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The Clar number of a benzenoid hydrocarbon and linear programming

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It is shown that the Clar number of a benzenoid hydrocarbon H (defined as the number of circles in a Clar formula, or equivalently as the maximum number of mutually resonant hexagons of H) can be determined by mixed-integer programming. Moreover, linear programming appears to suffice in practice to find in moderate computing time the Clar number of pericondensed hydrocarbons with more than a thousand hexagons.

1. Introduction

It has long been known that many chemical properties of a benzenoid hydrocarbon can be explained in terms of the number of circles in a Clar formula for this molecule, or in other words, in terms of its maximum number of mutually resonant hexagons [1–10]. In ref. [11] it was proposed to call this number the *Clar number* of a benzenoid hydrocarbon. Note that the Clar number is equal to the degree of the sextet polynomial [7,12–14], as well as of the Clar polynomial [15,16], which have both been much studied in connection with description of resonance relations among individual hexagons of benzenoid hydrocarbons. When the Clar number increases within a series of isomeric benzenoid hydrocarbons one observes increased stability, as well as a change of color from dark blue-green to red, yellow or white [5,6,10]. Such observations, and many others, led Clar to devise his aromatic sextet theory. Aihara [1] examined 52 benzenoid hydrocarbons with a unique Clar structural formula and concluded that the Clar number gives a rough estimate of the Dewar-type resonance energy [17,18]. Many papers discuss Clar formulas from both the chemical and mathematical points of view [19–36]. For recent surveys of aromatic sextet theory, see ref. [6,37].

Yet, while some upper bounds are known [11,38], no general method appears to have been proposed to determine the Clar number of a benzenoid hydrocarbon. There is also no general method to draw a Clar formula. Only the case of multiple chain-like molecules (catacondensed benzenoids) has been completely solved [16,39]. It turns out however, as shown below, that mixed-integer programming

[40,41], and, in practice, linear programming (which may be viewed as a subcase of mixed-integer programming) allow to solve efficiently this problem even for very large molecules (pericondensed benzenoids with more than a thousand hexagons). Integer optimal solutions were obtained for all test problems when solving the linear programming relaxation of the mixed-integer program (in which integrality constraints on the variables are omitted). We conjecture that this property holds for all benzenoid hydrocarbons. Moreover, this mixed integer programming approach can be extended to determine all Clar formulae of a benzenoid hydrocarbon.

This paper is organized as follows. We present some basic definitions in section 2. The mixed-integer programming model for determining a Clar structural formula as well as the Clar number of a benzenoid hydrocarbon is given in section 3. Computational results are also presented in that section. Finally in section 4 we give an upper bound for the objective value of the mixed-integer linear program and show that the conjecture on integral solutions mentioned above is closely related to a conjecture of ref. [11].

2. Definitions

The skeleton of a benzenoid hydrocarbon (in which hydrogen atoms are suppressed) may be described by a graph called *benzenoid system*. Such a graph is defined as a finite connected subgraph of the infinite hexagonal lattice without cut vertices and nonhexagonal interior faces (see fig. 1a). A *generalized benzenoid system* is defined in a similar way, but omitting the last restrictions, i.e., cut vertices and nonhexagonal interior faces are allowed (see fig. 1b). Note that a benzenoid system is also a generalized benzenoid system, but the converse is not true.

A Kekulé structure or *perfect matching* of a generalized benzenoid system is a set of disjoint edges covering all vertices. Up to now, no benzenoid hydrocarbons which do not correspond to benzenoid systems with a Kekulé structure have been synthesized, even as transient species [6]. In this paper, all (generalized) benzenoid

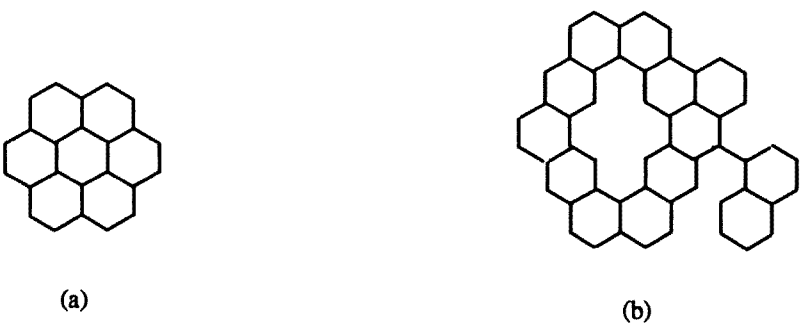


Fig. 1. A benzenoid system and a generalized benzenoid system.

systems considered are assumed to have a Kekulé structure. Since the Clar formulas and the Clar number of a benzenoid hydrocarbon are determined by its topological structure, we focus our discussion on (generalized) benzenoid systems.

A set of disjoint hexagons of a benzenoid system (or of a generalized benzenoid system) is *resonant* if a Kekulé structure can be written in which each hexagon in the set contains three double bonds (i.e., three bonds which belong to the Kekulé structure). A resonant set is *maximum* if its cardinality is maximum. The hexagons in a resonant set are said to be *mutually resonant*.

Clar proposed to represent resonant hexagons in a benzenoid system by drawing circles in them following some rules. The resulting diagrams are called Clar structural formulae (or Clar formulae for short). Rules for obtaining a Clar formula for a (generalized) benzenoid system are as follows (Gutman and Cyvin [6,42]):

(a) Circles are never drawn in adjacent hexagons (two hexagons are adjacent if they have an edge in common);
(b) The generalized benzenoid system obtained by deleting the vertices of all hexagons containing a circle must have a perfect matching (or Kekulé structure) or must be empty;
(c) The number of circles is maximum subject to (a) and (b).

Drawing a Kekulé structure in the generalized benzenoid system obtained by deleting all hexagons with a circle is straightforward (see fig. 2). Moreover such a Kekulé structure is unique [43].

It follows from these rules that a set S of disjoint hexagons of a benzenoid system H (or of a generalized benzenoid system) is a maximum resonant set if and only if there is a Clar formula of H in which the set of hexagons possessing circles is S.

3. A mixed integer linear program for Clar formula

The problem of determining the Clar number of a benzenoid hydrocarbon will be solved by using techniques of mathematical programming. This discipline aims at finding optimal solutions to constrained optimization problems. The easiest and best known case is linear programming [44,45] in which the function to be optimized (called the objective function) is linear and the constraints are linear inequal-

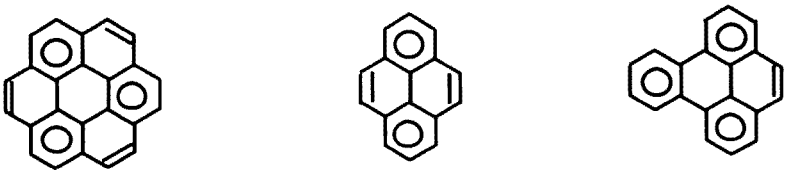


Fig. 2.

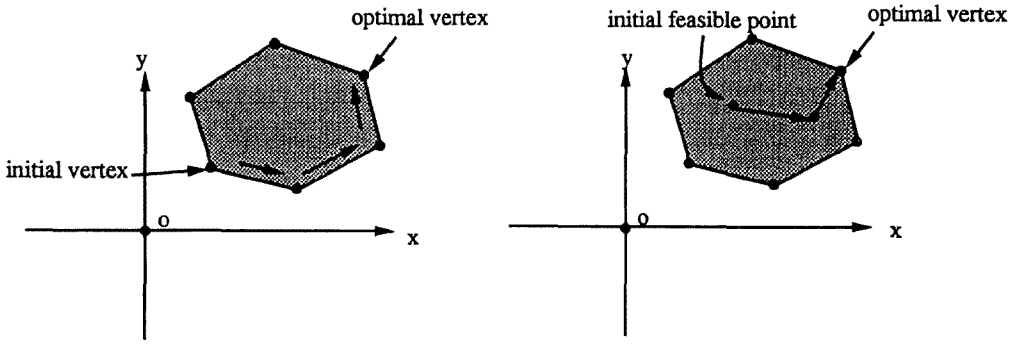
ities or equations. The set of feasible solutions, i.e. those vectors satisfying the constraints, defines a convex polyhedron. It is well known that an optimal solution of a linear program always occurs at a vertex of this polyhedron. The classical method to solve linear program is the *simplex method* [44,45] and consists in finding a first vertex of the polyhedron and then proceeding iteratively from this vertex to an adjacent one (i.e. one on an edge of the polyhedron going through that vertex) with a better value of the objective function, until the optimal vertex is reached (see fig. 3a). Recently different algorithms which prescribe a trajectory going through the interior of the polyhedron, known as *interior point methods* [46,47], have been devised (see fig. 3b). They tend to perform better than the simplex method on large problems. Both the simplex algorithm and an interior point method will be used. In addition we will consider a more complex type of problem from mathematical programming, i.e. linear programs in 0-1 or mixed variables, in which in addition to the above constraints some or all of the variables are restricted to take only the values 0 or 1. A *branch and bound* approach [40,41] to the solution of such problems is described below.

3.1. MIXED INTEGER PROGRAM

All results given in this section can be extended to generalized benzenoid systems in a straightforward way.

Any vertex of a benzenoid system H for which a Clar formula is known must either (i) belong to a hexagon containing a circle, or (ii) not belong to such a hexagon and be an end vertex of a double bond. We now translate this property in mathematical terms.

Let us associate with each hexagon h of H a 0-1 variable y_h which is equal to 1 if h contains a circle and equal to 0 otherwise. Moreover, let us associate with each edge (i,j) joining vertices i and j of H, a variable $x_{i,j}$ which is equal to 1 if this edge is not one of a hexagon containing a circle and is a double bond in the given Clar formula, and is equal to 0 otherwise. Let $N(i)$ and $H(i)$ denote, respectively, the index



(a) Illustration of simplex method

(b) Illustration of interior point method

Fig. 3.

sets of the vertices adjacent to vertex i and of the hexagons containing vertex i in H. Let $V(H)$ and $E(H)$ denote the vertex set and the edge set of H, respectively. Then the y_h, $x_{i,j}$ so defined satisfy all the constraints of the following integer linear program (ILP), and therefore form a feasible solution for this program (we will see that this feasible solution is also optimal):

$$\textit{maximize } z = \sum_{h \in H} y_h$$

subject to the constraints :

$$\sum_{j \in N(i)} x_{i,j} + \sum_{h \in H(i)} y_h = 1 \quad \textit{for } i \in V(H) \qquad (ILP)$$

$$x_{i,j}, y_h \in \{0,1\} \qquad \textit{for } (i,j) \in E(H) \textit{ and } h \in H .$$

So the Clar number of H is less than or equal to the optimal objective value of ILP. On the other hand, for any optimal solution (X^*, Y^*) of this integer linear program, we may draw a circle in the hexagon h if $h_h^* = 1$ in Y^* and a double bond on the edge (i,j) if $x_{i,j}^* = 1$ in X^*. Then a Clar formula is obtained. Thus the optimal objective value of the integer linear program is exactly the Clar number of H. Therefore the feasible solution of the integer linear program obtained from a Clar formula is also an optimal solution to the program. Summarizing these results, we have:

THEOREM 1

There is a one-to-one correspondence between Clar formulae of a benzenoid system H and optimal solutions of the integer linear program ILP.

In fig. 4, we illustrate this correspondence by an example. Moreover, the integrality constraints on the $x_{i,j}$ variables can be relaxed to $0 \leqslant x_{i,j} \leqslant 1$. The reason is

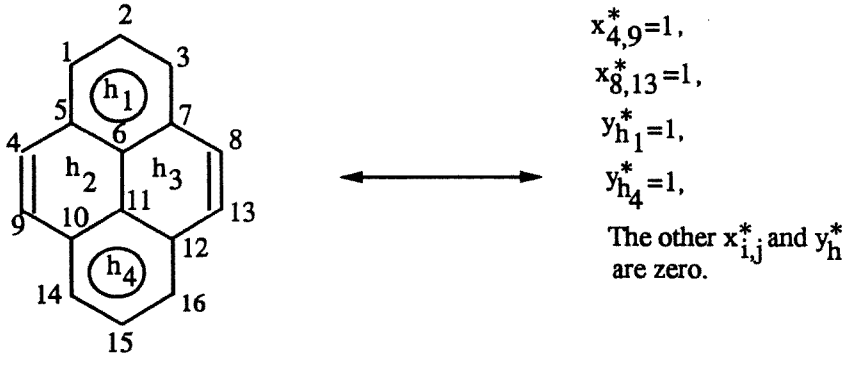


Fig. 4. Correspondence between a Clar formula and an optimal solution of ILP.

the following: Let (X^*, Y^*) be an optimal solution of the mixed-integer program (MIP) obtained by relaxing the constraints that the $x_{i,j}$ be equal to 0 or 1 to $0 \leqslant x_{i,j} \leqslant 1$; let H' be the subgraph of H obtained by deleting the hexagons which correspond to the y_h^*'s equal to 1 in Y^*; then H' is a bipartite graph and the $x_{i,j}^*$'s of X^* which are not 0 form a fractional matching [41] of H', i.e. $\sum_{j \in N(i)} x_{i,j}^* = 1$ for each vertex i of H'. So by a well-known theorem [48–50] H' has a perfect matching or, in other words a Kekulé structure; thus the hexagons corresponding to $y_h^* = 1$ in Y^* are mutually resonant; since the objective value of MIP is at least as large as that of the integer linear program ILP (as some constraints of ILP have been relaxed to obtain MIP), the hexagons with $y_h^* = 1$ form a maximum resonant set. From a maximum resonant set, a Clar formula can be drawn easily. By using a similar reasoning as above we can prove the following theorem (the proof of which is omitted here):

THEOREM 2

Let (RLP) be the linear program obtained by relaxing the constraints $y_h = 0$ or 1 to $0 \leqslant y_h \leqslant 1$ in MIP. Then the hexagons which correspond to the variables y_h equal to 1 in any feasible (but not necessary optimal) solution of RLP form a resonant set. Thus the number of variables y_h equal to 1 in any feasible solution of RLP is less than or equal to the Clar number of the corresponding benzenoid system H.

3.2. SOLVING MIP

We first describe the general idea of the solution method for the mixed integer linear program MIP given in the previous subsection. This program is solved by first relaxing the integrality constraints on the y_h variables to $0 \leqslant y_h \leqslant 1$ and solving the resulting linear program (denoted by RLP in theorem 2). This provides an upper bound on the Clar number. Then, if some variable y_h takes a fractional value in the optimal solution of this relaxed problem, branching is done by fixing y_h at 0 or at 1, thus obtaining two linear programming subproblems. By noting that any feasible solution to these subproblems is also a feasible solution to RLP, the conclusion of theorem 2 is also valid for the subproblems. Further branching on each subproblem takes place unless an integer solution is found or the optimal value of the linear program corresponding to the subproblem is less than or equal to the number of variables y_h equal to 1 in the best solution yet found (this is justified by theorem 2; the number of y_h equal to 1 in the best solution yet found is less than or equal to the Clar number of H).

We now state the above more formally:

Let RLP denote the linear program obtained by relaxing $y_h = 1$ or 0 to $0 \leqslant y_h \leqslant 1$ in MIP.

Method (solving MIP):
Initial Step: Nodeset = {RLP}.

Step 1: Determine an optimal solution for each (as yet unsolved) linear program in Nodeset. Let Q be the linear program in Nodeset which has the maximum objective function value. Let (X^*, Y^*) be an optimal solution for Q. If all the components of Y^* which correspond to the hexagons of H are integers, then the hexagons whose corresponding variables are 1 in Y^* form a maximum resonant set of H. Stop. Otherwise let N be the number of variables y_h equal to 1 in Y^*. Delete the nodes other than Q which have an optimal objective function value less than or equal to N. Proceed to Step 2.

Step 2: If Y^* has a non-integer component which corresponds to a hexagon s of H, then let y_s^* be such a component. Add the constraints $y_s = 0$ and $y_s = 1$ to Q one at a time thus defining two new linear programs Q_0 and Q_1 (This operation is called branching). Set Nodeset to be Nodeset $\cup \{Q_0, Q_1\} - \{Q\}$. Return to Step 1.

It turns out that in all of the many examples which we have solved, the initial linear programming upper bound on the Clar number was always tight and the corresponding optimal solution integer. So the mixed integer program was solved as a linear program, i.e., without branching. In other words, in none of the instances considered did the mixed integer program have an integrality gap [40,41] (This linear program does not have a coefficient matrix of one of the known forms which guarantee the absence of such a gap for *any* objective function, i.e., it is not totally unimodular nor perfect [40,41]. See ref. [41] for undefined terms.)

Several benzenoid systems are presented in fig. 5, each of them (except for two generic ones) with a Clar formula and computing CPU time on a SUN/SPARC station necessary to find it. The efficient interior point linear programming code OB1 [47] was used to get an optimal solution (not necessarily at a vertex of the polyhedron of feasible solutions of RLP) followed by some simplex interations to get a basic optimal solution (i.e., one corresponding to a vertex of the polyhedron). All problems in fig. 5 could be solved in less than half a minute of computing time each. In fig. 6, we present three further benzenoid systems with their number of hexagons (over a thousand) and their Clar number (since these benzenoid systems are too large, we are unable to draw a Clar formula for them in the diagram). We also report the number of iterations to get an optimal solution by the following methods: (1) by OB1 only; (2) first by OB1 to get an optimal solution, which may not be basic (i.e., a solution which corresponds to a vertex of the polyhedron of feasible solutions) followed by the simplex method to get a basic optimal solution; (3) by the simplex method only. When the number of iterations of the simplex method following the use of OB1 is 0, this means the initial vertex for the simplex method which is found from the optimal solution obtained by OB1 is optimal, and therefore no further iterations are needed. Computing times are presented for all these strategies. For our test problems, the OB1 code was much faster than the simplex method.

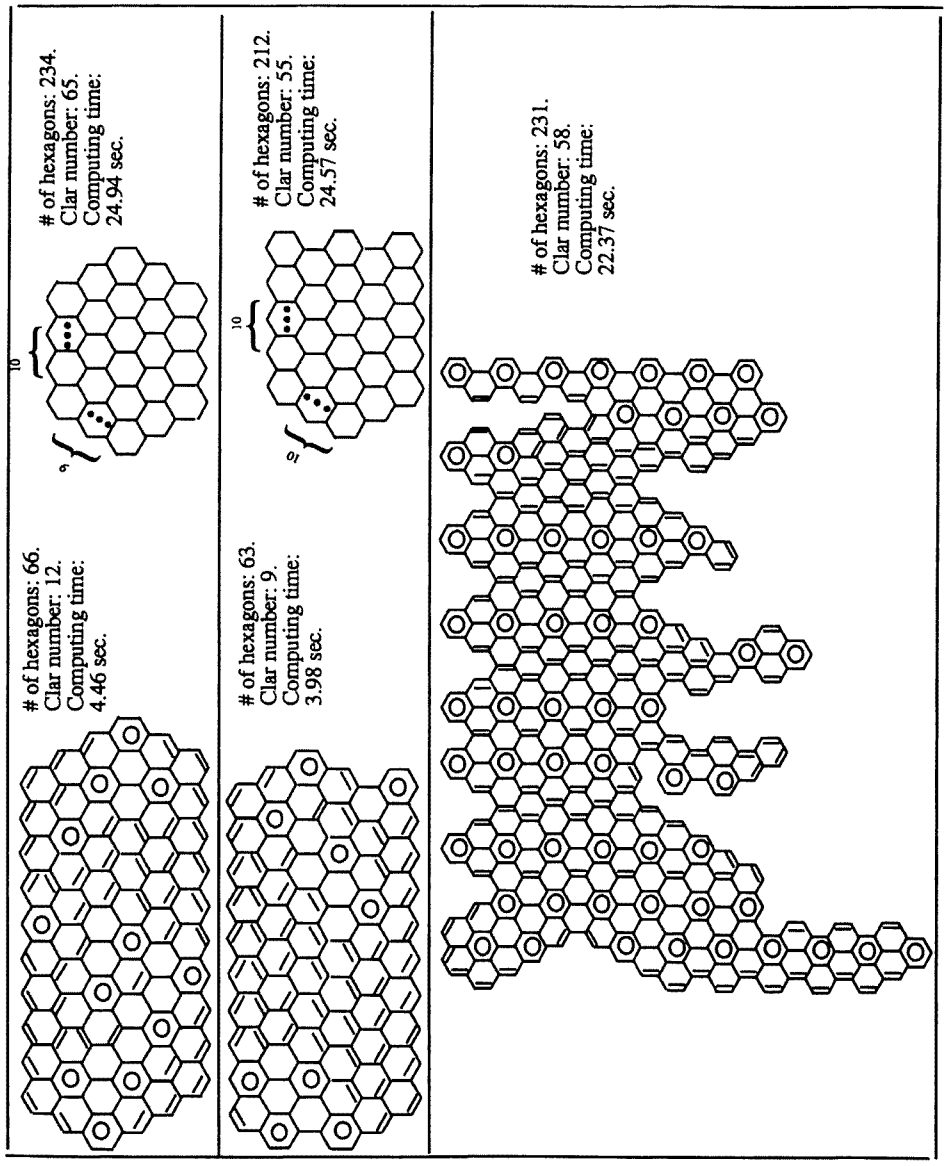
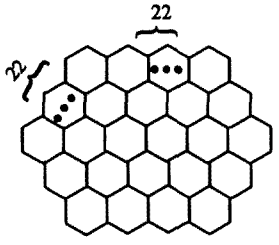
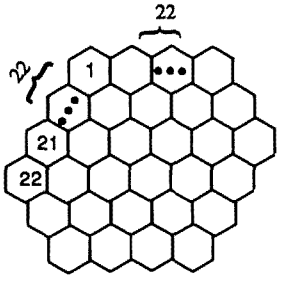


Fig. 5. Clar formulae of various benzenoid systems and computing times for obtaining them (OB1 followed by the simplex method).



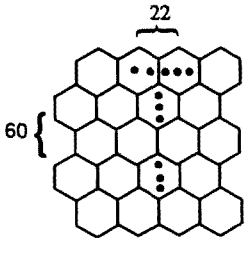
# of hexagons: 1395 Clar number: 363

	Iterations	CPU Time (Sec.)
OB1	11	42.12
OB1-Simplex	OB1: 11 Simplex: 0	235.55
Simplex	Phase 1: 2842 Phase 2: 3985	949.42



# of hexagons: 1344 Clar number: 352

	Iterations	CPU Time (Sec.)
OB1	10	40.08
OB1-Simplex	OB1: 10 Simplex: 0	227.73
Simplex	Phase 1: 2424 Phase 2: 3926	839.31



# of hexagons: 1320 Clar number: 60

	Iterations	CPU Time (Sec.)
OB1	9	24.26
OB1-Simplex	OB1: 9 Simplex: 0	66.88
Simplex	Phase 1: 106 Phase 2: 488	42.66

Fig. 6. Computing times for determining the Clar number and a Clar formula of large pericondensed benzenoid systems using the simplex algorithm and an interior point method for linear programming (OB1).

3.3. ENUMERATION OF CLAR FORMULAE

If all Clar formulae must be found, only slight and standard modifications need to be made in the way to solve the mixed integer program given above. Specifically, subproblems cannot be deleted anymore if the bound given by the solution of the current linear programming relaxation is equal to the current value of the best known solution (i.e., to the Clar number as soon as one Clar formula has been found). But several shortcuts which accelerate the solution are possible and are par-

ticularly useful if there are many Clar formulae (in which case the computing time increases considerably).

First, the problem can be decomposed if the related benzenoid system has fixed bonds (a bond or edge is *fixed* if it belongs to all of the Kekulé structures or to none of them). A normal component of H is a maximal connected subgraph which has no fixed bonds. Note that any hexagon which contains a circle in a Clar formula cannot have fixed bonds. It has often been observed [6,51] and proved rigorously in ref. [52] that if H has fixed bonds it has at least two normal components and all its normal components are normal benzenoid systems (i.e. benzenoid systems with no fixed bonds). A linear algorithm to find all fixed bonds of benzenoid systems has also been given in ref. [53]. Thus all normal components of H can be found in linear time. Clar formulae for each normal component are then found. All Clar formulae of H are obtained by combining in all possible ways one Clar formula from each of its normal components.

Second, each time a Clar formula is found one can add to the mixed integer program the constraint

$$\sum_{h \in C} y_h \leq |C| - 1 ,$$

where C is the index set of hexagons containing a circle. This constraint forbids to obtain again this Clar formula but not any other one. The accumulation of such constraints gives tighter and tighter bounds until it is shown that all Clar formulae have been enumerated. However, this time fractional solutions are obtained for the linear programming relaxation and branching is needed to get integer ones. The different phases of the determination of all Clar formulae for a benzenoid hydrocarbon H are illustrated in fig. 7.

4. Upper bound for the optimal objective function value of RLP

Up to now we have not found a proof that the optimal objective function value of RLP is equal to the Clar number of the corresponding benzenoid system, but we conjecture that this is indeed the case. We next present an upper bound on the optimal objective function value of RLP. If a conjecture (which will be recalled later) given by us in ref. [11] is true, then the optimal objective function value of RLP is exactly the Clar number of the corresponding benzenoid system. Should this be the case the problem of finding the Clar number of a benzenoid system could be solved as a linear program.

More definitions are needed. Note that a (generalized) benzenoid system H is a bipartite graph. We color the vertex set of H in two colors (black and white) such that two adjacent vertices have different colors.

A *cut* of a (generalized) benzenoid system H is a non-self-intersecting curve C (which may be closed or not) in the plane such that (a) C intersects H only at edges,

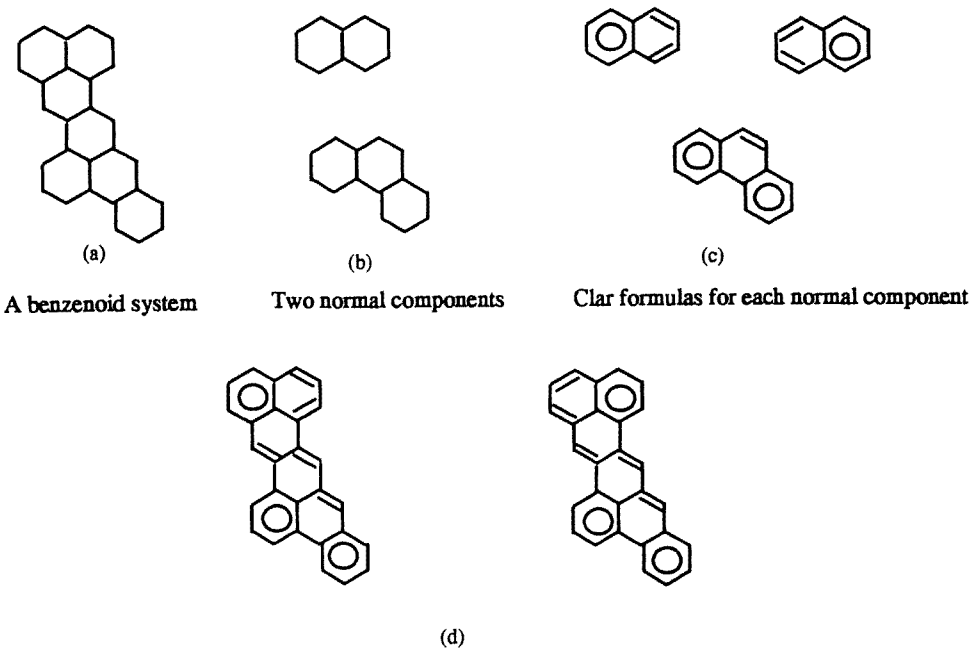


Fig. 7. Determination of all Clar formulae of a benzenoid system.

(b) removal of all the edges intersecting C leads to a disconnected subgraph $H - C$ such that the end vertices of each edge intersecting C belong to different connected components of $H - C$, and (c) the black end vertices of the edges intersecting C are on one side and the white ones are on the other side of C (see fig. 8 for several examples of cuts). Note that $H - C$ may have more than two connected components. So this definition is slightly different from the definition of cuts given

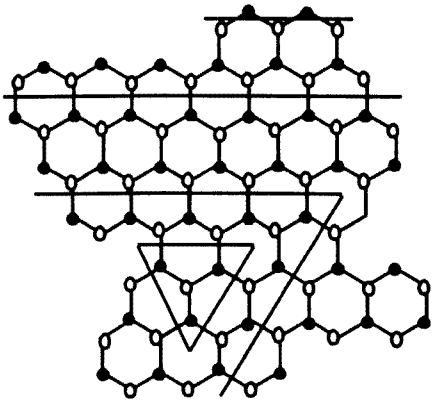


Fig. 8. Cuts of a benzenoid system.

in ref. [54], where it is required there that $H - C$ have two connected components only.

The *black side* (*white side*) of a general cut C is the union of the connected components of $H - C$ which contain no white (black) cut-boundary vertices. Two cuts are equal, by definition, if they intersect the same set of edges.

A set $\mathcal{C}$ of cuts of a (generalized) benzenoid system H is a *cover* if each hexagon of H intersects with at least one cut in $\mathcal{C}$. A cover $\mathcal{C}$ is *perfect* if each hexagon of H intersects with exactly one cut in $\mathcal{C}$.

Let M be a Kekulé structure and C be a cut of a (generalized) benzenoid system H. Let $m(C)$ be the number of edges in M which intersect C. The following is a basic property of a cut which is proved in ref. [11]:

THEOREM 3

Let C be a cut of a (generalized) benzenoid system H. Then $m(C)$ is independent of M.

Let $\mathcal{C}(H)$ be a set of cuts of a (generalized) benzenoid system H and $c(\mathcal{C}(H)) = \sum_{C \in \mathcal{C}(H)} m(C)$. An immediate consequence of theorem 3 is the following.

COROLLARY 1

$c(\mathcal{C}(H))$ remains the same for all Kekulé structures of H.

Let $\mathcal{A}(H)$ be the set of all covers of a (generalized) benzenoid system H and $CL(H) = \min\{c(\mathcal{C}) : \mathcal{C} \in \mathcal{A}(H)\}$. Let $O(H)$ be the optimal objective function value of the linear relaxation RLP of ILP for a benzenoid system H. Then we have

THEOREM 4

For a benzenoid system H, $O(H) \leqslant CL(H)$.

Before giving the proof, we need the following definition: let s be a hexagon of H. The three edges of s are said to be in a proper position if they are the right vertical edge and the nonvertical edges which are adjacent to the left vertical edge of s (see fig. 9). Note that by this definition, each edge e belongs to at most one hexagon for which it is in a proper position.

Let H be a benzenoid system. Let $P(H)$ be the perfect matching polytope of H, i.e., is the set of all solutions of the following system:

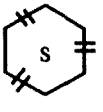


Fig. 9. Edges of a hexagon in proper position.

$$\sum_{j \in N(i)} x_{i,j} = 1 \quad \text{for } i \in V(H),$$

$$0 \leqslant x_{i,j} \leqslant 1 \quad \text{for } (i,j) \in E(H).$$

Since H is a bipartite graph, $P(H)$ is an integral polytope (ref. [41] p. 108), i.e., each vertex of $P(H)$ is an integer vector. There is a one-to-one correspondence between vertices of $P(H)$ and perfect matchings of H defined in the following way: a vertex X of $P(H)$ corresponds to a perfect matching M such that if $x_{i,j} = 1$ then (i,j) belongs to M.

For a feasible solution X of RLP, let X' be the vector constructed in the following way: if there is a hexagon s in which the edge (i,j) is in the proper position then let $x'_{i,j} = x_{i,j} + y_s$, otherwise let $x'_{i,j} = x_{i,j}$ (actually this procedure can be easily reversed). One can check easily that X' belongs to $P(H)$.

Proof of theorem 4

Let $\mathcal{C}$ be a cover of H. Let C be any cut which belongs to $\mathcal{C}$. Let (X, Y) be a feasible solution of RLP and $X' = (x'_{i,j})$ be the corresponding vector in $P(H)$ obtained as stated above. Then

$$\sum_{s \text{ intersects } C} y_s \leqslant \sum_{(i,j) \text{ intersects } C} x'_{i,j}.$$

Since X' is a vector in $P(H)$, it is a convex combination of some vertices of $P(H)$, i.e., there are nonnegative numbers $k_1, k_2, \ldots, k_m$ and vertices $X_1, X_2, \ldots, X_m$ of $P(H)$ such that $X' = k_1X_1 + k_2X_2 + \ldots + k_mX_m$ and $k_1 + k_2 + \ldots + k_m = 1$. Let $X_r = (x^r_{i,j})(r = 1, 2, \ldots, m)$. Then

$$\sum_{(i,j) \text{ intersects } C} x'_{i,j} = k_1 \sum_{(i,j) \text{ intersects } C} x^1_{i,j} + k_2 \sum_{(i,j) \text{ intersects } C} x^2_{i,j} + \ldots$$

$$+ k_m \sum_{(i,j) \text{ intersects } C} x^m_{i,j}.$$

By theorem 3,

$$\sum_{(i,j) \text{ intersects } C} x^1_{i,j} = \sum_{(i,j) \text{ intersects } C} x^2_{i,j} = \ldots = \sum_{(i,j) \text{ intersects } C} x^m_{i,j} = m(C).$$

So

$$\sum_{s \text{ intersects } C} y_s \leqslant m(C)$$

and thus

$$\sum_s y_s \leqslant c(\mathcal{C}).$$

Since the choices of $\mathcal{C}$ and (X, Y) are arbitrary, $O(H) \leqslant \sum y_s \leqslant CL(H)$. The proof is completed. □

COROLLARY 2

Let $cn(H)$ denote the Clar number of a benzenoid system H. Then $cn(H) \leqslant O(H) \leqslant CL(H)$.

Proof

This immediately follows from theorem 1 and that the optimal objective function value of RLP is greater than or equal to that of MIP.

In ref. [11], we conjectured that $cn(H) = CL(H)$. If this is true, it immediately implies the conjecture of the present paper, i.e., $cn(H) = O(H)$.

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