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Topological Properties of Benzenoid Systems. XXI. Theorems, Conjectures, Unsolved Problems*

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The main known mathematical results (in the form of 32 theorems and 5 conjectures) about benzenoid systems are collected. A few new results (seven theorems) are proved. Seven unsolved problems are also pointed out.

The paper contains results on the basic properties of benzenoid graphs, on the number of Kekulé structures and on Clar's resonant sextet formulas.

INTRODUCTION

Benzenoid systems are the geometric figures obtained by arranging congruent regular hexagons in a plane, so that two hexagons are either disjoint or have a common edge. Benzenoid systems must (by definition) be superimposable with a hexagonal (graphite) lattice. Hence the perimeter of a benzenoid system can be viewed as a cycle on the hexagonal lattice. In the literature benzenoid systems are sometimes called polyhexes or hexagonal animals or hexagonal systems.

Throughout the present paper we shall assume that the benzenoid systems have no holes, i. e. that they divide the plane into an (infinite) external region and a certain number of internal regions, all of which must be regular hexagons. Consequently, corannulenes (kekulene etc.) and related compounds are out of the scope of the present work. It should be mentioned, however, that a great part of the results which are collected here do not hold (or, at least, need substantial modifications) if benzenoid systems with holes were included into the consideration.

A benzenoid system is a natural mathematical representation of a benzenoid hydrocarbon. Therefore, benzenoid systems are of certain interest for theoretical chemistry. Topological properties of benzenoid systems are of considerable importance in various quantum mechanical models of the electronic structure of benzenoid hydrocarbons, especially in resonance theory, Hückel molecular orbital theory, Clar's aromatic sextat theory and the theory of conjugated circuits. From the references cited it will become evident that this topic has a relatively long history in theoretical organic chemistry. Never-

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theless, the great majority of the presently known results has been obtained quite recently.

For review of topological properties of benzenoid hydrocarbons see ref. 1.

A benzenoid system can be viewed as a graph. Then we speak about benzenoid graphs. Throughout this paper we will always refer to the graph-theoretical representation of benzenoid systems and, consequently, we will use a pertinent graph-theoretical terminology.

Our notation will be the following. A benzenoid graph will be denoted by B. It has n vertices, $v_1, v_2, \ldots, v_n$, and m edges. The edge connecting the vertices v_r and v_s will be labelled by e_{rs}. The number of hexagons in B is h. The number of Kekulé structures in the corresponding benzenoid hydrocarbon will be denoted by $K = K(B)$. This is, on the other hand, equal to the number of perfect matchings[1] of the graph B.

A benzenoid graph B is *cata-condensed* if no three hexagons of B have a common vertex. Otherwise, B is *peri-condensed*. A cata-condensed benzenoid graph B is said to be *non-branched* if every hexagon of B has at most two neighbours. Otherwise, B is a *branched* cata-condensed benzenoid graph.

An ordered h-tuple $(S_1, S_2, \ldots, S_h)$ of symbols L and A can be associated with every non-branched cata-condensed benzenoid graph B. If the i-th hexagon of B is annelated in a linear mode (resp. angular mode), we set $S_i = L$ (resp. $S_i = A$), $i = 2, \ldots, h-1$. In addition we define $S_1 = S_h = L$. Such an h-tuple will be called the L,A-sequence of the benzenoid graph B and will be denoted by $LA(B)$.

In the following we will present the main (but certainly not all) known mathematical properties of benzenoid graphs (without proof), together with a few new results (with proof). We will also point out several unsolved problems and conjectures.

BASIC PROPERTIES

A benzenoid graph B is bipartite and planar. It may contain cycles of size 6, 10, 12, 14, 16, 18 etc. Its vertices have degree two or three.

The vertices of B which lie on the perimeter are called *external*. All other vertices are said to be *internal*. Let the number of internal vertices of B be denoted by n_i.

1. Theorem[2,3]

A benzenoid graph is cata-condensed if and only if, $n_i = 0$.

2. Theorem[4]

Let n_2 and n_3 be the number of vertices of degree two and three, respectively, in the benzenoid graph B. Then,

$$n_2 = 2h + 4 - n_i,$$

$$n_3 = 2(h-1),$$

and consequently,

$$n = n_2 + n_3 = 4h + 2 - n_i,$$

$$m = n + h - 1 = 5h + 1 - n_i.$$

3. Theorem[5]

The graph B has $2h + 4 - n_i$ external vertices of degree two and $2h - 2 - n_i$ external vertices of degree three. Hence the perimeter of B contains

$4h + 2 - 2n_i$ vertices. At least six edges of the perimeter connect a pair of bivalent vertices.

4. Theorem[6]

There exist benzenoid graphs having any number of vertices, except for $n < 6$, $n = 7$, 8, 9, 11, 12 and 15.

5. Theorem[6]

The parameters n and h in a benzenoid graph vary within the ranges

$$2h + 1 + \{\sqrt{12h - 3}\} \leqslant n \leqslant 4h + 2,$$
$$\{(n - 2)/4\} \leqslant h \leqslant n + 1 - \{(n + \sqrt{6n})/2\},$$

where $\{x\}$ denotes the smallest integer being greater than or equal to x. All values of n and h within the above ranges occur in benzenoid systems.

6. Theorem[7]

In the interior of every $(4k + 2)$-membered cycle, $k \geqslant 1$, the number of vertices is even (or zero). In the interior of every $(4k)$-membered cycle, $k \geqslant 3$, there is an odd number of vertices.

Let e be an edge of a benzenoid graph B. If the graph $B^0 = B\text{-}e$, obtained by deletion of the edge e from B, is also a benzenoid graph, then we will say that B is *e-transformable* to B^0.

7. Theorem

A benzenoid graph B has a Hamiltonian cycle if and only if B is either cata-condensed or *e*-transformable (in one or more steps) to a cata-condensed benzenoid graph.

Proof

Since by Theorem 1 all vertices of a cata-condensed benzenoid graph are external, they all lie on the perimeter and thus the perimeter of a cata-condensed system is a Hamiltonian cycle.

Consider now the case when B is peri-condensed. If B is *e*-transformable to a cata-condensed benzenoid graph B^0, then the perimeter of B^0 is the Hamiltonian cycle of B. This proves the »if« part of Theorem 7.

If B has a Hamiltonian cycle, then this cycle can be viewed as the perimeter of some cata-condensed benzenoid graph B^0. The graph B differs from B^0 by having only some additional edges. The deletion of these edges from B is just the required *e*-transformation. This proves the »only if« part of Theorem 7.

It can be also demonstrated that the Hamiltonian cycle of a benzenoid graph (provided it exists) is unique.

Let $\Phi(B, x)$ be the *characteristic polynomial* and $\alpha(B, x)$ the *matching* (or *acyclic*) *polynomial* of B. These polynomials can be written in the form

$$\Phi(B, x) = \sum_{k=0}^{[n/2]} (-1)^k q(B, k) x^{n-2k}$$

and

$$\alpha(B, x) = \sum_{k=0}^{[n/2]} (-1)^k p(B, k) x^{n-2k}.$$

Then the coefficients $q(B, k)$ and $p(B, k)$ are non-negative for all values of k.

8. Theorem[3,8,9]

$$q(B, 1) = p(B, 1) = m,$$

$$q(B, 2) = p(B, 2) = [(n + h - 2)^2 - n - 7h + 6]/2,$$

$$q(B, 3) = p(B, 3) + 2h,$$

$$q(B, 4) = p(B, 4) + 2h^2 + 2h(n - 15) + 2n + 4.$$

9. Theorem[9]

$q(B, k) = 0$ if and only if $p(B, k) = 0$.

10. Theorem[9]

$q(B, k) \geqslant p(B, k)$ for all values of k.

The (unique) non-branched cata-condensed benzenoid graph whose L,A-sequence is $(L, L, \ldots, L)$ is called the *linear polyacene* graph.

11. Conjecture

Among cata-condensed benzenoid graphs with equal number of hexagons, the linear polyacene graph has minimal $q(B, k)$ and $p(B, k)$ values for all k.

Closed analytical formulas for the eigenvalues (i. e. the zeros of the characteristic polynomial) of linear polyacene graphs were obtained by Coulson[10]. Analytical formulas for the eigenvalues of other calsses of benzenoid graphs are not known.

Concluding this section we would like to point out two fundamental problems in the theory of benzenoid systems. The definition of a benzenoid system given in the introduction has a metric (geometric) nature rather than a non-metric (topological) nature.

12. Problem

It is not known how to define benzenoid graphs by using exclusively graph-theoretical notions.

This problem has been considered in ref. 11.

13. Problem

How many benzenoid systems (with a given number of hexagons) exist?

Harary offers US $ 100 for the solution of this difficult enumeration problem[12].

NUMBER OF KEKULÉ STRUCTURES

For various methods for the enumeration of Kekulé structures in benzenoid systems see refs. 1,13—15.

14. Theorem[16]

If B is a benzenoid graph, then

$$K(B) \cdot K(B - v_r - v_s) = K(B - v_r - v_s)^2 + \sum_Z K(B - Z)^2,$$

where Z is a cycle of B and the summation goes over all cycles of B, containing the edge e_{rs}.

15. Theorem[16]

If B is a benzenoid graph, then B has either no Kekulé structures or the number of Kekulé structures is greater than one. In addition, if $K(B) = 2$, then B is the benzene graph.

16. Theorem[5]

If B has Kekulé structures, then every edge of B connecting a pair of bivalent vertices corresponds to a double bond in at least one Kekulé structure.

17. Theorem[17]

If B is cata-condensed, then

$$h + 1 \leqslant K(B) \leqslant 2^{h-1} + 1.$$

The left-hand side of the above inequality provides the best possible lower bound for the number of Kekulé structures of cata-condensed systems.

A simple recursive method for the enumeration of Kekulé structures in cata-condensed benzenoid graphs (both branched and non-branched) have been developed by Gordon and Davison[18].

18. Theorem[18]

The number of Kekulé structures of a non-branched cata-condensed benzenoid system is fully determined by its L,A-sequence.

19. Theorem[18,19]

If $LA(B) = (S_1, S_2, \ldots, S_h)$, then $K(B)$ is equal to the first component of the two-dimensional vector $\mathbf{M}_1 \mathbf{M}_2 \ldots \mathbf{M}_h \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, with the matrices $\mathbf{M}_i$, $i = 1, \ldots, h$ being defined as

$$\mathbf{M}_i = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \text{ if } S_i = L$$

and

$$\mathbf{M}_i = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \text{ if } S_i = A.$$

20. Theorem

The L,A-sequences $(L,L,L,\ldots,L,L)$ and $(L,A,A,\ldots,A,L)$ determine the minimal and the maximal K-value of a non-branched cata-condensed benzenoid graph with h hexagons.

Proof

Note first that for x and y being arbitrary numbers, $x \geqslant y$,

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \leqslant \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}.$$

Consequently, for $(S_1, S_2, \ldots, S_h)$ being an arbitrary S,A-sequence,

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}^h \begin{pmatrix} 1 \\ 1 \end{pmatrix} \leqslant M_1 M_2 \ldots M_h \begin{pmatrix} 1 \\ 1 \end{pmatrix} \leqslant \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}^{h-2} \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

Theorem 20 follows now immediately from Theorem 19.

21. Theorem[18] If $LA(B) = (L,L,L,\ldots,L,L)$, then

$$K(B) = h + 1.$$

If $LA(B) = (L,A,A,\ldots,A,L)$ then

$$K(B) = 2^{-(h+2)}[(1+\sqrt{5})^{h+2} - (1-\sqrt{5})^{h+2}]/\sqrt{5}.$$

Additional interesting combinatorial formulas for the number of Kekulé structures of various classes of benzenoid systems can be found in refs.[18,20-23].

22. Theorem[24]

If a benzenoid graph B possesses a linear polyacene fragment of length b, then $K(B)$ is a linear function of the parameter b.

23. Problem

It is not known which benzenoid systems have Kekulé structures. In other words, we need a relatively simple and efficient graph-theoretical characterization of those benzenoid graphs for which $K = 0$. (According to Theorem 17, if $K(B) = 0$, then B must be peri-condensed.)

24. Problem

Which of the benzenoid systems (with a given number of hexagons) have the maximal and minimal (but non-zero) numbers of Kekulé structures?

25. Conjecture

If $K(B) = 3$, then B is the napthalene graph. If $K(B) = 4$, then B is the anthracene graph. If $K(B) = 5$, then B is either the tetracene or the phenanthrene graph.

26. Conjecture

There is a finite number of benzenoid graphs for which $0 < K \leqslant 8$. (It can be demonstrated that the number of benzenoid graphs for which $K = 9$ is infinite.)

27. Theorem[25]

A benzenoid graph B has no Kekulé structures if and only if B has an eigenvalue equal to zero, i. e. if $\Phi(B, 0) = 0$.

28. Theorem[26]

Let $\mathbf{A}$ be the adjacency matrix of the benzenoid graph B. Then

$$\det A = (-1)^{n/2} K(B)^2$$

29. Theorem[27-30]

If v_r and v_s are adjacent vertices of B, then

$$(A^{-1})_{rs} = K(B - v_r - v_s)/K(B).$$

If v_r and v_s are not adjacent, then the above equation is not always fulfilled[7].

CLAR'S SEXTET FORMULAS

The definition of Clar's sextet formulas of benzenoid hydrocarbons can be found in ref. 31.

Let B be a benzenoid graph and $H_1, H_2, \ldots, H_h$ be its hexagons. We say that the hexagon H_i is resonant in B if $K(B - H_i) \neq 0$. We say that the hexagons $H_1, H_2, \ldots, H_k$ are mutually resonant in B if they are mutually disjoint (i. e. no pair of hexagons has common vertices) and if $K(B - H_1 - H_2 - \ldots - H_k) \neq 0$.

30. Theorem

If the hexagons $H_1, H_2, \ldots, H_k$ are mutually resonant, then the hexagons $H_1, H_2, \ldots, H_j$, $j < k$, are also mutually resonant.

Proof

Since an isolated hexagon (i. e. the benzene graph) has two Kekulé structures, it follows from $K(B - H_1 - \ldots - H_k) \neq 0$ that $K(B - H_1 - \ldots - H_j)$ must be greater than $K(B - H_1 - \ldots - H_k)$ by at least 2^{k-j}. Hence $B - H_1 - \ldots - H_j$ has Kekulé structures which means that the hexagons $H_1, \ldots, H_j$ are mutually resonant.

31. Theorem

If H_i is not resonant, i. e. if $K(B - H_i) = 0$, then H_i is not mutually resonant with any other hexagon.

Proof

Assuming $K(B - H_i - H_j) \neq 0$, and applying Theorem 30 we conclude that $K(B - H_i) \neq 0$, a contradiction.

32. Theorem

The hexagons $H_1, H_2, \ldots, H_k$ are mutually resonant if and only if they are pairwise resonant.

Proof

The »only if« part of Theorem 32 follows immediately from Theorem 30. In order to prove the »if« part, note that when a hexagon H_i is resonant in B, then some other hexagons cannot be mutually resonant with H_i. Let these hexagons be labelled by H_j, $j \in A_i \subset \{1, 2, \ldots, h\}$. These hexagons form a neighbourhood of the hexagon H_i. All other hexagons of B which lie »outside« this neighbourhood are independent of H_i in the sense that a hexagon H^0 is resonant in B if and only if it is resonant in B_i, where B_i is the benzenoid graph containing the hexagons of B which lie »outside« of H_i.

Now if the hexagons $H_1, \ldots, H_k$ are pairwise resonant, then they are also pairwise independent (in the above sense). But then they are mutually independent and thus mutually resonant.

This proves Theorem 32.

33. Theorem

If B has no Kekulé structures, then no hexagon of B is resonant.

Proof

Since every hexagon itself has two Kekulé structures, $K(B - H_i) \neq 0$ would imply $K(B) \neq 0$, a contradiction.

The number of Clar's formulas of B, containing k sextets, will be denoted by $s(B, k)$. By definition[31], $s(B, 0) = 1$ for all benzenoid graphs B.

34. Theorem

If B has a Hamiltonian cycle, then $s(B, 1) = h$.

Proof of this result is lengthy and is based on the fact that the deletion of a hexagon from B causes the decomposition of the Hamiltonian cycle of B into two parts, with $2b$ and $n - 6 - 2b$ vertices, each of which has a Kekulé structure. (The case $b = 0$ can also occur and has to be considered separately.)

Because of Theorem 7, the above result implies that all hexagons of a cata-condensed benzenoid system are resonant.

The proof of Theorem 32 contains the basic ideas of the *Clar graph* concept[32]. If B is a benzenoid graph composed of the hexagons $H_1, H_2, \ldots, H_h$, then the Clar graph of B is the graph $C(B)$ whose vertices are $H_1, H_2, \ldots, H_h$. Two vertices H_i and H_j are adjacent in $C(B)$ if $j \in A_i$, $i = 1, 2, \ldots, h$.

35. Theorem[32]

If $k > 1$, then $s(B, k)$ is equal to the number of selections of k independent vertices in $C(B)$.

The sextet polynomial of B is[31]

$$\sigma(B, x) = \sum_{i=1}^{S(B)} s(B, k)\, x^k,$$

with $S(B)$ denoting the maximal value of k for which $s(B, k) \neq 0$.

36. Theorem[31,33]

If B is cata-condensed, then

$$\sigma(B, 1) = \sum_{k=0}^{S(B)} s(B, k) = K(B).$$

37. Theorem[31,34]

If B is cata-condensed, then

$$\sigma'(B, 1) = \sum_{k=0}^{S(B)} k\, s(B, k) = \sum_{i=1}^{h} K(B - H_i).$$

38. Problem

It is not known how to generalize the above two theorems to the case of peri-condensed benzenoid systems.

39. Theorem[32,35]

If B is non-branched cata-condensed, then $C(B)$ is the line graph of a tree. If B is branched cata-condensed, then $C(B)$ is not a line graph.

The construction of the tree mentioned in Theorem 39 is based on the L,A-sequence of B. An interesting consequence of Theorem 39 is[32] that if B is non-branched cata-condensed, then all the zeros of its sextet polynomial are real and negative numbers.

40. Problem

It is not known which conditions must a graph fulfil in order to be the Clar graph of some benzenoid system.

41. Problem

It is not known which peri-condensed benzenoid graphs have the property that their Clar graph is a line graph. It is also not known which sextet polynomials have real zeros.

42. Theorem[36,37]

If B is a non-branched cata-condensed system with $LA(B) = (L,A,A,\ldots,A,L)$, then

$$s(B,k) = a_k = \binom{h+1-k}{k}$$

where a_k is the number of Kekulé structures of B in which there are exactly $2k$ double bonds of the type C=CH.

Few years ago Aihara[38] observed that for a great number of benzenoid systems, the following statement holds.

43. Conjecture[38] Let

$$F(B) = S(B)\,K(B) - 2\sum_{i=1}^{h} K(B-H_i).$$

Then whenever $s(B,S(B)) = 1$, the function $F(B)$ is equal to zero or, at least, small comparable to $K(B)$.

We demonstrate now that Aihara's conjecture is true under some special conditions and give support for its general validity. Assuming that B is cata-condensed and using Theorems 36 and 37, we transform the function $F(B)$ into the form

$$F(B) = \sum_{k} [S(B) - 2k]\,[s(B,S(B)-k) - s(B,k)],$$

with the summation going over all k, such that $2k < S(B)$. According to the assumption in the conjecture, the relation

$$s(B,S(B)-k) = s(B,k)$$

is fulfilled for $k = 0$. If this equality holds for all values of k, i. e. if the coefficients of the sextet polynomial are symmetric, then $F(B) = 0$ and Aihara's conjecture is true. Clearly, the conjecture will be valid whenever the coefficients of the sextet polynomial are (at least) nearly symmetric.

44. Conjecture

For all benzenoid graphs B there exists a constant $k_o = k_o(B)$, such that

$$s(B,k-1) \leqslant s(B,k) \quad \text{for} \quad k \leqslant k_o,$$

$$s(B,k) \geqslant s(B,k+1) \quad \text{for} \quad k \geqslant k_o.$$

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SAŽETAK

Topološka svojstva benzenoidnih sustava. XXI. Teoremi, hipoteze, neriješeni problemi

I. Gutman

Prikupljeni su važniji poznati matematički rezultati o benzenoidnim sustavima i izloženi u obliku 32 teorema i 5 hipoteza. Dokazan je i stanovit broj novih rezultata. Ukazano je na neke neriješene probleme.

Rad sadržava rezultate o osnovnim svojstvima bezenoidnih grafova, o broju Kekuléovih struktura i o Clarovim sekstetnim formulama.