match no. 24 pp. 201-206 1989

Some Properties of Generalized Benzenoid Systems

Rong-qin Sheng
Shanghai Institute of Computer Technology
546 Yu Yuan Road, Shanghai
People's Republic of China

(Received: March 1988)

ABSTRACT

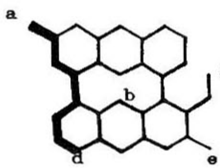
Definitions and some properties of generalized benzenoid systems are given. An invariant in Kekuléan generalized benzenoid systems is derived. An algebraic formula for the invariable triple of ref.[2] is established by means of the invariant.

1. INTRODUCTION

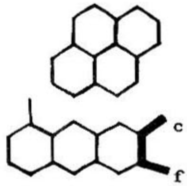
The topological theories of benzenoid molecules play an important role in chemical literature, and have also mathematical interests. A number of results have been obtained; the readers should consult ref.[3], where a systematical review was given.

The present paper will deal with a generalization of benzenoid systems.

A generalized benzenoid system is obtained by deleting some vertices and some edges from a benzenoid system. A generalized system may be unconnected; each independent conjugated subsystem is called a component. A benzenoid system is a special case of a generalized benzenoid system. Fig.1 shows two examples.



I



II

Fig.1 Examples of generalized benzenoid systems

In fact, the generalized benzenoid systems have many properties similar to benzenoid systems. It is clear that theorems derived for generalized benzenoid systems are also valid for the benzenoid systems.

2. SOME BASIC PROPERTIES OF GENERALIZED BENZENOID SYSTEMS

It is clear that a generalized benzenoid system is Kekuléan if and only if its components are all Kekuléan.

If a connected generalized system is Kekuléan, then the number of its vertices is even.

Consider a generalized benzenoid system G drawn such that some of its edges are vertical. Then a peak is defined as a vertex which has at least one non-vertical incident edge and lies above all its neighbours. A valley is a vertex which has at least one non-vertical incident edge and lies below all its neighbours.

A monotonic path in G is a path connecting a peak and a valley, such that when starting at the peak one always goes downwards. Two paths are independent when they have no vertices in common. In Fig.1, a,b,c are peaks, d, e,f valleys, g is not a peak, the heavy lines are monotonic paths.

In each Kekulē pattern of a generalized benzenoid system,when starting at a peak, first along a double bond, then alternately through single and double bonds, always downwards, a valley must be reached. Therefore a peak must have a monotonic path to a valley, and two such paths must be independent.

Conversely, if G has a constellation of independent monotonic paths, double bonds are drawn in the non-vertical edges lying in the monotonic paths and in the vertical edges not lying in the monotonic paths, a Kekulē pattern is obtained.

From the above discussion we have

THEOREM 1. Let G be a generalized benzenoid system. G is Kekulēan if and only if G has at least one constellation of independent monotonic paths.

THEOREM 2. If G is a Kekuléan generalized benzenoid system, then there is a one-to-one correspondence between a constellation of independent monotonic paths and Kekulé structures.

COROLLARY 1. A Kekuléan generalized benzenoid system possesses an equal number of peaks and valleys.

Assume again that the generalized system is oriented with some of its edges vertical. Two segments (upper and lower) are produced by cutting horizontally through a number of edges with a cut. The cut edges are called tracks, their number is denoted by tr(L) if the cut is L.

The numbers of peaks and valleys for the upper segment with respect to a cut L are respectively denoted by p(L) and v(L). Furthermore, seg(L)= p(L)-v(L).

THEOREM 3. If G is a Kekuléan generalized benzenoid system, then for any cut L, $0 \leqslant seg(L) \leqslant tr(L)$.

3. AN INVARIANT

In this section we deal with Kekuléan generalized benzenoid systems. For a cut L, the numbers of double bonds and single bonds in corresponding tracks are respectively denoted by d(L) and s(L). Then we have

THEOREM 4. d(L) = tr(L)- seg(L).

Proof. Deleting the s(L) edges corresponding to the s(L) single bonds, we get another Kekuléan generalized system G'

(See Fig.2). Considering the cut L, the number of valleys in the upper segment of G' increases by s(L), and the correspon-ding tracks of G' are all double bonds or empty. Hence there are no monotonic paths through L, and the upper segment must have an equal number of peaks and valleys, i.e. seg(L)-s(L)=0, and d(L)=tr(L)-seg(L).

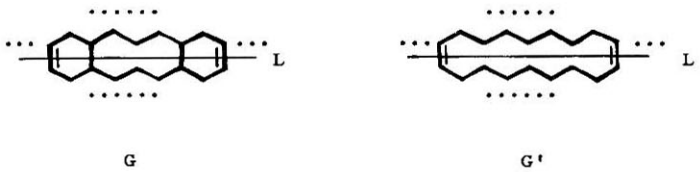


Fig.2 Illustration of Theorem 4

Theorem 4 exposes the fact that for a given Kekuléan generalized benzenoid system and a certain cut, the number of double bonds in corresponding tracks for all Kekulé patterns is an invariant.

THEOREM 5. If G is a Kekuléan generalized benzenoid system, L is a cut, then

(a) The corresponding tracks are all fixed single bonds if and only if tr(L) = seg(L);

(b) The corresponding tracks are all fixed double bonds if and only if seg(L)=0.

Theorem 5 (b) is an improvement of Theorem VI of ref. [1].

4. AN FORMULA FOR INVARIABLE TRIPLE

Ref. [2] presented an invariant in a given Kekuléan benzenoid. It is the invariable triple (a,b,c), a,b,c are respectively the numbers of double bonds in three different orientations A, B, C.

Let the cuts be $\left\{ L_A^{(i)},\ 1 \leqslant i \leqslant r \right\}$, $\left\{ L_B^{(i)},\ 1 \leqslant i \leqslant s \right\}$, $\left\{ L_C^{(i)},\ 1 \leqslant i \leqslant t \right\}$. By Theorem 4 we have the following formula.

THEOREM 6.

$$a = \sum_{i=1}^{r} \left(tr(L_A^{(i)}) - seg(L_A^{(i)})\right),$$

$$b = \sum_{i=1}^{s} \left(tr(L_B^{(i)}) - seg(L_B^{(i)})\right),$$

$$c = \sum_{i=1}^{t} \left(tr(L_C^{(i)}) - seg(L_C^{(i)})\right).$$

ACKNOWLEDGEMENT

I am thankful to Prof. S.J. Cyvin for useful suggestions.

REFERENCES

[1] S.J. Cyvin and I. Gutman, J.Mol.Struct.(THEOCHEM) 150(1987)157.

[2] F. Zhang, R. Chen, X. Guo and I. Gutman, J.Serb.Chem.Soc. 51(1986)537.

[3] I. Gutman, Bull.Soc.Chim.Beograd 47(1982)453.