match no. 24 pp. 215-222 1989

DISTRIBUTION OF THE CONVEX PAIRS IN A BENZENOID OR QUASI-BENZENOID SYSTEM

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(Received: July 1988)

Abstract. A structural character of the benzenoid systems is derived. Distribution of the convex pairs in a benzenoid or quasi-benzenoid system is pointed out, in order to emphasize the simplicity and rapidity of the algorithm reported in ref. [1] for determining whether a given benzenoid system possesses the Kekulé structures or not.

1. Introduction

The importance of finding rapid ways to recognize whether a given benzenoid system is Kekuléan or not is well known [3-5] . Only two simple and generally applicable algorithms have been found. The first one is given by Sachs [2] . More recently the present author [1] put forward an algorithm which is much simpler and faster than that of Sachs.

The present paper is concerning the convex pairs, defined in ref. [1], and their distribution in a benzenoid or quasi-benzenoid system. A structural property of the benzenoid systems is reported.

2. Some related concepts and consequences

Let B be a benzenoid system. Denote respectively by n_2 and n_3 the numbers of the external vertices of degree two and three in B. It is well known

$$n_2 = n_3 + 6 \ . \quad (1)$$

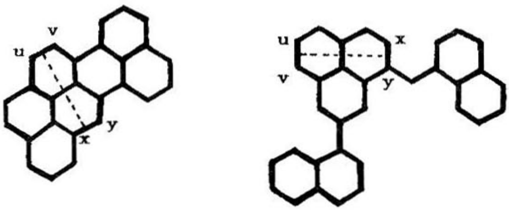
Q is called a quasi-benzenoid system if it satisfies:

(i) Q consists of benzenoid subunits joined by one or more acyclic lines on the hexagonal lattice;

(ii) By regarding the benzenoid units as vertices and the acyclic lines as edges, the corresponding joining graph is a tree, which is called the incidence tree of Q, denoted by T(Q).

In a quasi-benzenoid system, the vertices and edges lying on the perimeters of the benzenoid subunits and the acyclic lines are called external.

Let u,v,x,y be four external vertices of a (quasi)benzenoid system Q. u and x are respectively adjacent to v and y, the cut orthogonal to the edge $\{u,v\}$ going through the interior of Q intersects the edge $\{x,y\}$. Then u,v,x,y form a rectangular set. If u,v are of degree two, and at least one of x and y is of degree two, then u,v form a convex pair. Fig. 1 depicts above concepts.



(a) (b)

Fig. 1. (a) A benzenoid system in which (u,v) is a convex pair because u, v and y are of degree two. (b) A quasi-benzenoid system in which (u,v) is a convex pair because u, v and x are of degree two.

The procedure of the algorithm, reported in ref. [1], consists of the deletion of a convex pair followed by the deletion of pendent vertices (if any) together with their first neighbours. The procedure ends when an isolated vertex is created or when all vertices are pairwise deleted. In the former case the benzenoid system examined is non-Kekuléan; in the latter case it is Kekuléan.

It is known [1] that a benzenoid system possesses at least six convex pairs, and a quasi-benzenoid system possesses at least 4k convex pairs if its incidence tree has k leaves. Note that it always holds $k \geq 2$.

3. Upper and lower concave vertices

Let B be a benzenoid system oriented with some of its edges vertical. v is an external vertex of degree three, v_1, v_2 and

v_3 are its adjacent vertices, $\{v,v_1\}$ is internal and vertical, $\{v,v_2\}$ and $\{v,v_3\}$ are external. If v lies above v_1 (see Fig. 2a), then v is called an upper concave vertex (UCV); if v lies below v_1 (see Fig. 2b), then v is called a lower concave vertex (LCV).

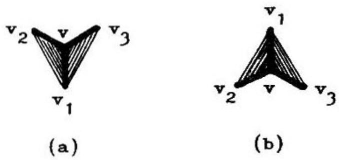


Fig. 2. (a) v is an UCV. (b) v is a LCV. The hatched parts lie in the interior of B.

Denote respectively by n_p, n_v, n_u and n_l the numbers of peaks, valleys, UCVs and LCVs.

THEOREM 1. $n_p = n_u + 1$, (2)

$n_v = n_l + 1$. (3)

Proof. It is easy to see that (3) is equivalent to (2) by the rotation of 180°. Hence we shall prove (2) only.

Denote by h the number of all hexagons in a benzenoid system. We use mathematical induction.

When h=1, the only corresponding benzenoid system is a regular hexagon, obviously (2) holds.

Assume (2) holds for $h \leqslant k$, we shall verify that (2) holds for h = k+1 :

Let B be a benzenoid system with h = k+1. The numbers of peaks and UCVs are respectively denoted by n_p and n_u. In the lowest line of hexagons, choose the first hexagon from the left, denoted by X. Then there are seven possible contact cases, as indicated in Fig. 3.

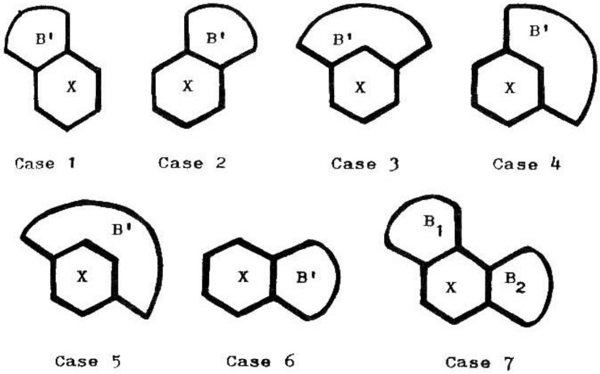


Fig. 3. Seven possible contact cases.

In each of the Cases 1-5, B is obtained by adding the hexagon X to a benzenoid system B' with h=k. The numbers of peaks and UCVs are unchanged under the addition. By the assumption (2) holds for B', hence (2) is valid for B.

In Case 6, B is also obtained by adding X to B' with h=k. The numbers of peaks and UCVs in B' are denoted by n'_p and n'_u, respectively. We have $n_p = n'_p + 1$, $n_u = n'_u + 1$. By the assumption $n'_p = n'_u + 1$. Hence $n_p = n_u + 1$.

In Case 7, X joins two benzenoid systems B_1, B_2 with $h < k$. Denote respectively by $n_p^{(i)}$ and $n_u^{(i)}$ the numbers of peaks and UCVs in B_i, i=1,2. We have

$n_p = n_p^{(1)} + n_p^{(2)}$, $n_u = n_u^{(1)} + n_u^{(2)} + 1$. By the assumption

$n_p^{(i)} = n_u^{(i)} + 1$, $i=1,2$. Therefore $n_p = n_u + 1$.

Consequently, (2) is valid for all benzenoid systems, and so is (3). The proof is completed.

4. Distribution of the convex pairs

The edge joining two vertices of a convex pair is called a convex edge; or, equivalently, an edge is called a convex edge if its both vertices form a convex pair.

THEOREM 2. A benzenoid system possesses at least two convex edges in each of its three edge directions.

Proof. Consider a benzenoid system B oriented with some of its edges vertical. Because non-vertical directions can be transformed into the vertical direction by the rotations, it only needs to be verified that B possesses at least two vertical convex edges.

Let V_{ext} = the set of external vertices,

V_1 = the set of the external vertices which have vertical, external incident edges,

V_2 = the set of peaks, valleys, UCVs and LCVs.

It is easy to know that

$$V_1 \cap V_2 = \emptyset \quad , \quad V_1 \cup V_2 = V_{ext} \; . \tag{4}$$

Denote respectively by $n_2(S)$ and $n_3(S)$ the numbers of the vertices of degree two and three in S, where S is a set constituted by some external vertices in B.

By (1), (4) and Theorem 1,

$$n_2(V_1) - n_3(V_1) = 4. \tag{5}$$

Consider all the rectangular sets contained by V_1, denoted by $R_1, R_2, \ldots, R_m$, we have

$$R_i \cap R_j = \phi, \quad 1 \leq i < j \leq m, \qquad \bigcup_{i=1}^{m} R_i = V_1 . \tag{6}$$

Hence $$\sum_{i=1}^{m} \left[n_2(R_i) - n_3(R_i) \right] = n_2(V_1) - n_3(V_1). \tag{7}$$

Denote respectively by t_1 and t_2 the numbers of the rectangular sets which are contained by V_1 and have three and four vertices of degree two. Then the number of vertical convex edges is equal to t_1+2t_2 .

By (6), we get

$$\sum_{i=1}^{m} \left[n_2(R_i) - n_3(R_i) \right] \leq 2t_1 + 4t_2 . \tag{8}$$

By (5), (7) and (8), we obtain $t_1+2t_2 \geq 2$. This completes the proof.

By Theorem 2, we can easily deduce the following theorem:

THEOREM 3. If Q is a quasi-benzenoid system, its incidence tree T(Q) has k leaves, then Q possesses at least k convex edges in each of its three edge directions.

In Theorem 3, it always follows $k \geq 2$, therefore a quasi-benzenoid system possesses at least two convex edges in each of its three edge directions.

Theorem 2 and Theorem 3 show the fact that it is quite easy to search a convex pair (or a convex edge) in a benzenoid or quasi-benzenoid system.

References

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