CROATICA CHEMICA ACTA CCACAA **55** (4) 347—369 (1982)

YU ISSN 0011—1643
CCA-1340 UDC 541.62;547.53
Original Scientific Paper

Application of Reduced Graph Model to the Enumeration of Kekulé Structures and Conjugated Circuits of Benzenoid Hydrocarbons

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Received January 18, 1982

The reduced graph model which represents an alternative way of depicting hexagonal networks is reviewed. This model is exploited in several enumeration problems of benzenoid systems. It is used as a basis for »pencil and paper« algorithms for counting Kekulé structures, conjugated circuits and cata-condensed isomers of benzenoid hydrocarbons.

INTRODUCTION

We have recently developed a **reduced graph model** as an alternative way to represent benzenoid-type networks.[1] This model has shown itself to be very useful for computer enumeration and generation of Kekulé structures in benzenoid hydrocarbons. Since Kekulé structures are important quantities in the resonance theory and lattice statistics, the reduced graph model appears to be an interesting approach in further applications. Consequently we decided to test the reduced graph model in connection with some other enumeration problems of benzenoid systems. However, since the problem of enumerating the Kekulé structures is continually being discussed in the literature,[2-16] we have also decided to report on this question from another angle and to show how the reduced graph model could easily be used not only for cata- but also for peri-condensed benzenoid hydrocarbons. Therefore, we will be discussing the enumeration of Kekulé structures, conjugated circuits and cata-condensed isomers of benzenoid hydrocarbons by means of the reduced graph model. The number of Kekulé structures and the number of conjugated circuits are quantities needed in the structure-resonance theory[17-20] and in the conjugated circuits model of Randić.[21-26] The conjugated circuits model was also independently introduced by Gomes.[26a]

The counting of all benzenoid systems for a given number of benzene rings, is supposed to be an unsolvable problem.[27-30] Therefore, we decided to attack the problem by means of the reduced graph model and to see how the model could be used in this area. However, our paper will deal in this case only with cata-condensed benzenoid hydrocarbons.

THE REDUCED GRAPH MODEL OF BENZENOID HYDROCARBONS

Ordinarily benzenoid hydrocarbons are represented by hydrogen-suppressed[31] bipartite[32] planar[32] molecular graphs[33] which are called benzenoid graphs.[34] They are usually denoted by the symbol G. A standard convention is used for the construction of these graphs, *i. e.* vertices replace carbon atoms and edges replace carbon-carbon bonds.[33] In our previous work[1] and in contrast to some other work in this field,[35,36] the single bonds are represented by a single connecting line and the double bonds by two connecting lines. Consequently, the vertex valency[32-34] in these graphs is either 3 or 4. Thus, vertices belonging simultaneously to two rings necessarily have valency 4.

Since benzenoid graphs are planar graphs, we need to define the planarity of graphs. A graph is planar if it is isomorphic to some plane graphs. If a graph can be embedded in a plane in such a way that no pair of its edges cross, it belongs to the class of plane graphs.[32] A plane graph partitions the plane into one infinite (external) and several finite (internal) regions. These finite regions are called faces.[32] The edges limit the faces of the graph, which are hexagons in benzenoid graphs.

A vertex can belong either to the interior of an arbitrary cycle or it can lie on the boundary of the infinite region of the graph. The former vertices are called internal vertices, while the latter are called external vertices (see Figure 1). The interior of a graph is a finite region which is not bounded to the infinite region.

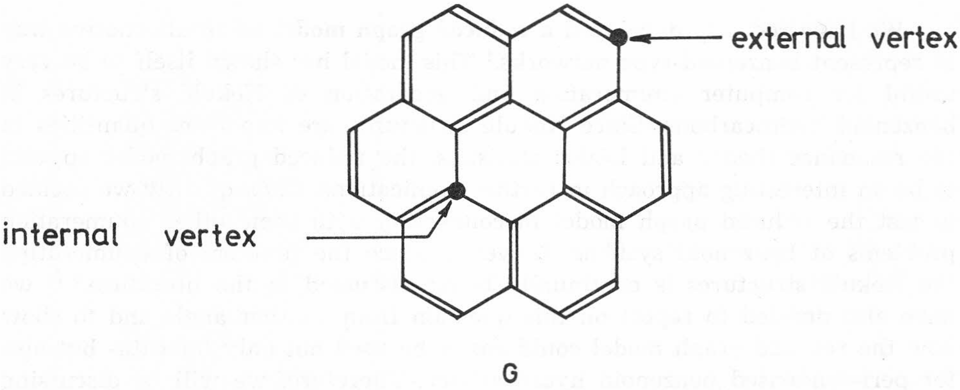
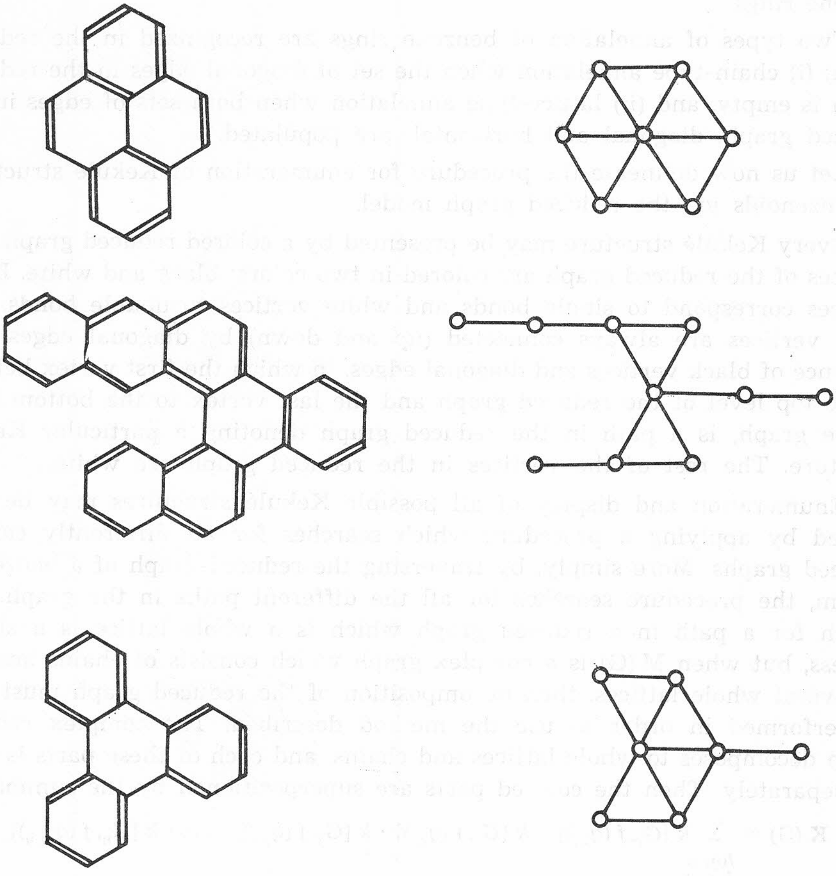


Figure 1. External and internal vertices

All internal vertices have valency 4. External vertices may have valencies 3 or 4.

Every benzenoid hydrocarbon may be presented as part of an infinite hexagonal planar lattice. Three sets of parallel edges, (vertical, left and right) arranged in rows, are recognized in the lattice. A new infinite triangular planar lattice T may be produced from the lattice H. This can be done in the following way. The vertices of the lattice T are the vertical edges of H. Two vertices of T are connected if (a) the corresponding edges belong to the same ring in H, or if (b) the corresponding edges are in the adjacent rings of H, and their distance is one. The lattice T has two disjunctive sets of edges that are called »diagonal« and »horizontal« edges. The degree of vertices in T is 6. If the same operation is performed on the benzenoid graph G, the graph M (G) is obtained. The graph M (G) represents a »reduced« graph of G. Some examples of benzenoid graphs and the corresponding reduced graphs are presented in Figure 2.



benzenoid graph G reduced graph M(G)

Figure 2. Examples of reduced graphs

The reduced graph model of benzenoid hydrocarbons has great potential for treating various types of isomer enumeration problems of these hydrocarbons. This will be demonstrated on subsequent pages.

KEKULÉ STRUCTURES AND REDUCED GRAPHS

Recently we had reported[1] on a novel algorithm for enumeration and display of Kekulé structures in benzenoid hydrocarbons, which was based on the search of paths in the binary tree generated from the reduced graph of the molecule. This algorithm is also applicable to some non-benzenoid hydrocarbons, alternant and non-alternant, if they can be reduced or enlarged to benzenoid structures by the appropriate graph-theoretical transformations.[37,38] This does not alter the number of Kekulé structures. The essentials of the reported algorithm will be summarized below. However, before proceeding to the discussion of the algorithm for enumeration of Kekulé structures in benzenoid systems, we need to describe the kinds of annelation found in the benzene rings.

Two types of annelation of benzene rings are recognized in the reduced graph: (*i*) chain-type annelation when the set of diagonal edges in the reduced graph is empty, and (*ii*) lattice-type annelation when both sets of edges in the reduced graph, diagonal and horizontal, are populated.

Let us now delineate the procedure for enumeration of Kekulé structures of benzenoids via the reduced graph model.

Every Kekulé structure may be presented by a colored reduced graph. The vertices of the reduced graph are colored in two colors: black and white. Black vertices correspond to single bonds and white vertices to double bonds. The black vertices are always connected (up and down) by diagonal edges. The sequence of black vertices and diagonal edges, in which the first vertex belongs to the top level of the reduced graph and the last vertex to the bottom level of the graph, is a path in the reduced graph denoting a particular Kekulé structure. The rest of the vertices in the reduced graph are white.

Enumeration and display of all possible Kekulé structures may be performed by applying a procedure which searches for all differently colored reduced graphs. More simply, by traversing the reduced graph of a benzenoid system, the procedure searches for all the different paths in the graph. The search for a path in a reduced graph which is a whole lattice is a simple process, but when M (G) is a complex graph which consists of chains and one or several whole lattices, then decomposition of the reduced graph must first be performed in order to use the method described. The complex reduced graph decomposes to whole lattices and chains, and each of these parts is colored separately. Then the colored parts are superpositioned by the summation,

$$\mathrm{K}(\mathrm{G}) = \sum_{\substack{f(q_{i,j})\\ f(q_{j,k})\\ \vdots \\ f(q_{m,n})}} k\,[\mathrm{G}_i, f(q_{i,j})] \cdot k\,[\mathrm{G}_j, f(q_{i,j})] \cdot k\,[\mathrm{G}_j, f(q_{j,k})] \cdot \ldots \cdot k\,[\mathrm{G}_n, f(q_{m,n})] \qquad (1)$$

where $k\,[\mathrm{G}_i, f(q_{i,j})]$ is a coloring of the graph (M (G_i), while $f(q_{i,j})$ is some coloring of the path $q_{i,j}$ in the colored superimposed structure consisting of M (G_i) and M (G_j). If the composite graph M (G) consist of only M (G_i) and M (G_j), then the product $k\,[\mathrm{G}_i, f(q_{i,j})] \cdot k\,[\mathrm{G}_j, f(q_{i,j})]$ represents a Kekulé structure of G. The set of all possible Kekulé structures is equal to the sum of all colorings of the paths $q_{i,j}, q_{j,k}, \ldots, q_{m,n}$. The path q are sequences of vertices and diagonal edges which decompose the reduced graph M (G) into subgraphs M (G_i), M (G_j), M (G_k), . . ., M (G_m), M (G_n). The possible colors of the vertices in path $q_{i,j}$ are presented in Table I.

TABLE I

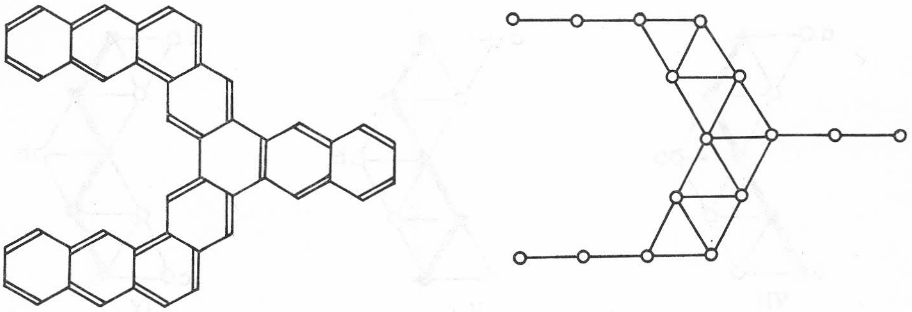
The colors of the vertices on the path $q_{i,j}$

Color of the vertex in G_i	Color of the vertex in G_j	Color of the vertex in G
black	black	$\emptyset$
black	white	black
white	black	black
white	white	white

The procedure described was implemented in a computer program.[1,39] The output of the program is the set of all possible Kekulé structures labelled and displayed. This method for enumeration of Kekulé structures may be simplified and used straightforwardly without the aid of a computer. In what follows we will discuss how to obtain the number of Kekulé structures by the »pencil and paper« method.

THE »PENCIL AND PAPER« METHOD FOR ENUMERATION OF KEKULÉ STRUCTURES IN BENZENOID HYDROCARBONS

Let us consider a sufficiently complex benzenoid structure such as the one presented in Figure 3.



benzenoid graph G **reduced graph M(G)**

Figure 3. An example of the complex benzenoid hydrocarbon and the corresponding reduced graph

The corresponding reduced graph consists of three chains and one whole lattice. Let us assign these constituent parts of the reduced graph M(G) as M(G_1), M(G_2), M(G_3) and M(G_4). Coloring the chains M(G_2), M(G_3) and M(G_4) produces three differently colored structures for every chain. Coloring the whole lattice M(G_1) produces 10 differently colored lattices as is shown in Figure. 4.

The vertices at which the chains join the whole lattice are denoted by *a*, *b* and *c*. The terminal vertices of the chains which represent the points of attachments to the lattice are colored twice with black and once with white (see Figure 5).

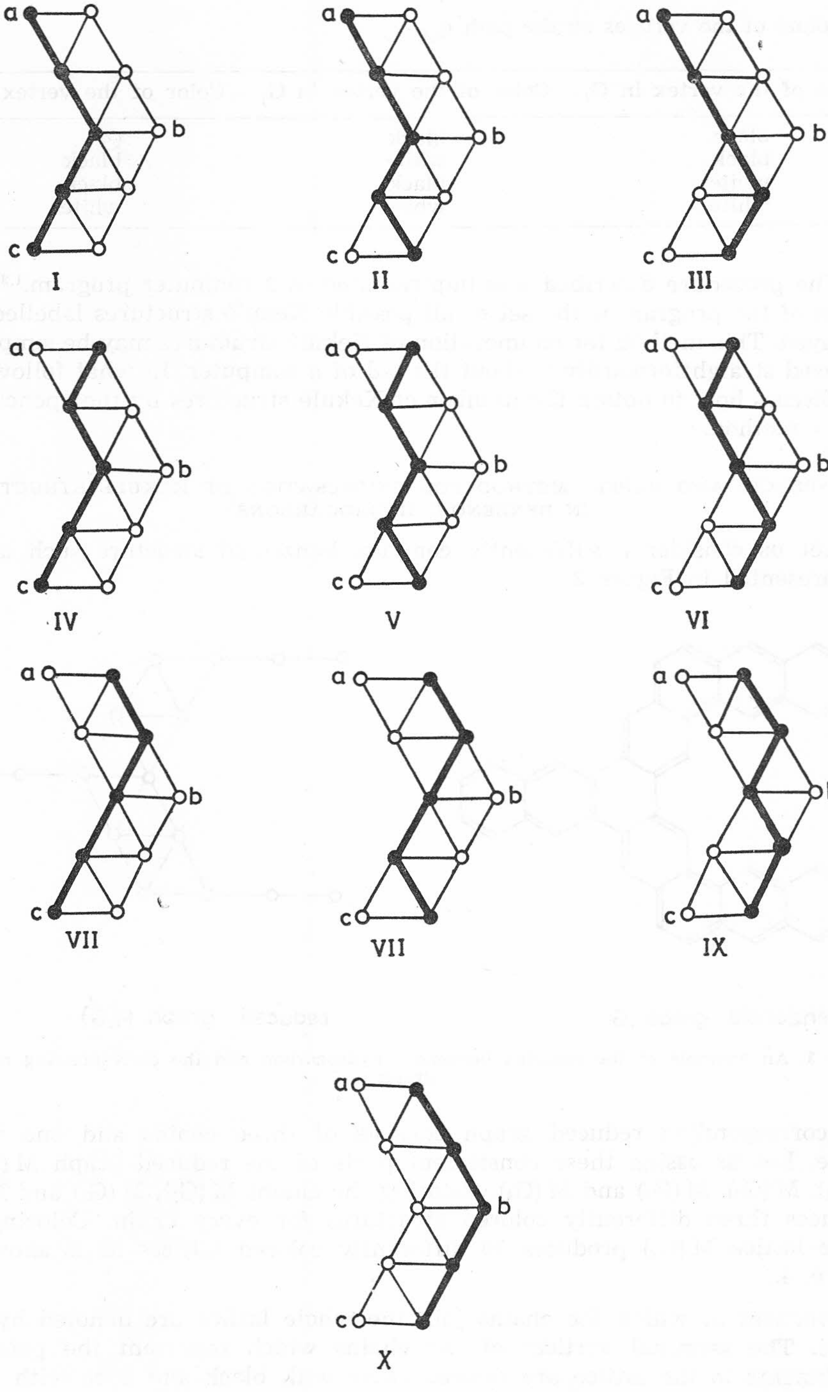


Figure 4. The path count in the M (G$_1$) lattice

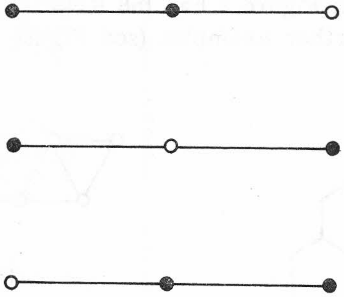


Figure 5. Coloring of the $M(G_i)$ ($i = 2, 3, 4$) chain

If $M(G)$ is a chain of v vertices then it can be colored differently v times. The terminal vertices are colored black v-1 times, and once white.

Let us now calculate the number of colored reduced graphs obtained by joining $M(G_1)$ and $M(G_2)$, $M(G_3)$ and $M(G_4)$.

vertex a

Vertex a is colored black, thus, only one of the $M(G_2)$ chains can be superpositioned and only one new structure is generated.

vertex b

Vertex b is colored white, thus, $M(G_1)$ and all three differently colored structures that correspond to the $M(G_3)$ chain may be joined and 3 new structures generated.

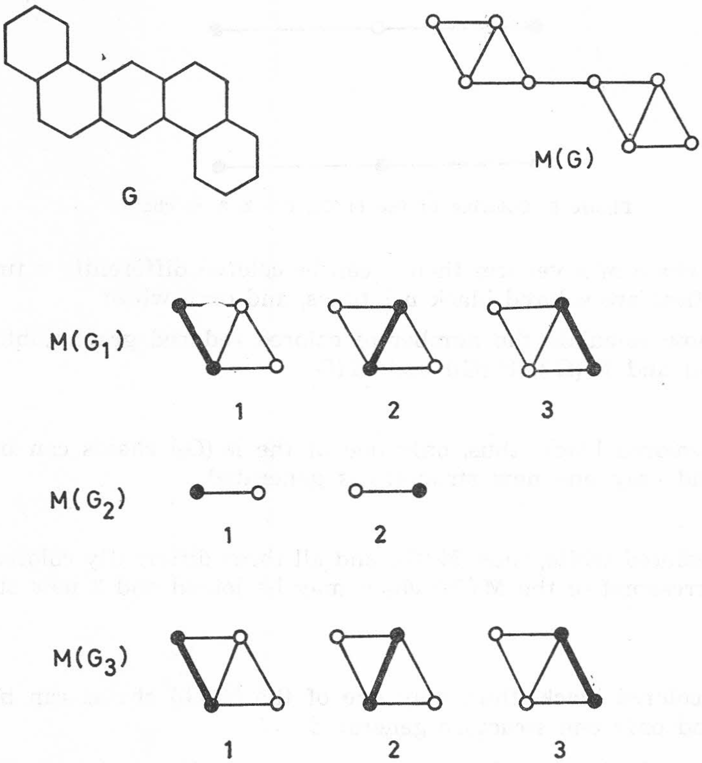
vertex c

Vertex c is colored black, thus, only one of the $M(G_4)$ chains can be superpositioned and only one structure generated.

Applying the rule of product (1) we can compute the number of differently colored reduced graphs that can arise from superpositioning $M(G_1)$ lattices and $M(G_2)$, $M(G_3)$ and $M(G_4)$ chains:

$M(G_1)$	Product $a \cdot b \cdot c$	Coloring of the terminal vertices
I	$1 \cdot 3 \cdot 1 = 3$	Vertex b is white
II	$1 \cdot 3 \cdot 3 = 9$	Vertices b and c are white
III	$1 \cdot 3 \cdot 3 = 9$	Vertices b and c are white
IV	$3 \cdot 3 \cdot 1 = 9$	Vertices a and b are white
V	$3 \cdot 3 \cdot 3 = 27$	Vertices a, b and c are white
VI	$3 \cdot 3 \cdot 3 = 27$	Vertices a, b and c are white
VII	$3 \cdot 3 \cdot 1 = 9$	Vertices a and b are white
VIII	$3 \cdot 3 \cdot 3 = 27$	Vertices a, b and c are white
IX	$3 \cdot 3 \cdot 3 = 27$	Vertices a, b and c are white
X	$3 \cdot 1 \cdot 3 = 9$	Vertices a and c are white
Total	156	

Therefore the molecule in Figure 3 has 156 Kekulé structures. This procedure is illustrated for two further examples (see Figure 6).



	$M(G_2)_1$ $M(G_3)_{1,2,3}$	$M(G_2)_2$ $M(G_3)_{1,2,3}$
$M(G_1)_1$	3	2
$M(G_1)_2$	3	2
$M(G_1)_3$	0	2

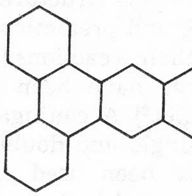
$K(G) = 6 + 6 = 12$

continued on page 355

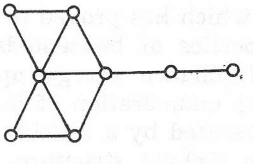
Figure 6

The advantage of this method over the earlier techniques for enumeration of Kekulé structures[3-16] is that the method is general and therefore, it covers all kinds of geometrically planar benzenoid structures.

Figure 6 continued from page 354

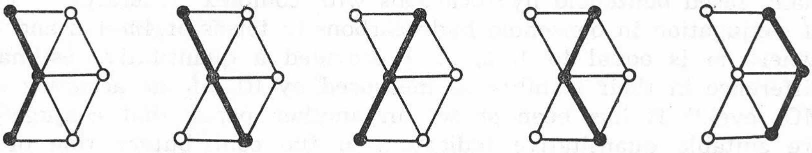


G



M(G)

$M(G_1)$



$M(G_2)$

	$M(G_2)_{1,2,3}$
$M(G_1)_1$	3
$M(G_1)_2$	3
$M(G_1)_3$	3
$M(G_1)_4$	3
$M(G_1)_5$	1
K =	13

Figure 6. Examples of computing the number of Kekulé structures without the use of computer

REDUCED GRAPHS AND CONJUGATED CIRCUITS

Kekulé structures have been used as a basis for deriving the resonance energies, RE, by means of two approaches. In the work of Herndon and Ellzey[17] the resonance energies of benzenoid hydrocarbons were calculated by using a set of equally-weighted Kekulé structures. The quality of the calculated RE was on the level of Dewar's semiempirical SCF MO results.[17,19] In addition, Herndon has used Kekulé structures as a foundation for his structure-resonance theory which has proved to be useful for interpreting and predicting a number of properties of benzenoids and for rationalizing their reactions.[17–20] In the other resonance energy approach, Kekulé structures have been used as a basis for enumeration of individual conjugated circuits.[21] A conjugated circuit is represented by a regular alternation of formally single and double bonds in a given Kekulé structure. Conjugated circuits have been used as essential elements for deriving the resonance energies of conjugated hydrocarbons.[21–23,25] In the expressions of RE the main features are the numbers of conjugated circuits with different numbers of CC bonds. By using the model of conjugated circuits Randić was able to predict, with remarkable accuracy, the RE's of many fused benzenoid hydrocarbons with complex structure.[21,25] The analysis of conjugation in benzenoid hydrocarbons in terms of $4m + 2$ and $4m$ circuits (where m is equal to 1, 2, ...) provided a quantitative estimate for the difference in their stability as measured by RE of the accuracy of the SCF MO level.[21] It has been shown in another paper that conjugated circuits are suitable quantitative indicators of the contributory role of individual Kekulé structures in the aromatic stability of the molecule.[26] Individual Kekulé structures each provide a different contribution to the total RE of a molecule. It was also noted that it is the conjugated circuits, not fragments such as individual bonds or rings, which are the essential structural elements to consider when discussing the properties of conjugated hydrocarbons.[21–26,40,41]

The search for conjugated circuits as well as their enumeration demands a list of all Kekulé valence structures of a compound. While there is no difficulty in deriving all Kekulé structures for a compound consisting of a few condensed rings, the situation is quite different when larger molecules are analysed. However, the problem of obtaining all Kekulé forms of such complex benzenoid hydrocarbons has been successfully solved by adopting the procedure described in section 3 to computer use.[1,39] The complete set of Kekulé structures is generated in the form of colored reduced graphs and corresponding benzenoid graphs. Comparison of the properties of the reduced graphs and conjugated circuits in a particular Kekulé structure has shown that the recognition and enumeration of conjugated circuits is far more easy and reliable if colored reduced graphs are used instead of the Kekulé structures. Let us now illustrate this by examining some examples. First we must recognize the basic forms of conjugated circuits represented as reduced graphs which will be analysed in the reduced graph of the molecule.

(a) Reduced graphs as a chain

When the reduced graph is a chain, the colorings have the property of a conjugated circuit, R_n (see Figure 7).

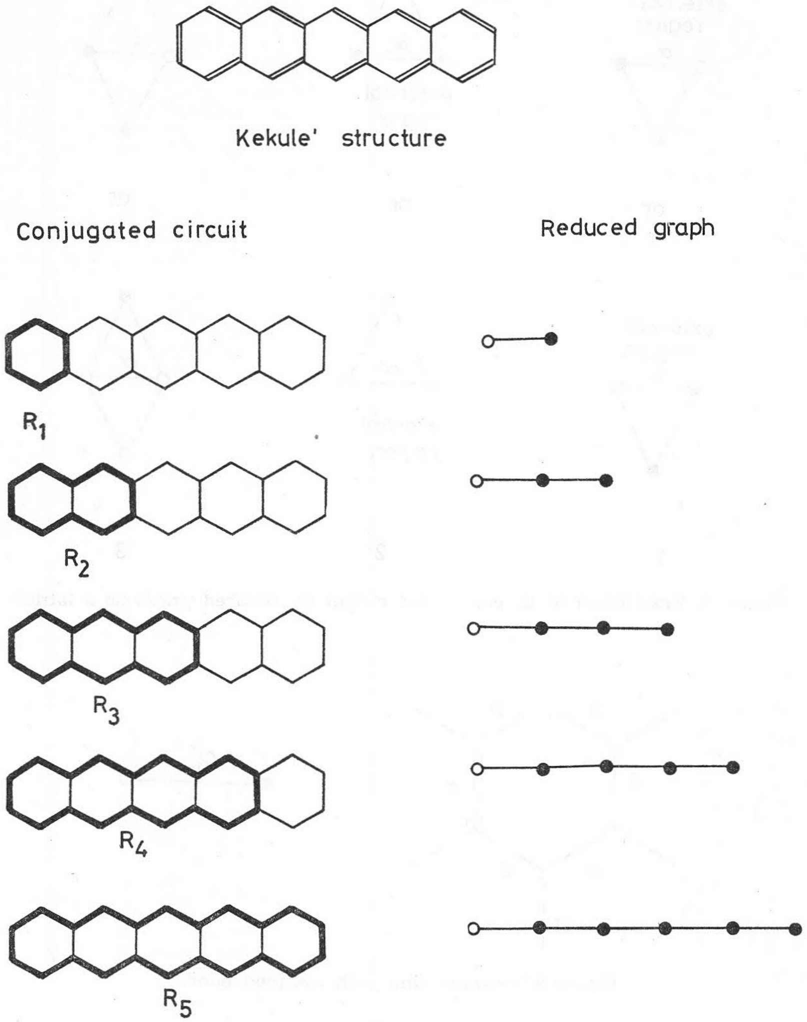


Figure 7. Reduced graphs representing the conjugated circuits

(b) Reduced graphs as a lattice

When the reduced graphs is a whole lattice, then R_1 may be found in three different environments. This is illustrated in Figure 8.

The dotted lines mean that the edge ●——○ lies in a triangle in which two black colored vertices are present. Let us explain this statement. In Figure 9 a benzene ring is given with the assigned bonds as *a, b, c, d, e* and *f*. If the bonds *a* and *b* are on the border of the external region, then bond *f* is single (the black vertex in the corresponding reduced graph) and bond *c* is double (the white vertex in the corresponding reduced graph) by definition.

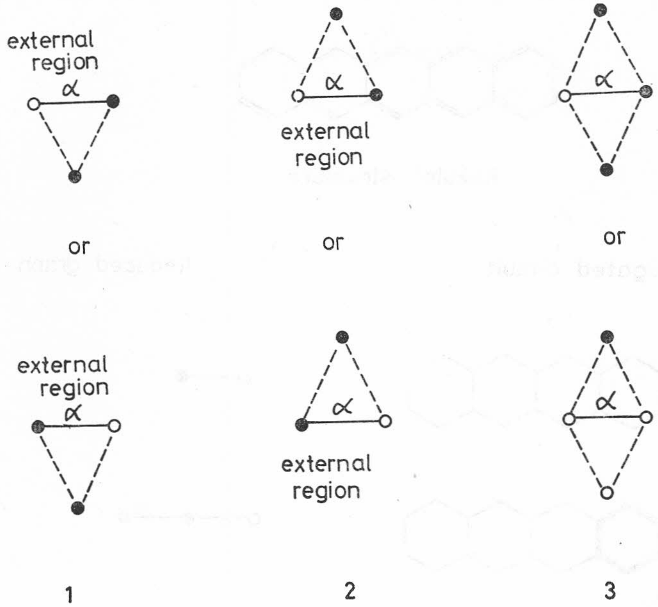


Figure 8. Description of R_1 conjugated circuit by reduced graph as a lattice

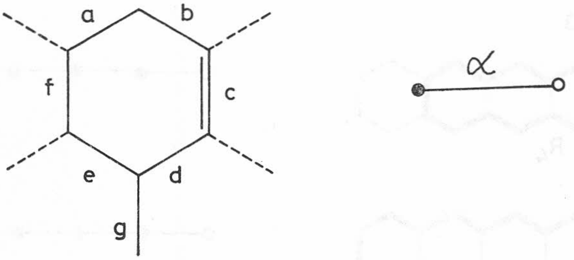


Figure 9. Benzene ring with assigned bonds

Bond *a* is then obviously double since there are no valency constraints regarding the vertex at which bonds *a* and *b* join, *i. e.* this vertex must have valency 3. The ring would be a conjugated circuit R_1 only if bond *g* is single and consequently bond *e* double. Or, in other words, the reduced graph consisting of the edge α and the adjacent vertices is a representation of a conjugated circuit R_1 only when it is part of a triangle in which two black vertices are present. When the benzene ring is part of the internal region of the graph, then the edge α is a diagonal of a square in which there are three black vertices and one white vertex.

Conjugated circuits of the R_2-type are represented by colored reduced graphs which are diamond-shaped, *i. e.* have the shape of a rhombus (see Figure 10).

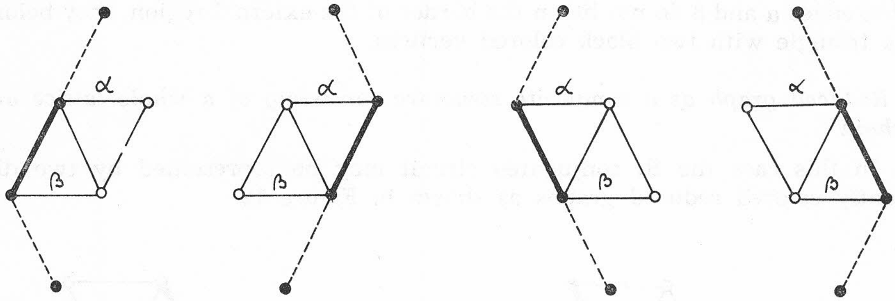


Figure 10. Description of R_2 conjugated circuit by reduced graph as a lattice

The edges denoted by α and β are on the border of the external region or are parts of triangles with two blue colored vertices.

Conjugated circuits of the R_3-type in the form of colored reduced graphs are given in Figure 11.

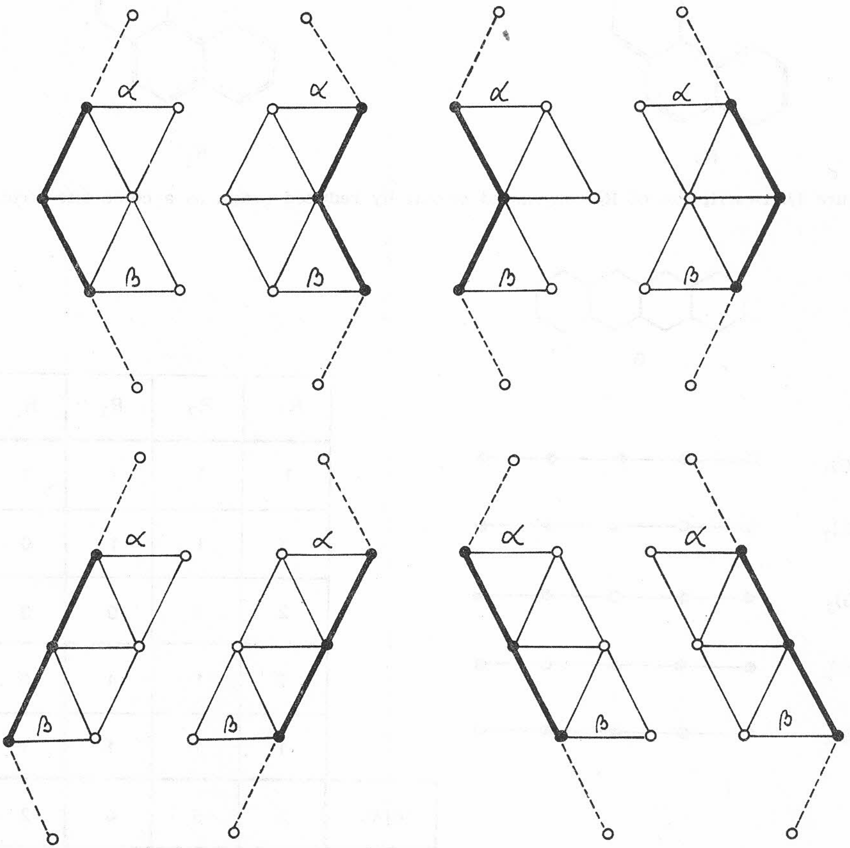


Figure 11. Description of R_3 conjugated circuit by reduced graph as a lattice

When edges α and β do not lie on the border of the external region, they belong to a triangle with two black colored vertices.

(c) Reduced graph as a composite structure consisting of a whole lattice and a chain

In this case the R_3 conjugated circuit may be represented by two differently colored reduced graphs as shown in Figure 12.

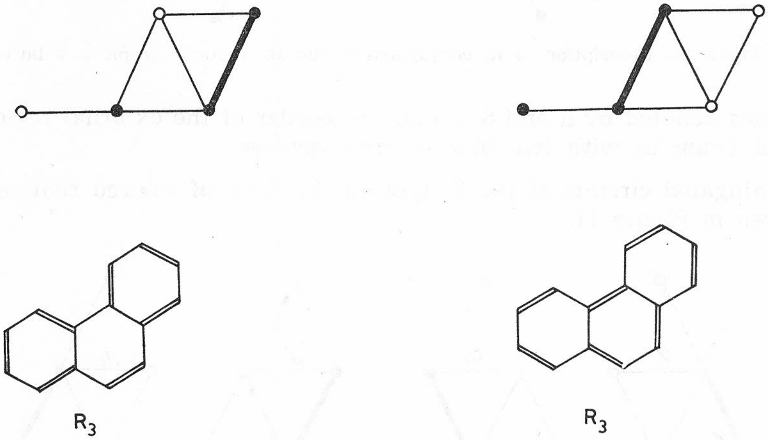
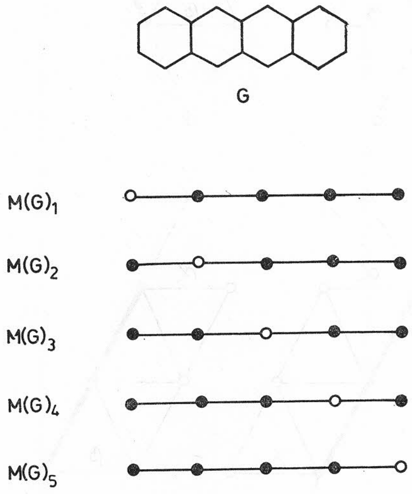


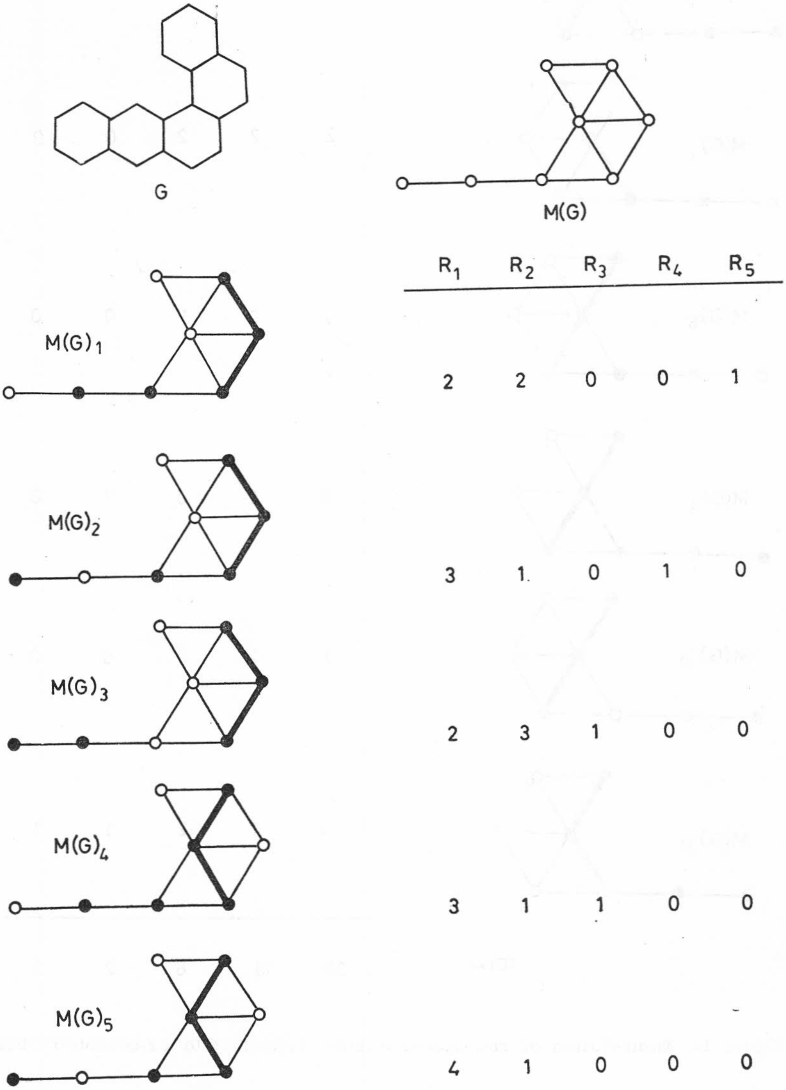
Figure 12. Description of R_3 conjugated circuit by reduced graph as a composite structure



	R_1	R_2	R_3	R_4
	1	1	1	1
	2	1	1	0
	2	2	0	0
	2	1	1	0
	1	1	1	1
TOTAL	8	6	4	2

Figure 13. Enumeration of conjugated circuits belonging to tetracene

How this procedure works when one wants to use it for the enumeration of conjugated circuits is shown in Figure 13 and Figure 14.



	R_1	R_2	R_3	R_4	R_5
$M(G)_1$	2	2	0	0	1
$M(G)_2$	3	1.	0	1	0
$M(G)_3$	2	3	1	0	0
$M(G)_4$	3	1	1	0	0
$M(G)_5$	4	1	0	0	0

continued on page 362

Figure 14

Figure 14 continued from page 361.

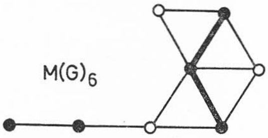
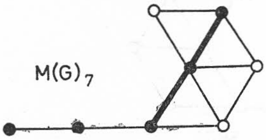
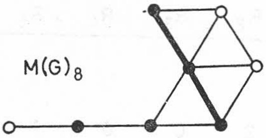
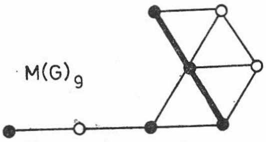
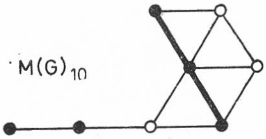
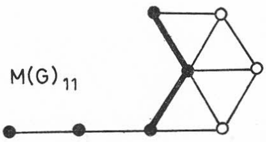
$M(G)_6$		4	1	0	0	0
$M(G)_7$		2	2	2	0	0
$M(G)_8$		2	2	1	0	0
$M(G)_9$		3	2	0	0	0
$M(G)_{10}$		3	2	0	0	0
$M(G)_{11}$		2	1	2	1	1
	TOTAL	30	18	6	2	2

Figure 14. Enumeration of conjugated circuits belonging to 1,2-benzotetraphene

Some additional results are presented in condensed form in Figure 15.

Results in Figure 13, Figure 14 and Figure 15 agree fully with Randić's original enumerations.

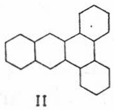
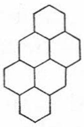
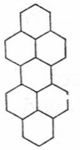
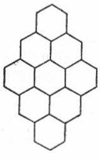
Molecular graph G	Number of conjugated circuits R_n	Number of Kekulé structures
 I	$R_1 = 40$ $R_2 = 20$ $R_3 = 10$ $R_4 = 4$ $R_5 = 2$	$K = 13$
 II	$R_1 = 42$ $R_2 = 14$ $R_3 = 6$ $R_4 = 3$ $R_5 = 1$	$K = 13$
 III	$R_1 = 24$ $R_2 = 18$ $R_3 = 14$ $R_4 = 10$	$K = 10$
 IV	$R_1 = 58$ $R_2 = 42$ $R_3 = 24$ $R_4 = 22$ $R_5 = 16$	$K = 18$
 V	$R_1 = 60$ $R_2 = 48$ $R_3 = 36$ $R_4 = 36$ $R_5 = 26$	$K = 20$

Figure 15. Enumeration of conjugated circuits belonging to 3,4,5,6-dibenzophenanthrene (I), 1,2,3,4-dibenzoanthracene (II), anthanthrene (III), peropyrene (IV), and 5,6,12,13-dibenzoperopyrene (V).

REDUCED GRAPHS AND THE ENUMERATION OF CATA-CONDENSED POLYHEXES

Enumeration of the number of structural isomers of benzenoid hydrocarbons is a very challenging problem.[28] Studies in pure mathematics, where such systems are known as hexaminoes or hexagonal animals,[42] have shown that it will be difficult to develop a general formula for obtaining their number. However, some computer calculations have yielded results for the first eight benzenoids, which are also known in the literature as arenes or polyhexes.[43,44] Another computer program by Lunnon[45] has enabled computations to be made for polyhex systems containing up to twelve hexagons (benzene rings). Recently, Knop and co-workers[46] have developed an algorithm for the enumeration of polyhexes which has been adapted to computer calculations. It produced all polyhexes up to 12 benzene rings and its results differ slightly from those of Lunnon in the cases of overlap. From the reported results it is evident that the number of possible structures increases very sharply with increasing N, the number of benzene rings in the structure. The benzenoid cata-condensed structures for $N \leqslant 8$ have been drawn in the form of their inner dual graphs by Balaban and Harary.[47] It is interesting to note here that Smith,[48] in his discussion on capacitive energy and ionization potentials of benzenoid hydrocarbons has drawn these molecules in a short-hand notation which is identical to the Balaban-Harary graphs. Thus, unconsciously, he was the first to use this graph-theoretical depiction of benzenoid systems. General formulae are available for enumerating the members of particular classes of catacondensed benzenoids, i. e. those that are in the form of unbranched chains,[47,49] or of branched chains.[50]

While studying the properties of the reduced graphs, we have arrived at a result which shows that they could be used for developing a systematic and reliable procedure for the enumeration and display of the set of all possible isomeric benzenoid hydrocarbons. It must be noted that the computer enumerations already reported represent only a few possible ways of producing a solution to the problem of »cell-growth« with hexagonal animals. For example, in these papers no account has been taken of hydrogen atoms, whose total number will vary among the structures for a given N value. However, attempts have also been made in this direction.[51]

We tried to solve this problem by defining a set of basic reduced graphs. The elements of the set containing the basic reduced graphs are: chains of one or two benzene rings, and lattices constructed of two, three and four benzene rings. Cata-condensed structures of up to 6 benzene rings are constructed by systematically combining the elements of the basic set. These results are presented in Figure 16.

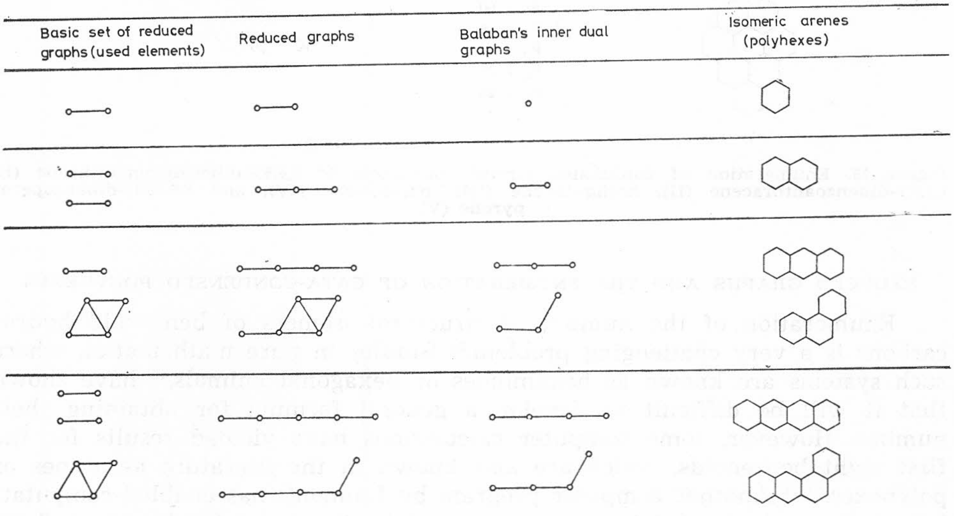


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Figure 16

Figure 16 continued from page 364

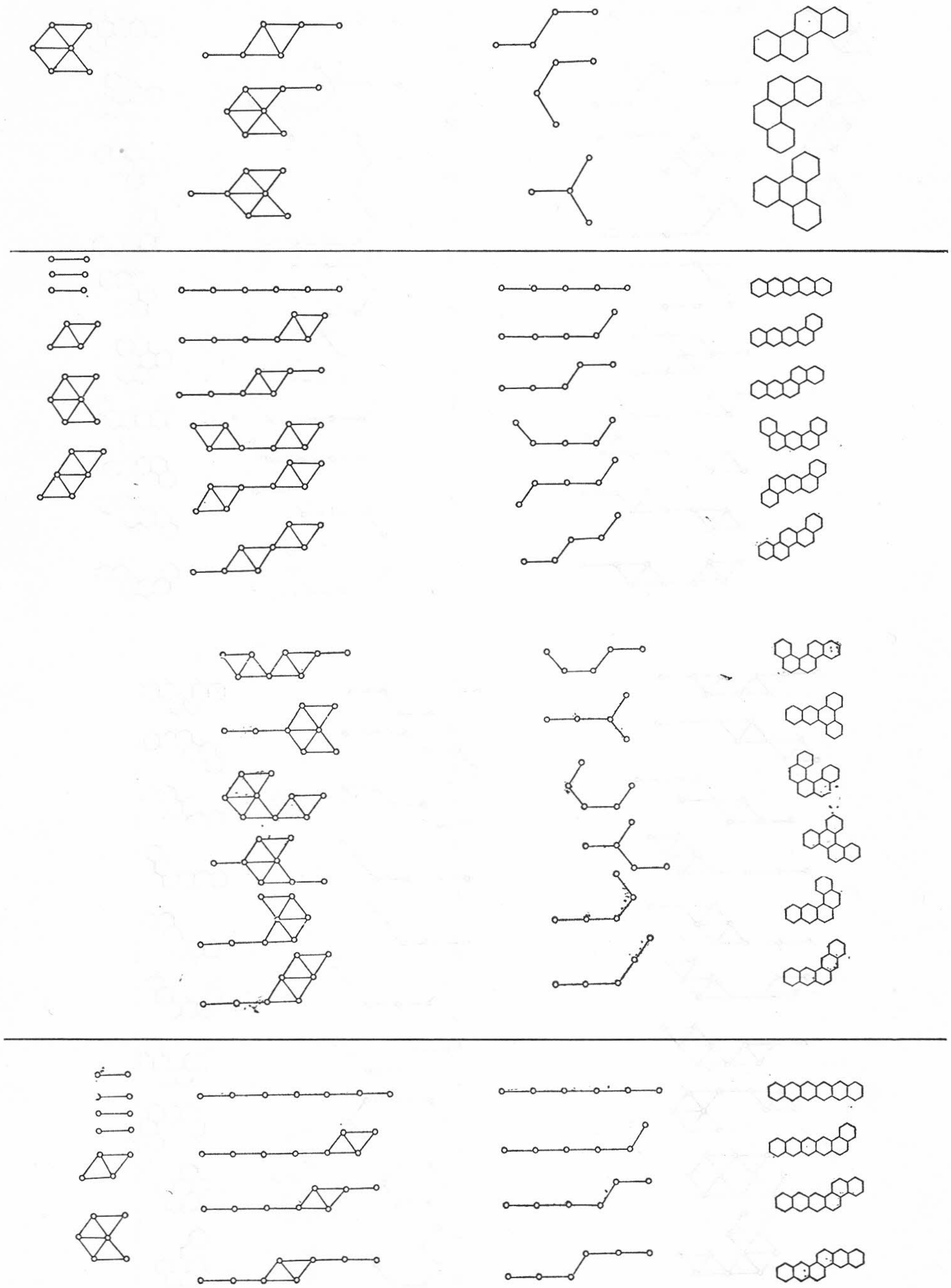

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Figure 16

Figure 16 continued from page 365

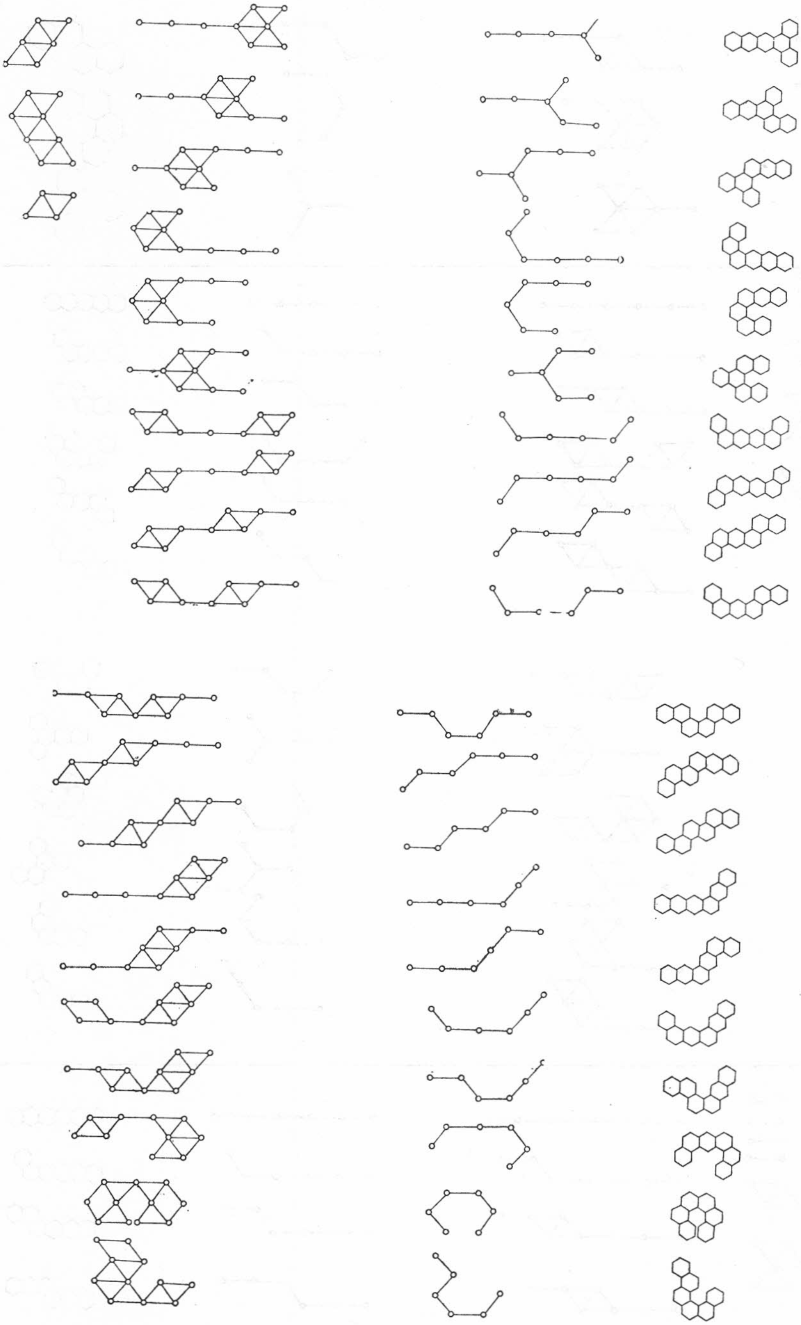

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Figure 16

Figure 16 continued from page 366

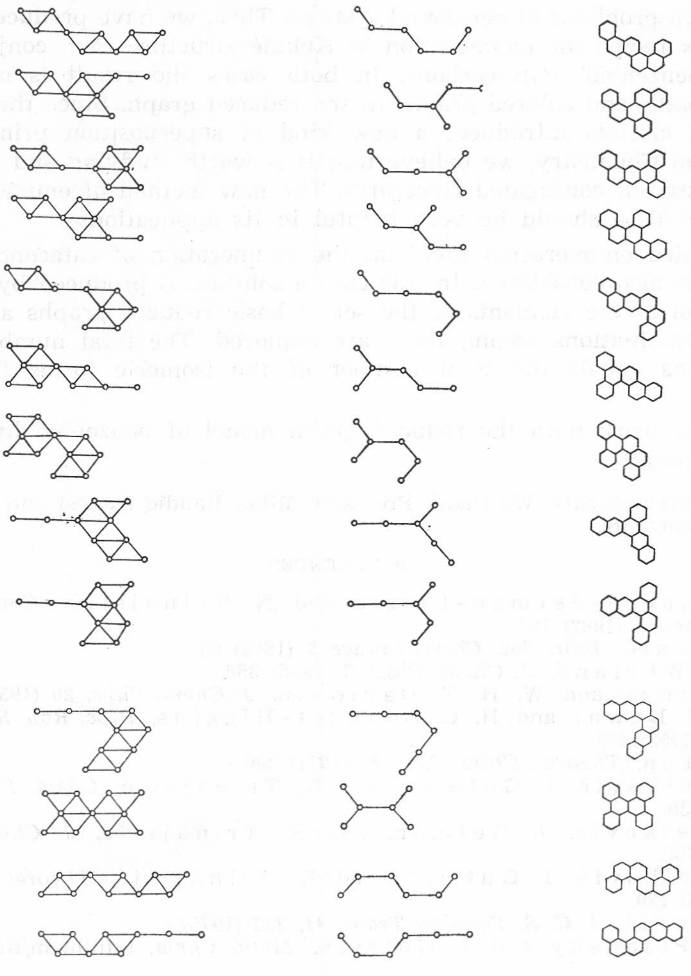

Figure 16. Enumeration of cata-condensed polyhexes by using the reduced graph approach

The results reported indicate that the suggested procedure gives an alternative solution to the problem of enumerating the cata-condensed hexagonal animals. At the same time these results point out that the problem of enumeration and display of the higher members (N > 6) of cata-condensed arene isomers may be solved in a simpler way if the polyhexes consisting of more than six rings are partitioned into substructures with two or three benzene rings.

CONCLUSION

In this paper we have expanded further the reduced graph model which appears to be very useful in providing an alternative graph theoretical representation of benzenoid hydrocarbons as well as for computer representation of benzenoids. The convenient features of the model are used in several enumeration problems of benzenoid systems. Thus, we have produced a »pencil and paper« recipe for enumeration of Kekulé structures and conjugated circuits of benzenoid hydrocarbons. In both cases the result is obtained by counting paths and colored graphs in the reduced graph. Since the use of the conjugated circuits introduces a new kind of superposition principle novel to Quantum Chemistry, we believe that it is worth studying and applying to the chemistry of conjugated structures. The new method of enumeration that is proposed here should be very helpful in its applications.

The third enumeration problem: the enumeration of catacondensed benzenoids was also considered. In this case a solution is produced by systematic combination of the elements of the set of basic reduced graphs and then all possible combinations among these are explored. The total number of these combinations equals the total number of the isomeric forms for a given molecule.

Further work with the reduced graph model of benzenoid hydrocarbons is in progress.[52]

Acknowledgements. We thank Professor Milan Randić (Ames) and the referees on their comments.

REFERENCES

1. B. Džonova-Jerman-Blažič and N. Trinajstić, *Computers and Chemistry* **6** (1982) 121.
2. A. Kekulé, *Bull. Soc. Chim. France* **3** (1865) 98.
3. G. W. Wheland, *J. Chem. Phys.* **3** (1935) 356.
4. M. Gordon and W. H. T. Davidson, *J. Chem. Phys.* **20** (1952) 428.
5. M. J. S. Dewar and H. C. Longuet-Higgins, *Proc. Roy. Soc. (London)* **A 214** (1952) 482.
6. T. F. Yen, *Theoret. Chim. Acta* **20** (1971) 399.
7. D. Cvetković, I. Gutman, and N. Trinajstić, *Chem. Phys. Lett.* **16** (1972) 535.
8. D. Cvetković, I. Gutman, and N. Trinajstić, *J. Chem. Phys.* **61** (1974) 2700.
9. D. Cvetković, I. Gutman, and N. Trinajstić, *Theoret. Chim. Acta* **34** (1974) 129.
10. M. Randić, *J. C. S. Faraday Trans. II,* 232 (1975).
11. O. E. Polansky and I. Gutman, *Math. Chem.* (Mulheim/Ruhr) **8** (1980) 269.
12. L. Pauling, *Acta Cryst.* **B 36** (1980) 1898.
13. J. V. Knop and N. Trinajstić, *International J. Quantum Chem.* **S 14** (1980) 503.
14. I. Gutman, *Math. Chem.* (Mulheim/Ruhr) **11** (1981) 1.
15. I. Gutman, *Bull. Soc. Chim.* (Belgrade) **46** (1981) 411.
16. N. Trinajstić, *Chemical Graph Theory,* CRC, Boca Raton, Chapter 10, in press.
17. W. C. Herndon and M. L. Ellzey, Jr., *J. Am. Chem. Soc.* **96** (1976) 6631.
18. W. C. Herndon, *J. Am. Chem. Soc.* **98** (1976) 887.
19. W. C. Herndon, *Israel J. Chem.* **20** (1980) 270.
20. W. C. Herndon, *J. Org. Chem.* **46** (1981) 2119.
21. M. Randić, *Chem. Phys. Lett.* **38** (1976) 68.
22. M. Randić, *J. Am. Chem. Soc.* **99** (1977) 444.
23. M. Randić, *Tetrahedron* **33** (1977) 1905.
24. M. Randić, *Mol. Phys.* **34** (1977) 849.
25. M. Randić, *International J. Quantum Chem.* **17** (1980) 549.
26. M. Randić, *Pure Appl. Chem.* **52** (1980) 1587.

26a. J. A. N. F. Gomes, D. Phil. Thesis, University of Oxford 1976.

27. F. Harary and R. C. Read, *Proc. Edinburgh Math. Soc. Ser. II* **17** (1970) 1.

28. F. Harary and E. M. Palmer, *Graphical Enumeration*, Academic, New York 1973, Chapter 10.
29. A. T. Balaban, in: *Chemical Applications of Graph Theory*, edited by A. T. Balaban, Academic, New York 1976, p. 63.
30. K. Balasubramanian, J. J. Kauffman, W. S. Koski, and A. T. Balaban, *J. Comput. Chem.* **1** (1980) 149.
31. L. Spialter, *J. Chem. Docum.* **4** (1964) 261, 269.
32. F. Harary, *Graph Theory*, Addison-Wesley, Reading, Mass. 1971, second printing.
33. I. Gutman and N. Trinajstić, *Topics Curr. Chem.* **42** (1973) 49.
34. A. Graovac, I. Gutman, and N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules, Lecture Notes in Chemistry*, Springer, Berlin, 1977, Vol. 4.
35. I. Gutman, *Croat. Chem. Acta* **46** (1974) 269.
36. I. Gutman, *Theoret. Chim. Acta* **45** (1977) 309.
37. D. Cvetković, I. Gutman, and N. Trinajstić, *Croat. Chem. Acta* **44** (1972) 365.
38. M. Randić, *Croat. Chem. Acta* **47** (1975) 71.
39. B. Džonova-Jerman-Blažič, Ph. D. Dissertation, University of Zagreb, 1980.
40. J. A. N. F. Gomes, *Croat. Chem. Acta* **53** (1980) 561.
41. J. A. N. F. Gomes, *Theoret. Chim. Acta* **59** (1981) 333.
42. W. S. Golomb, *Polyminoes*, Scribner, New York 1965.
43. A. T. Balaban, *Tetrahedron* **25** (1969) 2949.
44. D. Klarner, *Fibonacci Quart.* **3** (1965) 9.
45. W. F. Lunnon, in: *Graph Theory and Computing*, edited by R. C. Read, Academic, New York 1972, p. 87.
46. J. V. Knop, K. Szymanski, Ž. Jeričević, and N. Trinajstić, *J. Comput. Chem.*, in press.
47. A. T. Balaban and F. Harary, *Tetrahedron* **24** (1968) 2505.
48. F. T. Smith, *J. Chem. Phys.* **34** (1961) 793.
49. D. H. Rouvray, *J. South African Chem. Inst.* **26** (1973) 141.
50. R. C. Read and F. Harary, *Proc. Edinburgh Math. Soc.* **17** (1980) 1.
51. J. R. Dias, *J. Chem. Inf. Comp. Sci.* **22** (1982) 139.
52. B. Džonova-Jerman-Blažič and N. Trinajstić, work in progress.

SAŽETAK

Primjena modela reduciranog grafa na prebrojavanje Kekuléovih struktura i konjugiranih krugova benzenoidnih ugljikovodika

B. Džonova-Jerman-Blažič i N. Trinajstić

Model reduciranog crteža (grafa) pretstavlja alternativni način prikazivanja heksagonalnih struktura. U ovom je radu taj model upotrebljen kao temelj nekoliko jednostavnih algoritama za prebrojavanje Kekuléovih struktura, konjugiranih krugova i kata-kondenziranih izomera benzenoidnih ugljikovodika.