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Normal Benzenoids are Reducible

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Abstract: A simple method is proposed for deleting a hexagon from a normal benzenoid to yield a new normal one.

In this paper all the terms and definitions are applied in consistence with those in [1-7].

Consider a benzenoid G. An edge on the contour of G is called an external edge. A hexagon X having external edges is called an external hexagon. An external hexagon X with mode L, E, F, B or D having 5,3,1,4,2 external edges is denoted by X_L, X_E, X_F, X_B, X_D, respectively. (See Fig.1)

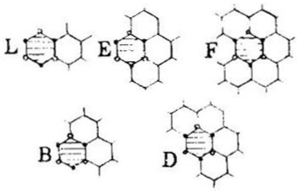


Fig.1 Five modes of external hexagons

A normal benzenoid G is a Kekuléan benzenoid system having no fixed-bond edges. It is well known that all normal benzenoids are stable compounds.

As preliminary information, we quote the following theorems.

<u>Theorem 1</u> [1] A benzenoid system G is normal if and only if there exists a Kekulé structure K where the contour C_e of G is a conjugated circuit.

Theorem 2[1] A benzenoid system G is normal if and only if the remainder system G' of G produced by deleting all the vertices on the contour C_e of G is Kekuléan (one-factorable).

Here, G' is called the maximum internal subgraph of G. G' may be a generalized benzenoid system and may be disconnected.

Theorem 3[2] Suppose that a hexagon is added to a normal benzenoid G_1 with h-1 hexagons. If the added hexagon has mode L, E or F, then the generated benzenoid G_2 with h hexagons is normal; and if the added hexagon has mode B or D, the generated benzenoid is non-Kekuléan.

In the former case, an even number of vertices has been added to the molecular graph, and in the latter an odd number.

Consider a normal benzenoid G_1 drawn such that some of its edges are vertical. We can easily find one Kekulé structure K_1' of its maximum internal subgraph G_1'[8,9]. An example is shown in Fig.2. According to Sachs' one-to-one correspondence theorem[10], K_1' corresponds to a perfect P-V(peak-to-valley)path system of G_1' which is also shown in Fig.2. In a Kekulé structure, all the oblique edges in the corresponding P-V path system and all the vertical edges not in this system are of double-bond type; the others are of single bond type[8].

Fig.2 A Kekulé structure K_1' of the maximum internal subgraph G_1' of a normal benzenoid G_1

Using Theorem 2, we immediately have the following theorem.

Theorem 4 In a Kekulé structure of the maximum internal subgraph G_1' of G_1,if an alternating path (such as an alternating P-V path) is extended to and terminated in the contour C_e of G_1, and the path divides G_1 into two parts G_2 and G_3 which have the alternating path in common, then both G_2 and G_3 are normal.

The proof of the theorem is very simple. Because the interiors of G_2 and G_3 are Kekuléan, according to Theorem 2, both G_2 and G_3 are normal.

With regard to the inverse problem of Theorem 3, in[2], S.J.Cyvin and I.Gutman proposed two conjectures. In[6],we proved the two conjectures.Here we rewrite one of them as the following theorem.

Theorem 5 From an arbitrary normal benzenoid G_1 with h ($h > 1$) hexagons, one hexagon (with mode L, E or F) may be removed to yield another normal benzenoid G_2 with h-1 hexagons.

According to Theorem 4, obviously, a benzenoid G_2 yielded by deleting any one X_L from a normal benzenoid G_1 must be normal. Thus, to yield a new normal benzenoid G_2 from G_1, all X_L's are removable.

However a benzenoid G_2 yielded by deleting an X_E or an X_F from a normal benzenoid G_1 need not be normal (See Fig.3).

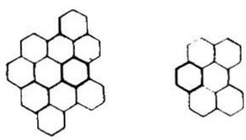


Fig.3 Deletion of a hexagon with mode E or F in a normal benzenoid G_1

How to select and to delete an X_E or X_F in G_1 with h ($h > 1$) hexagons to yield a new normal benzenoid G_2? In[2] we proposed a method, but the method is somewhat complicated. In this paper we propose a new simple method.

If an X (X_L, X_E, X_F) is deleted from a nomal benzenoid and the yielded benzenoid is still normal, then the X is called an N-removable one.

Consider a Kekulé structure K_1' of the maximum internal sub-graph G_1' of G_1. According to Theorem 4, if in an X_E of G_1, there is one double-bond edge belonging to K_1' (internal double-bond edge); or in an X_F, there are two internal double-bond edges belonging to K_1', then such an X_E or X_F (e.g. the hexagons marked by "△" or "▲" in Fig.4) is N-removable.

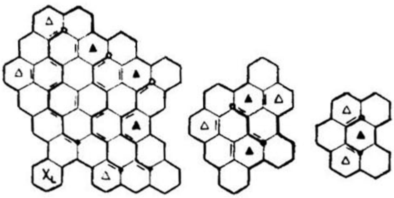


Fig.4 Some N-removable X_L's, X_E's and X_F's

To yield a new normal benzenoid G_2 from G_1, the method is as follows.

1) If there exist X_L's, then delete one of them. If there is no X_L, then go to step 2.

2) Find out a possible Kekulé structure K_1' of the maximum internal sub-graph G_1'. A P-V path system S_1' corresponds to K_1'.

3) If in S_1' there is a P-V path attached to a segment of the contour of G_1, then somewhere between the P-V path and the segment of the contour there exists at least one N-removable X_E (or X_F) which contains one (or two) oblique edges belonging to the P-V path. The proof is as follows.

In Fig.5a, denote the segment of the contour by ab whose ends a and b are adjacent to the ends p and v of the P-V path, respectively. The number of external edges of segment ab is odd (a and b have distinct colours).Hence there is at least one $X_E$or X_F attached to ab(X_E or X_F has an odd number of external edges).

Among them, every X_F contains two oblique edges belonging to the P-V path and is N-removable; the X_E's which contain one oblique edge belonging to the P-V path are N-removable; but the X_E's which have no oblique edge belonging to the P-V path need not be N-removable.

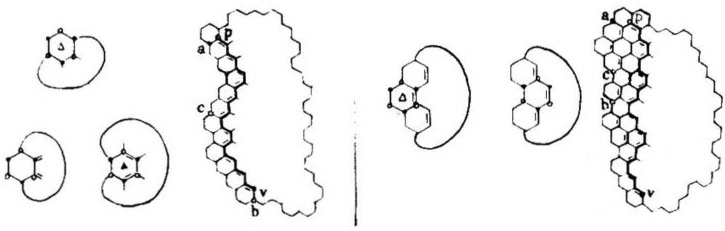
Assume that there is no X_F attached to ab and all the X_E's attached to ab have no oblique edge belonging to the P-V path. In these X_E's, among the external vertices of degree three, the one nearest to vertex a is vertex c. It has different colour from a. The number of external edges in segment ac is odd. Hence there exists at least one X_E or X_F attached to ac. This contradicts our assumption.

4) After step 2, if there is no P-V path attached to the contour tightly (see Fig.5b), then there exist some chains of external hexgons in which every hexagon has one internal vertical double-bond edge, and in every chain, there exists at least one N-removable X_E.The proof is analogy to that in step 3.

Fig.5b shows an example of such a chain which is attached to a segment of the contour of G_1.The ends of the segment are a and b. Since a has different colour from b, the number of external edges of ab is odd. There exists at least one X_E or X_F in the chain. Among them, X_E's are N-removable, but X_F's need not be so.

Assume that in such a chain, there is no X_E and all the X's having odd number of external edges are X_F's. Among the external vertices of these X_F's, let c be the vertex nearest to a. It has different colour from a. The number of external edges in segment ac is odd. Hence there exists at least one X_E or X_F attached to ac. This contradicts our assumption.

Fig 6. shows some examples about the reduction of normal benzenoids. In these examples, to yield new normal benzenoids. the successive deletion order of hexagons is given. Obviously, the order is not unique.



a b

Fig.5. Existence of N-removable X_E, X_F

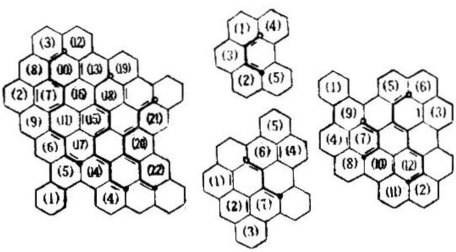


Fig.6 Deletion order of N-removable hexagons

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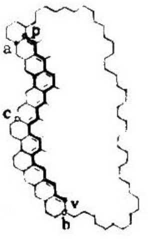
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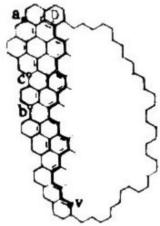
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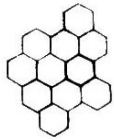

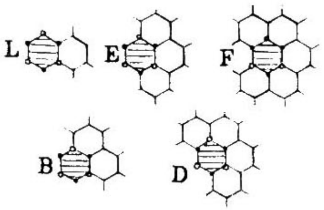
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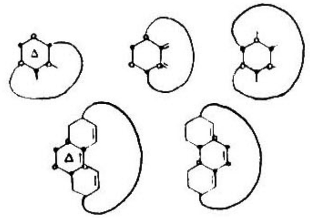
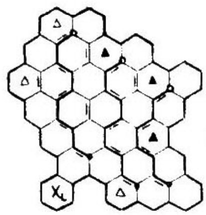
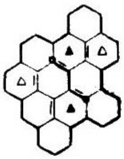
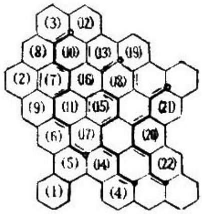



X_L

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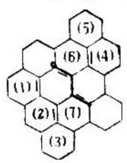
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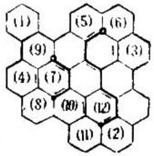
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