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SOME TOPOLOGICAL PROPERTIES AND GENERATION OF NORMAL BENZENOIDS

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ABSTRACT

The previous paper[1] on topological properties of benzenois and coronoids is supplemented, and the conjectures in[2] are proved.

KEY WORDS

Normal benzenoids - Building-up - Kekulé structure - Conjugated circuit

In this paper all the terms and definitions are applied in consistence with those in[1-5].

A normal benzenoid is a Kekuléan benzenoid system having no fixed-bond edges.

In[2],S.J.Cyvin and I.Gutman proposed the following conjectures.

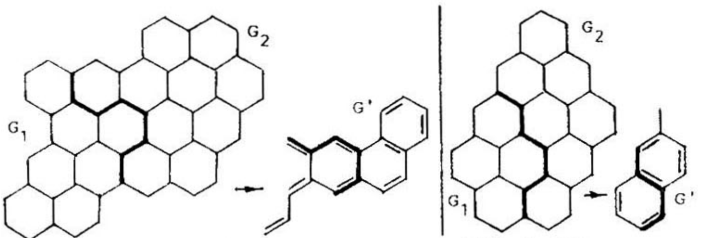
Conjecture A. All normal benzenoids with h hexagons ($h>1$) can be generated from the normal benzenoids with h-1 hexagons by adding a hexagon.

Conjecture B. From an arbitrary normal benzenoid with h hexagons ($h>1$), one hexagon may be removed to yield another normal benzenoid with h-1 hexagons.

These two conjectures have a connection with the generation and classified enumeration of benzenoids.

Discussion of the Building-up and Cut-off Processes

Let two benzenoids, G_1 with h_1 hexagons and G_2 with h_2 hexagons, touch each other and form a new benzenoid G with h ($h=h_1+h_2$) hexagons. We say that the two benzenoids are closely pieced together, and we call this process a building-up process (See Fig.1).



$m=8$, $n_1=26$
$n_2=34$, $n=52$

G is normal.

$m=7$, $n_1=16$
$n_2=26$, $n=35$

G is obvious non-Kekuléan.

Fig.1 Building-up processes

Theorem 1 (Building-up theorem A). If two normal benzenoids G_1 and G_2 are closely pieced together and have an odd number of common edges, then the produced benzenoid G is normal.

Proof:

According to theorem 7 in[1], both of the remainder systems G_1' and G_2' produced by deleting the external perimeters of G_1 and G_2, respectively, are Kekuléan.

Now let us consider G. The remainder G' produced by deleting the external perimeter of G is composed of three parts, G_1', G_2', and the common edges of G_1 and G_2. All the three parts are Kekuléan(See Fig.1). According to theorem 7 in[1], G is normal. Q.E.D.

Theorem 2 (Building-up theorem B). If two Kekuléan benzenoids G_1 and G_2 are closely pieced together, and have an even number of common edges, then the produced benzenoid G is obvious non-Kekuléan.

Proof:

Denote the number of common vertices of G_1 and G_2 by m, and the numbers of vertices in G_1, G_2 and G by n_1, n_2 and n, respectively. Both n_1 and n_2 are even and m is odd, so n is odd ($n=n_1+n_2-m$). Q.E.D.(See Fig.1)

There are five modes in which a new hexagon can be closely pieced together with (or added to) a benzenoid G_0 having h-1 hexagons to form a benzenoid G with h hexagons. These modes are denoted by L, E, F, B and D (See Fig.2).

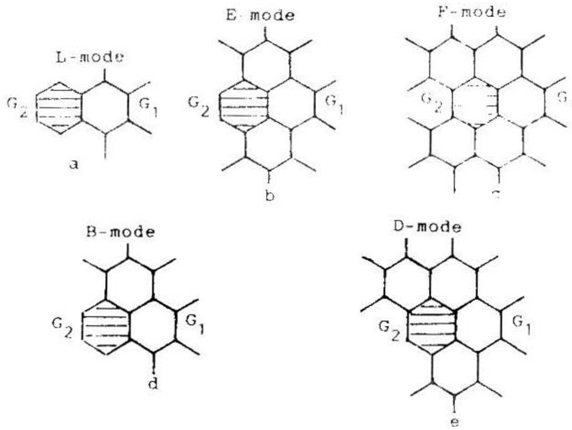


Fig.2 Five modes of closely pieced hexagons

From Theorems 1 and 2, we immediately have the following generation rules of benzenoids.

Theorem 3. A hexagon is added to a normal benzenoid G_1 with h-1 hexagons. If the addition mode is one of L, E and F. then the generated benzenoid G with h hexagons is normal (Fig.2a-c).

Proof:

For these modes, G_1 and G_2 have an odd number of common edges.

Theorem 4. A hexagon is added to a Kekuléan benzenoid G_1 with h-1 hexagons . If the addition mode is mode B or mode D. then the generated benzenoid G with h hexagons is obvious non-Kekuléan (Fig.2d,e).

Proof:

For these modes, G_1 and G_2 have an even number of common edges.

Now, go into the cut-off processes. We have the following results.

Theorem 5. From a Kekuléan benzenoid G with $h(h>1)$ hexagons, cut off any one Kekuléan benzenoid G_1 with h_1 hexagons to yield another benzenoid G_2 with $h_2(=h-h_1)$ hexagons. If the number of common edges of G_1 and G_2 is even, G_2 is obvious non-Kekuléan (Fig.3a).

Poof:

Using the same notation as in the proof of theorem 2, We have that $n_2(=n+m-n_1)$ is odd, because both n and n_1 are even and m is odd.

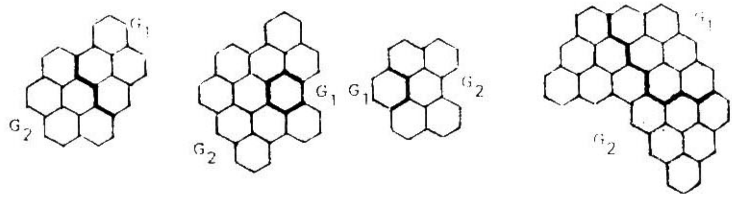
Now from a normal benzenoid G with h $(h>1)$ hexagons, cut off any one normal benzenoid G_1 with h_1 hexagons to form aother benzenoid G_2 with h_2 $(=h-h_1)$ hexagons. Even when the number of common edges of G_1 and G_2 is odd, G_2 needs not always be normal. Some examples are shown in Fig.3b-d.

There are two questions.

1) For an arbitrary normal benzenoid G with h hexagons $(h>1)$, is there a hexagon which can be removed from G to yield a normal benzenoid ?

2) If there is, how to find the hexagon in G ?

m =	5	6	4	10
n_1 =	16	6	6	22
n_2 =	19	36	20	42
n =	30	36	22	54



G_2 is obvious non-Kekuléan. | G_2 is essentially disconnected Kekuléan. | G_2 is concealed non-Kekuléan.

a b c d

Fig.3 Cut-off processes

The Proof of Cyvin-Gutman Conjectures and Some Other Results

<u>Theorem 6</u>. If a benzenoid G with h hexagons ($h>1$) is normal, then there exists a Kekulé structure K of G, in which both the external perimeter C_e and one of the hexagons touching with C_e are conjugated[6,7].

Proof:

According to Theorem 7 in[1], there is a Kekulé structure K_1 in which the external perimeter C_e is conjugated. Suppose that in K_1, there is no conjugated hexagons touching with C_e.

Step 1. In the interior of C_e, an alternating path can extend to and terminate on C_e. The path divides C_e into two parts. Each part with the path forms a circuit. There seem to exist two cases shown in Fig.4a,b. Case a is impossible, because both of the two circuits have odd edges. So we only need to consider the case b. In this case, one of the two circuits, say C_1 (shown by a heavy line in Fig.4b) is conjugated. Now, both of the circuits C_1 and C_e are conjugated in a Kekulé structure. If C_1 has a size more than one hexagon, we go into step 2.

Step 2. In the interior of C_1, an alternating path can extend to and terminate on C_1. There are five cases shown in Fig.5. For the cases in Figs.5a,b,c, one of the two newly produced circuits, C_2, which is drawn by heavy line, touchs with C_e and is conjugated. For the cases in Figs. 5a' and 5b', in which C_2 touching with C_e, is not conjugated, executing an RL transformation[1] of C_2' and an RL transformation of C_e, respectively,we can change C_2 into a conjugated circuit.

So in all five cases, we can obtain a conjugated circuit C_2 touching with the conjugated circuit C_e and enclosing a smaller area than C_1.

Using the method in step 2 continuously, we can obtain a smaller and smaller conjugated circuit touching with C_e, and finally we obtain a conjugated hexagon C_0 toudhing with the conjugated circuit C_e. Q.E.D.

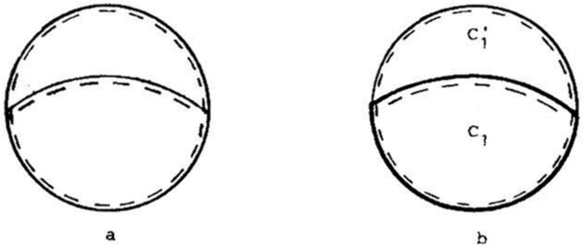


Fig.4 Step 1 of the proof of Theorem 6

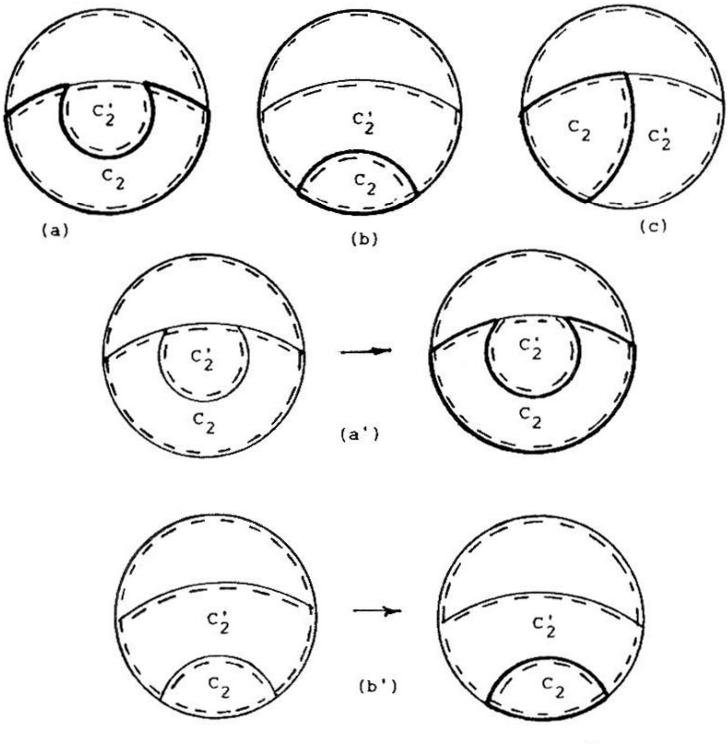


Fig.5 Step 2 of the proof of Theorem 6

If in step 1, executing an RL transformation[1] of C_e, we can change C_1' into a conjugated circuit, then, analogously to the above proof, we can prove that there exists a Kekulé structure of G in which both C_e and another hexagon C_0', which touchs with C_e and is in the interior of C_1', are conjugated.

Obviously, either C_0 or C_0' are coincident with one of the three modes L, E and F.

Using Theorem 6, we can easily give the proof of Cyvin-Gutman conjectures A and B. Now, we rewrite them as Theorems 7 and 8.

Theorem 7. From an arbitrary normal benzenoid G with h hexagons ($h>1$) one hexagon may be removed to yield another normal benzenoid G' with h-1 hexagons.

Proof:

According to Theorem 5, there exists a Kekulé structure K of G, in which both the external perimeter C_e of G and a hexagon C_0 touching with C_e are conjugated. Of course, the mode of C_0 is one of L, E and F. Our proof is only for the case of the E-mode. The proofs for the L- and the F- modes are fully analogous.

Executing an RL transformation[1] of C_0, we obtain a Kekulé structure K'(shown in Fig.6), in which uv is a double bond edge.

The remainder system G' produced by deleting the two vertices u and v has a Kekulé structure in which the external perimeter C_e' is conjugated. According to Theorem 7 in[1], G' is normal.

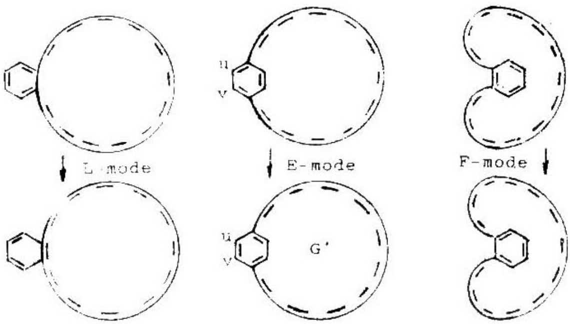


Fig 6 Illustration of the proof of Theorem 7

For an arbitrary normal benzenoid G with h (h>1) hexagons, Theorem 6 gives not only the proof of existence of the hexagon which can be removed from G to yield another normal benzenoid, but also the method for finding the hexagon in G.

From Theorem 7, we immediately have Theorem 8.

Theorem 8. All normal benzenoids with h hexagons(h>1) can be generated by adding one hexagon with modes L, E or F to the normal benzenoid with h-1 hexagons.

According to Theorems 3 and 8, to begin with the benzene, by using the L-, E- and F- mode additions,all the normal benzenoids can be generated.

However, Theorems 7 and 8 cannot be extended to the case of normal coronoids. An example is shown in Fig 7. Deleting any haxagon from the normal coronoid, we obtain a non-Kekuléan system. Therefore such a normal coronoid cannot be generated by adding one hexagon to a normal system with h-1 hexagons.

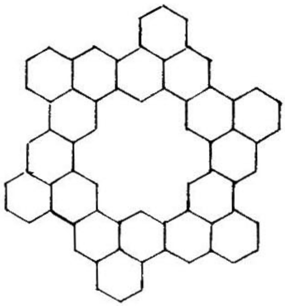


Fig.7 A coronoid

<u>Theorem 9</u>. If from an arbitrary normal benzenoid G with h hexagons (h>1) one deletes any one hexagon with one of the modes L, E and F, then the obtained remainder benzenoid G' must be Kekuléan.

Proof:

From the proof of Theorem 6 in the present paper, for h>1, there must exist at least two hexagons with modes L, E or F. Consider one of such hexagons, say C_0 with mode E. Our proof is only for the case of mode E. The proofs for modes L and F are fully analogous.

According to Theorem 5 in[1], there exists a Kekulé structure of G in which C_0 is conjugated and the edge uv is a double bond. Delete the vertices u and v. This has no effect on the Kekulé structure of the remainder G'(See Fig.8). Q E D

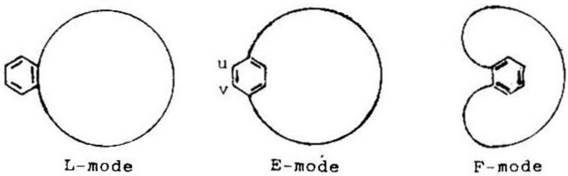


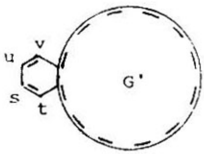
Fig. 8 Deletion of one hexagon with mode L, E or F

Furthermore, we have the following theorem.

Theorem 10. If from a normal benzenoid G having some hexagons with mode L, one deletes any one hexagon with mode L, then the obtained remainder benzenoid G' must be normal.

Proof:

According to theorem 7 in[1], there exists a Kekulé structure of G in which the external perimeter C_e is conjugated. As we can see in Fig.9, in the same Kekulé structure, C_0 is also conjugated and the edges uv and st are double bonds. The remainder G' produced by deleting uv and st has a conjugated external perimeter. According to theorem 7 in[1], G' is normal.



L-mode

Fig.9 Deletion of one hexagon with mode L

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