nature of individual rings based on the count of formal benzene valence structures within a larger system. It takes into account all conjugated circuits in a molecule, not only the dominant smallest such components, benzene rings.

We want firstly to introduce a convenient notation which summerizes information on conjugated circuits of a single Kekulé valence structure. This can be achieved as follows: Write down a molecular structure and insert label 1 for each formal benzene ring (1 indicates the size of conjugated circuits in the expression 4n + 2). Consider next conjugated circuits of size n = 2 and introduce label 2 for rings involved in such conjugated circuits, but only for the rings which have not already been assigned label 1. Continue the process by considering conjugated circuits of size n = 3 and assign labels 3 to circuits involved

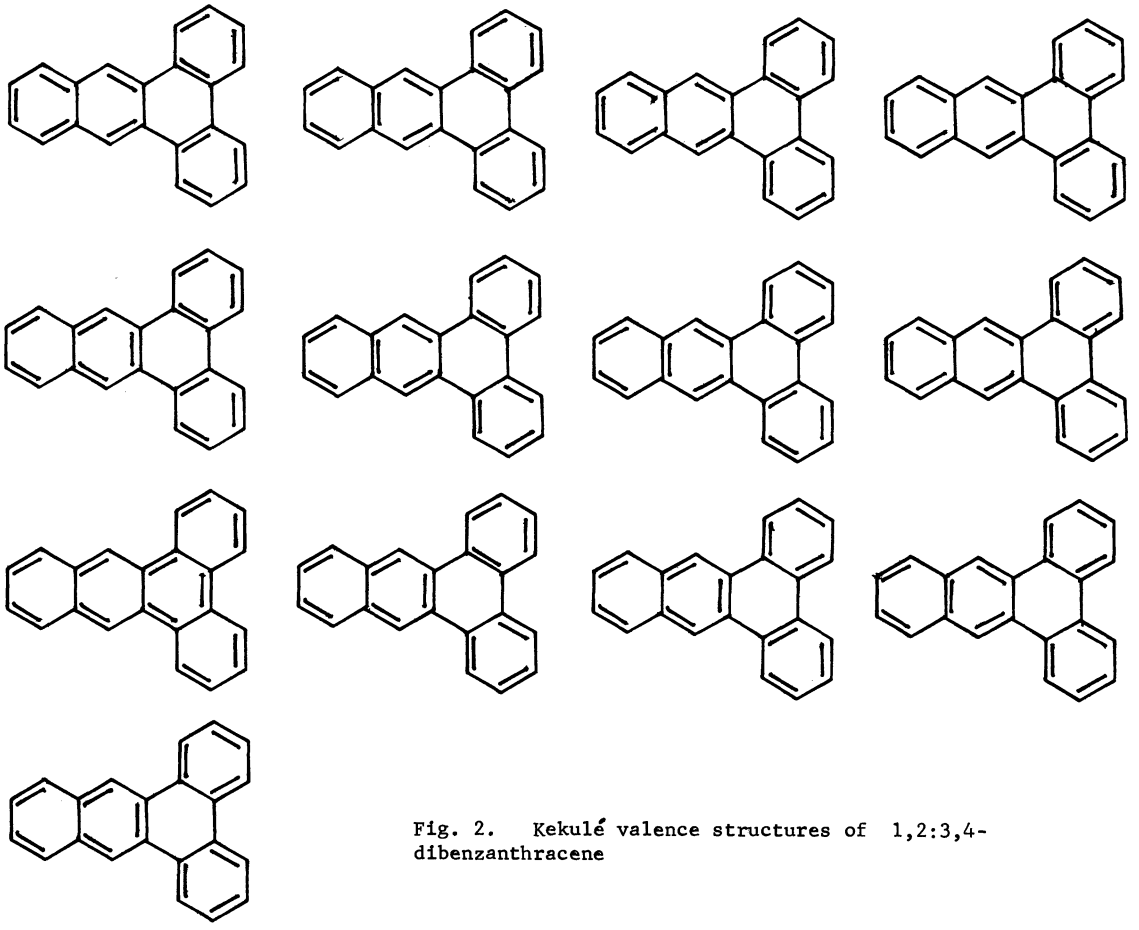
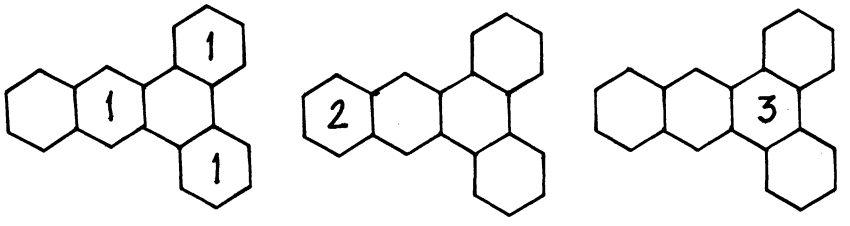


Fig. 2. Kekulé valence structures of 1,2:3,4-dibenzanthracene

if they have not been earlier given smaller labels. The process ends when all rings have been assigned a label. For dibenzanthracene Kekulé valence structure of Fig. 1 the indicated steps are illustrated below:



In this way each ring in the structure is assigned a single number, the number indicating the smallest conjugated circuit that encompasses the particular ring. The labeling of rings can be combined on a single molecular structure as illustrated for the 13 Kekulé structures of dibenzanthracene in Fig. 3. A glance at Fig. 3 clearly shows how individual rings play a different role in each of Kekulé structure. A superposition of the results for a single ring arising from all Kekulé structures will produce a characterization of the chosen ring. The present analysis differs from the previous simple characterization of the rings in conjugated hydrocarbons by the recognition of the role of larger conjugated circuits. For each ring separately we count how many times it appears with label 1, 2, 3, 4, and 5 and thus for each ring we obtain a sequence of integers, a code. For the four nonequivalent rings of 1,2:3,4-dibenzanthracene we have the results shown on the next page. Generally some rings will show a tendency of a prevailing benzenoid character, while others may involve different conjugated circuits equally and consequently will lack apparent similarity with a benzene ring. Rings A and B of dibenzanthracene already show that some differences among individual rings previously ignored surface when larger conjugated circuits are taken into account. Before embarking on a more detailed discussion of the ring codes and selected local molecular properties in catacondensed benzenoid systems we want to emphasize

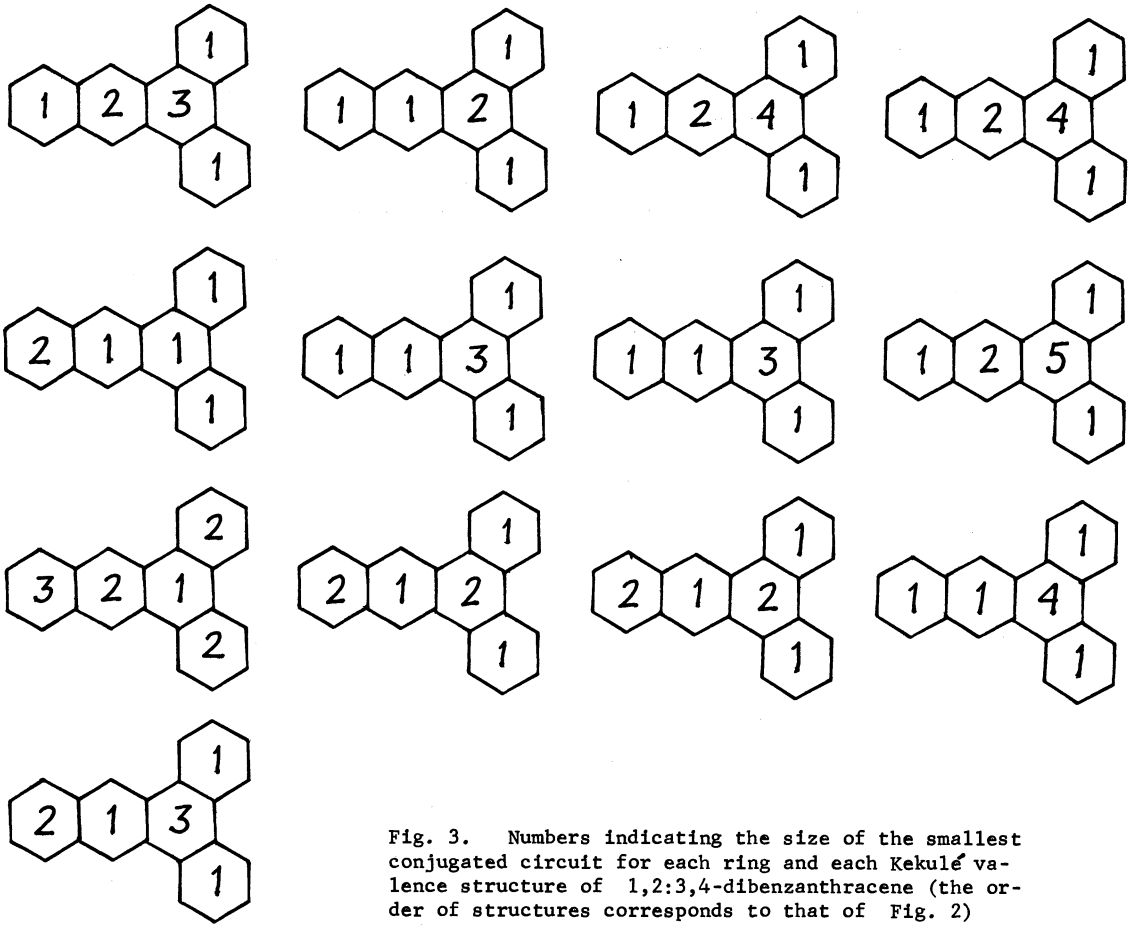
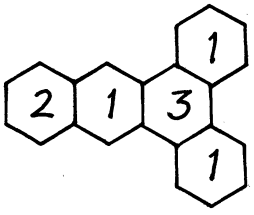


Fig. 3. Numbers indicating the size of the smallest conjugated circuit for each ring and each Kekulé valence structure of 1,2:3,4-dibenzanthracene (the order of structures corresponds to that of Fig. 2)

that the above analysis applies to a wide selection of compounds, including also nonbenzenoid hydrocarbons (e.g., biphenylene, azulene, heptalene), providing that the role of 4n conjugated circuits is also taken into account.



CATACONDENSED BENZENOID HYDROCARBONS

In this work we will confine our attention primarily to catacondensed benzenoid hydrocarbons. They represent the most primitive fused ring compounds. If the analysis proves useful for them one would be justified to expand such studies to more general compounds. In Table 1 we have listed the ring codes for benzenoid catacondensed hydrocarbons having four and less rings, while similar results for selected larger hydrocarbons are given in Table 2. The corresponding molecular carbon skeletons which include ring labels are shown in Figs. 4 and 5. Some regularities and properties of the ring codes can be learned from Table 1. The codes are not unique, for instance the code 2, 2, 1 appears in phenanthrene and tetracene. The corresponding rings in benzphenanthrene and chrysene have the same codes which indicates that occasionally this approach cannot discriminate among some isomers and their rings. Terminal rings tend to have a more pronounced benzenoid character. Qualitatively the most important aspect of Table 1 is the demonstration of the considerable diversity of codes, which means that we have a sensitive scheme capable to capture important structural variations. Besides merely encoding some innate structural features we propose that the

TABLE 1. Ring codes and ring resonance energies for selected benzenoid hydrocarbons

MOLECULE		Ring	Code	Ring RE	RE/Ring
1	Benzene		2	0.869	0.869
2	Naphthalene				0.661
			2, 1	0.661	
3	Anthracene				0.533
		A	2, 1, 1	0.521	
		B	2, 2	0.558	
4	Phenanthrene				0.651
		A	4, 1	0.744	
		B	2, 2, 1	0.466	
5	Tetracene				0.446
		A	2, 1, 1, 1	0.425	
		B	2, 2, 1	0.466	
6	Benzanthracene				0.579
		A	4, 2, 1	0.581	
		B	4, 3	0.602	
		C	2, 2, 2, 1	0.353	
		D	6, 1	0.780	
7	Benzphenanthrene				0.626
		A	6, 2	0.713	
		B	4, 3, 1	0.539	
8	Chrysene				0.626
		A	6, 2	0.713	
		B	4, 3, 1	0.539	
9	Triphenylene				0.680
		A	8, 1	0.800	
		B	2, 3, 3, 1	0.318	

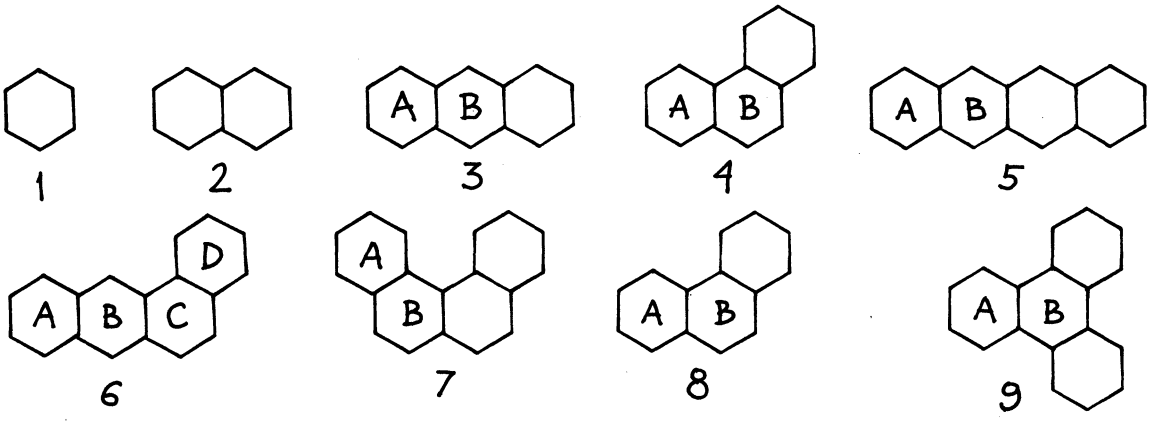


Fig. 4. Ring labels for benzenoid systems of Table 1.

count of conjugated circuits is a fundamental component in analysis of molecular properties. Earlier results on molecular resonance energies (RE) of smaller benzenoid systems fully justifies such a claim. More recently the conjugated circuits approach has been applied to much larger polycyclic benzenoid hydrocarbons (9) showing that size of a molecule is not detrimental factor. The partial contribution to the molecular resonance energy of a Kekulé valence structure can be readily found from Fig. 3 if symbols 1, 2, 3, ... are replaced by R_1, R_2, R_3, ... and the components added. For the first Kekulé structure of Fig. 2 we then obtain $(3R_1 + R_2 + R_3)/13$, while the second structure yields $(4R_1 + R_2)/13$ and so on. The partial contributions have to be divided by the number of Kekulé structures in order to produce the molecular RE. In this way we find for RE of dibenzanthracene $(42R_1 + 14R_2 + 5R_3 + 3R_4 + R_5)/13$. Hence one can view the molecular RE as an average RE of the participating

Kekulé valence structures. This reconfirms that benzenoid hydrocarbons cannot be adequately represented by a single Kekulé valence structure, but manifest themselves as a superposition of all such structures. Interestingly, already a simple averaging is producing a sufficiently accurate picture of some molecular properties, such as the molecular resonance energies. Now instead of summing the contributions of conjugated circuits for each Kekulé valence structure separately we can alternatively first add all contributions for the individual rings, and than add all ring contributions to derive the overall result for the molecule. From ring codes we immediately obtain the partial contributions for rings. In the case of dibenzanthracene we have

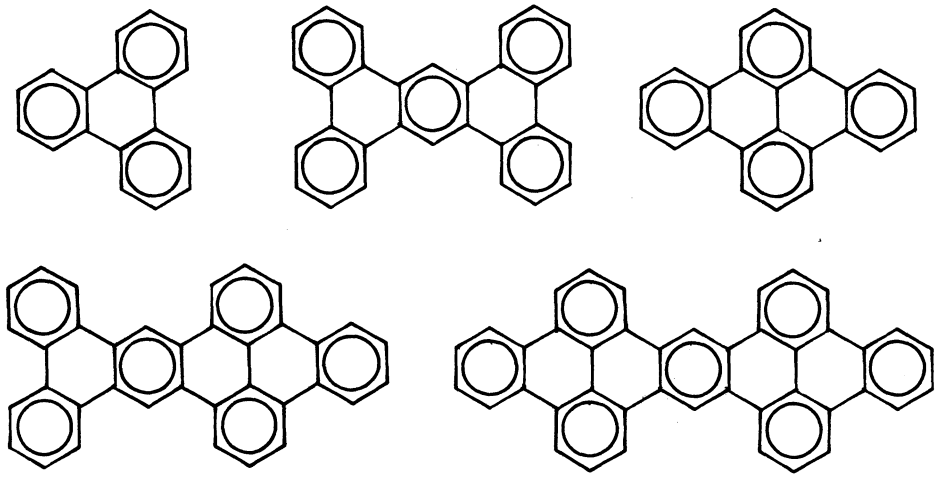
ring	resonance energy contribution
A	$(8R_1 + 4R_2 + R_3)/13$
B	$(8R_1 + 5R_2)/13$
C	$(2R_1 + 3R_2 + 4R_3 + 3R_4 + R_5)/13$
D	$(12R_1 + R_2)/13$

Molecular resonance energy is obtained as the sum: A + B + C + 2D . In order to obtain the numerical values for the RE one has to adopt some numerical values for the parameters R_1, R_2, R_3, etc. As discussed elsewhere (5), primarily to dispel some confusion that graph theory is "nothing but disguised Hückel MO method" we have deliberately selected available SCF MO calculations (10) for determining the magnitudes for the parameters R_n:

$R_1 = 0.869$ eV; $R_2 = 0.246$ eV; $R_3 = 0.100$ eV; $R_4 = 0.041$ eV.

Larger conjugated circuits are assumed to have negligible contributions. The agreement between the graph theoretical predictions and individually calculated SCF MO results was found to be within few hundredths of eV. Hence, one is justified in (a) considering only Kekulé valence structures in the study (i.e., ignoring the so called "long bond" structures); and (b) taking all Kekulé valence structures with a same weight. This does not mean that graph theoretical analysis cannot be extended beyond the above conditions, it only means that available data do not warrant at this moment such extensions.

The numerical values for the ring resonance energies in Table 1 imply the normalization which corresponds to averaging with respect to the number of Kekulé valence structures of the compound. This means that the ring code 6, 1 of benzanthracene and code 12, 2 of 1,2:3,4-dibenzphenanthrene (Table 2) indicate the same kind of ring when resonance energies are considered. The monotonic decrease of the parameters R_n with n leads to some regularities for the relative magnitudes of ring resonance energies. For instance rings with codes 1, 1; 2,1; 3,1; 4,1; ... give a monotonic sequence of ring RE: 0.558; 0.661; 0.713; 0.744; etc, which, as expected, converges to the limit 0.869, the RE of benzene. Among the rings of Table 1 the peripheral rings in triphenylene (RE = 0.800 eV) already approach the benzene limit, but in some larger benzenoid systems the similarity with the benzene ring is even more remarkable. Among the compounds studied in this paper, we find ring code 16, 1 in 1,2:3,4-dibenzanthracene (Table 2), but it is obvious that by considering even larger catacondensed benzenoid hydrocarbons the limit of benzene can be approached even more closely. The same can happen also for larger pericondensed systems. Many such large benzenoid compounds are known and particularly important class consists of compounds which Clar calls fully benzenoid (2). For these compounds one can write a valence structure in which a ring is either represented as an isolated sextet or is devoid of conjugation. Symbolically such rings have an inscribed circle or are empty:



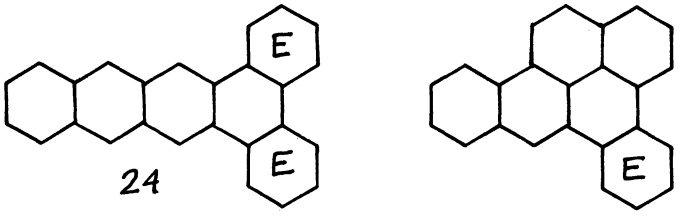
In comparing molecules, particularly molecules of different size, it is useful to evaluate the average ring resonance energy. This quantity can be viewed as a measure of the aromatic character of the molecule indicating the degree of delocalized conjugation. Benzene is the prototype of full delocalization, but as we go along the series of linearly fused benzene rings: naphthalene, anthracene, tetracene, and so on, as is well known, gradually pronounced differences with benzene emerge. The fully benzenoid compounds in this respect show an optimal local similarity with benzene in comparison with other molecules of a similar size with only a moderate decrease in the average ring resonance energies. The decrease of the average ring RE is related to the ratio of the number of "fully benzenoid" rings and "empty" rings. Hence, already such simple examination of molecular skeletons leads to a useful qualitative characterization of such compounds. Quantitatively the average ring resonance energy (RE/ring in Table 1) appears a plausible index for the degree of aromatic conjugation in benzenoid hydrocarbons. Such index is defined for all benzenoid systems, whether they are fully benzenoid or not. The qualitative ideas of Clar have found, in ring resonance energy and average ring resonance energy, the quantitative paragon.

RING CURRENTS

As an application of the concept of ring code, we will discuss the ring currents in fused ring compounds. The concept of ring currents, already considered by Pauling (11) over 40 years ago, is of interest in the computation of chemical shifts in NMR spectroscopy. Ring currents are not observable, but nevertheless proved useful for discussing magnetic properties of conjugated hydrocarbons. A number of publications reported the numerical values of ring currents for well over 300 rings in some 60 benzenoid systems (12-14). Although data are in abundance, it is significant how little was deduced from them concerning the origin for reported relative magnitudes as witnessed by the following quotations: "... in general, the ratios of the individual ring currents in the pentacyclic hydrocarbons to the benzene ring current do not differ drastically from unity..." (13), and "... in polycyclic molecules, the ring currents are, in general, greater than the ring currents in benzene, but fall rapidly with increase in condensation..." (14). We will see that with the help of the concept of conjugated circuits and the ring codes considerably more could be said about the relative magnitudes for the ring currents. In Table 2 we give ring codes and the ring currents (taken from the literature, ref. 13 and ref. 14) for a number of catacondensed benzenoid compounds having five and six fused rings. Molecular diagrams with labels for the rings listed in Table 2 are shown in Fig. 5. Immediately a number of interesting and important observations can be made regarding the relative values for the ring currents in these molecules:

(1) Nonequivalent rings (within a molecule) with the same code show the same ring current
(2) Rings with a same code in different molecules have the same ring current
(3) Rings with a dominant contribution from R_1 approach a ring current of 1.000
(4) Rings which have the smallest ring currents tend to have "long" codes (i.e., contributions from conjugated circuits of all sizes compatible with the structure)

We still are unable to discover fully the relationship between the codes and ring intensities and reduce such a relationship to some functional dependence. But it is remarkable that the simple graph theoretical approach already provides important guidance. There should be no doubts that the conjugated circuits play an important role here, since we find that rings in different molecules, such as rings A, B, C in molecules 12 and 13 have practically coinciding ring currents for the corresponding rings. Moreover, in molecule 14 we find rings which are nonequivalent but display same ring codes and same ring currents. The situation is even more impressive in the case of the "exposed" rings (E) of dibenzotetracene 24 and dibenzopyrene shown below



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since the compounds are hardly related, representing catacondensed and pericondensed systems respectively. Yet the rings E have the same code 16, 1 and approximately a same ring current (1.061 and 1.058 respectively). Ring currents of benzenoid hydrocarbons are calculated independently for each ring and for each molecule. Hence the observed coincidences convincingly demonstrate some common structural basis. We conclude that ring currents are transferable between rings of a same code, though a caution is needed when extending such considerations to pericondensed systems. There are indications that additional factors may influence the magnitudes of the ring currents: (1) While the same ring codes indicate the same ring current the opposite is not necessarily true. For example rings 4, 3, 3, 1 and 6, 4, 1 which involve a large participation of conjugated circuits of dif-

TABLE 2. Ring codes and the ring currents for selected catacondensed benzenoid hydrocarbons

Molecule	Ring	Code	Ring currents			
10 Pentacene						
	A	2, 1, 1, 1, 1	1.06			
	B	2, 2, 1, 1	1.30			
	C	2, 2, 2	1.35			
11 1,2-benztetracene						
	A	4, 2, 2, 1	1.09			
	B	4, 4, 1	1.32			
	C	4, 3, 2	1.35			
	D	2, 2, 2, 2, 1	0.85			
	E	8, 1	1.11			
12 1,2:5,6-dibenzanthracene						
13 1,2:7,8-dibenzanthracene						
	A	10, 2	1.14	1.14		
	B	4, 4, 3, 1	0.94	0.94		
	C	8, 4	1.29	1.29		
14 1,2:5,6-dibenzphenanthrene						
15 Picene						
16 3,4:5,6-dibenzphenanthrene						
	A	10, 3	1.15	1.15	1.16	1.15
	B	6, 5, 2	1.06	1.05	1.06	1.06
	C	8, 4, 1	1.16	1.15	1.16	
17 2,3:7,8-dibenzphenanthrene						
18 2,3:5,6-dibenzphenanthrene						
	A	6, 3, 2	1.12	1.12		
	B	6, 5	1.30	1.30		
	C	4, 3, 3, 1	0.99	1.00		
	D	6, 4, 1	1.08	1.08		
	E	8, 3	1.15	1.14		
19 Penthaphene						
	A	6, 3, 1	1.11			
	B	6, 4	1.23			
	C	2, 2, 3, 2, 1	0.78			
20 1,2:3,4-dibenzanthracene						
	A	8, 4, 1	1.12			
	B	8, 5	1.21			
	C	2, 3, 4, 3, 1	0.65			
	D	12, 1	1.08			
21 1,2:3,4-dibenzphenanthrene						
	A	12, 2	1.13	1.14		
	B	4, 5, 4, 1	0.85			
	C	8, 5, 1	1.09			
	D	10, 4	1.10			
22 1,2:7,8-dibenzotetracene						
23 1,2:9,10-dibenzotetracene						
	A	14, 2	1.121	1.119		
	B	4, 4, 4, 3, 1	0.877	0.876		
	C	8, 6, 2	1.299	1.298		
24 1,2:3,4-dibenzotetracene						
	A	8, 4, 4, 1	1.094			
	B	8, 8, 1	1.311			
	C	8, 5, 4	1.194			
	D	2, 3, 4, 4, 3, 1	0.603			
	E	16, 1	1.061			
25 3,4-benzopenthaphene						
	A	10, 5, 2	1.121			
	B	10, 7	1.257			
	C	4, 4, 5, 3, 1	0.839			
	D	12, 5	1.262			
	E	6, 6, 4, 1	0.951			
	F	14, 3	1.138			

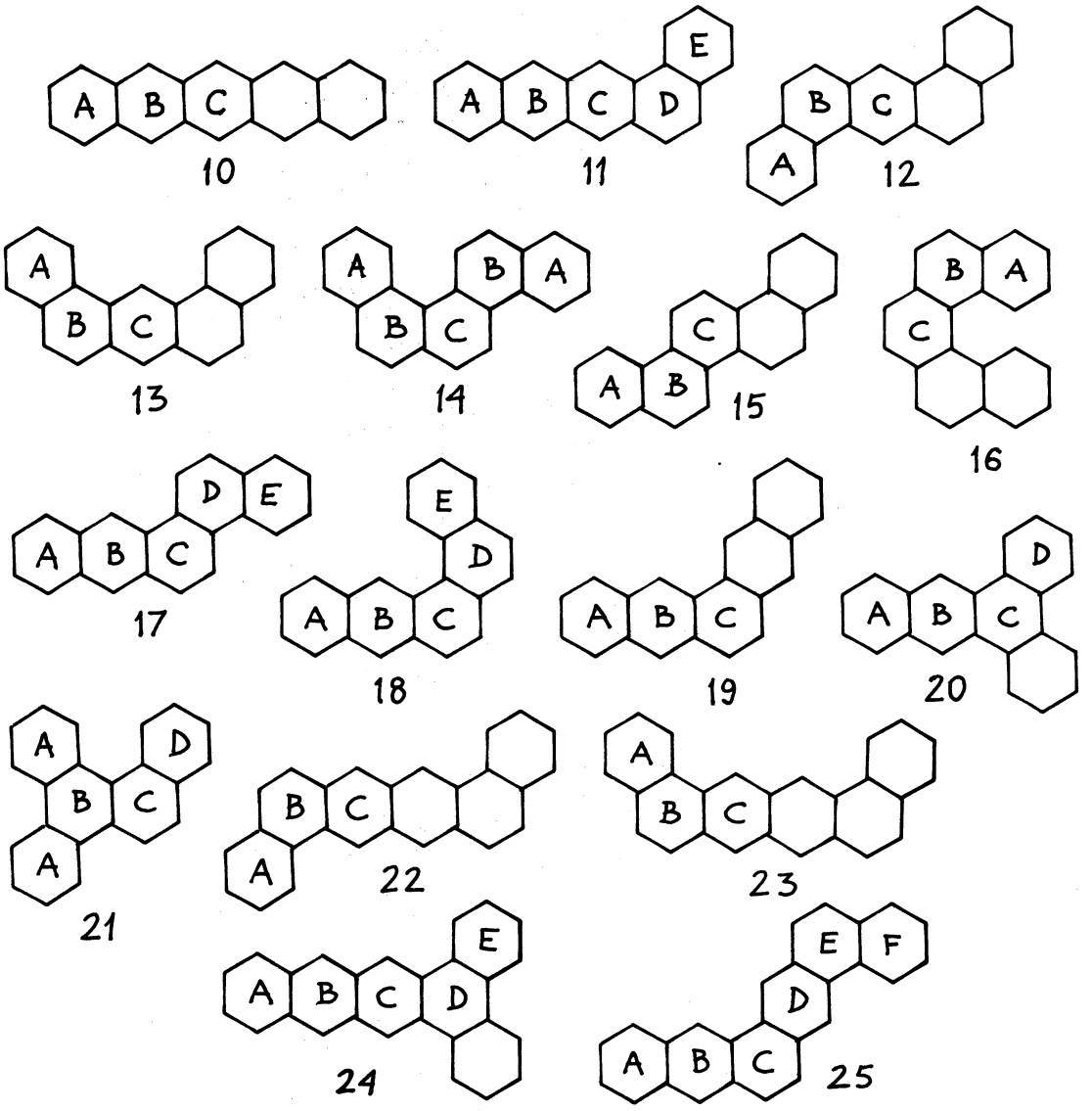
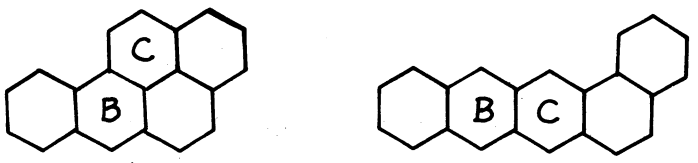


Fig. 5. Molecular diagrams and labeling of rings for benzenoid systems of Table 2.

ferent size have nevertheless ring currents close to the value of benzene ring; and (2) Occasionally rings having a same code (but belonging to less similar structures, e.g., catacondensed vs pericondensed benzenoid system) have profoundly different ring currents. For example, while rings B in 3,4-benzpyrene and 1,2-benztetracene



have a same code and reasonably similar ring currents (1.28 and 1.32 respectively) the rings C of the same compounds have also a same code but show very different ring currents (1.08 and 1.35 respectively). The origin of such discrepancies, be it spurious or genuine, need to be clarified. There are several factors which can possibly influence ring currents and which have not been here considered. In considering conjugated circuits we have registered for each ring only a presence of the smallest conjugated circuit involved. Then

the shape and the area of conjugated circuits may make an important difference for rings which have a same ring code. Finally disjoint conjugated circuits, the properties of which have been considered (15), may also play here some role.

The novel viewing on rings and ring contributions has still not resolved the issue of the relative magnitudes of ring currents in benzenoid systems. The problem has been challenge for a decade and more to quantum chemists and continue to be elusive. We are not surprised for the past lack of understanding of the relative magnitudes for ring currents. Strictly speaking the task is outside the usual scope of applied quantum mechanics since it is conceptual not computational. The concept of conjugated circuits definitely offered some guidance. To find explanation fully one needs more numerical results on additional rings and compounds. This part has to come from quantum mechanical calculations, it will not clarify the present difficulties, but may pave way to subsequent graph theoretical efforts and help in recognizing important factors. Graph theory normally does not produce new data, but hopefully can relate meaningfully the available data with a help of appropriate graph invariants. Combined quantum mechanical calculations and graph theoretical considerations are likely to further clarify the problem and possibly offer a complete understanding. The situation is a good illustration of the different character of the two important theoretical tools: quantum mechanics and graph theory.

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