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# THE NECESSARY AND SUFFICIENT CONDITIONS FOR BENZENOID SYSTEMS WITH SMALL NUMBER OF HEXAGONS TO HAVE KEKULÉ PATTERNS

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ABSTRACT. A concealed non-Kekuléan benzenoid system is said to be of type I if it satisfies Sachs' necessary conditions for benzenoid systems to have Kekulé patterns [1]. In this paper we prove that the smallest non-Kekuléan benzenoid system of type I is unique and contains exactly 14 hexagons. Furthermore, the necessary and sufficient conditions for benzenoid systems with $h<14$ to have Kekulé patterns are given.

Many investigations have been made to seek for necessary and sufficient conditions for the existence of Kekulé patterns in a benzenoid system [1-7]. In particular, [7] gave some fairly simple conditions, which are both necessary and sufficient. In the present paper, we give some simpler conditions for benzenoid systems with $h<14$ to have Kekulé patterns.

Let H be a benzenoid system (or a hexagonal system) drawn in the plane such that one of the three edge directions is vertical. The following concepts were first introduced in [1].

A straight line segment C with end points $p_1, p_2$ (possibly, $p_1=p_2$) is called a cut segment if (a) C is orthogonal to one of three edge directions, (b) each of $p_1$, $p_2$ is the centre of an edge, (c) if $p_1 \neq p_2$, then any point of C is either an interior or a boundary point of some cell (i.e. hexagon) of H, (d) the graph obtained from H by deleting all edges intersected by C has exactly two components (see Fig.1(a)).

Let $\mathbb{C}$ denote the set of edges of H intersected by C; $\mathbb{C}$ is called a cut of H. If C is a horizontal cut segment, the component of H-$\mathbb{C}$ lying at the upper bank of $\mathbb{C}$ is denoted by U($\mathbb{C}$), and the component at the lower bank is denoted by L($\mathbb{C}$).

A vertex of H which lies above (below) all the vertices which are adjacent to it is called the peak (valley) of H. The number of peaks (valleys) of H is denoted by p(H) (v(H)). And the number of peaks (valleys) of H which belong to the upper bank U($\mathbb{C}$) is denoted by p(H/U($\mathbb{C}$)) (v(H/U($\mathbb{C}$))).

Some necessary conditions for benzenoid systems to have Kekulé patterns were given in [1].

Lemma 1 [1]. Let H be a hexagonal system which has a perfect matching. Then, for each of the six possible positions and every horizontal cut $\mathbb{C}$, (i) $p(H)=v(H)$, (ii) $0 \leq p(H/U(\mathbb{C})) - v(H/U(\mathbb{C})) \leq |\mathbb{C}|$.

In [1], Sachs conjectured that the necessary conditions are also sufficient. But the conjecture is not true(see [2]).

In order to get some necessary and sufficient conditions for benzenoid systems to have perfect matchings, [7] generalized the concepts of the horizontal cut segment and the horizontal cut of H to the horizontal g-cut segment and the horizontal g-cut.

A broken line segment $C=p_1p_2p_3$ (possibly, $p_2=p_3$) is called a horizontal g-cut segment of H if (1) $p_1p_2$ is horizontal, (2) each of $p_1, p_3$ is the centre of an edge lying on the contour of H, and if $p_2 \neq p_3$, $p_2$ is the centre of a hexagon of H, (3) every point of C is either an interior or a boundary point of some hexagon of H, (4) if $p_2 \neq p_3$, the angle $p_1p_2p_3$ is $\pi/3$ (see Fig.1(b) ).

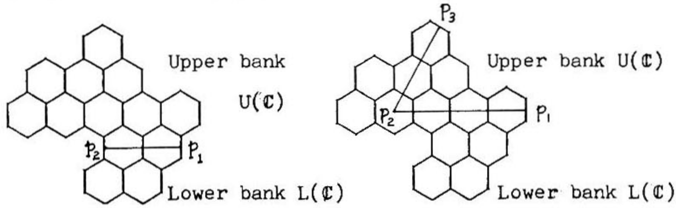


Fig.1(a) Fig.1(b)

In particular, if $p_2=p_3$, C becomes a horizontal cut segment.

For a horizontal g-cut segment $C=p_1p_2p_3$, let $\mathbb{C}_{12}$ and $\mathbb{C}_{23}$ denote the sets of edges of H intersected by straight line segments $C_{12}=p_1p_2$ and $C_{23}=p_2p_3$, respectively. Let $\mathbb{C}=\mathbb{C}_{12}\cup\mathbb{C}_{23}$. $\mathbb{C}$ is called a horizontal g-cut.

In particular, if $p_2=p_3$, $\mathbb{C}=\mathbb{C}_{12}$ becomes a horizontal cut.

Some fairly simple necessary and sufficient conditions were given in [7].

Theorem 2 [7]. Let H be a hexagonal system. Then H has a perfect matching if and only if , for each of its six possible and every horizontal g-cut $\mathbb{C}$,

(i) $p(H)=v(H)$,

(ii) $p(H/U(\mathbb{C}))-v(H/U(\mathbb{C}))\leqslant|\mathbb{C}_{12}|$ .

From theorem 2 and lemma 1 we can assert that there exist some concealed non-Kekuléan benzenoid systems which satisfy the conditions of lemma 1 but not (ii) of theorem 2. We call them the concealed non-Kekuléan benzenoid systems of type I. [2] gave a such example as shown in Fig.2.

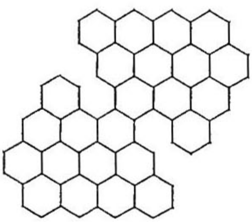

Fig.2

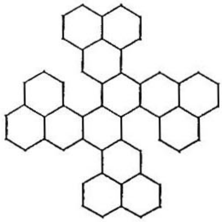

Fig.3

It is natural to investigate the smallest concealed non-Kekuléan benzenoid systems of type I. It can move us to find some simpler necessary and sufficient conditions for benzenoid systems with small number of hexagons to have Kekulé patterns.

Theorem 3. Let H be a smallest concealed non-Kekuléan benzenoid system of type I. Then (i) h=14, (ii) H is unique as shown in Fig.3.

Proof. Since H is of type I, there is a horizontal g-cut $C=p_1p_2p_3$ $(p_2\neq p_3)$ such that $p(H/U(C))-v(H/U(C))>|C_{12}|$.

If $|C_{12}|=|C_{23}|=1$, then $U(C)$ has only one vertex, and $p(H/U(C))-v(H/U(C))=0<|C_{12}|$, a contradiction. Hence either $|C_{12}|$ or $|C_{23}|$ is greater than one. Suppose that $|C_{12}|=2$, $|C_{23}|=1$ (see Fig.4(1)). Then the hexagon $s_1$ belongs to H. Otherwise, $p(H/U(C))-v(H/U(C))=1<|C_{12}|$, again a contradiction. We assert that the hexagon $s_2$ belongs to H, too. Otherwise the horizontal cut segment C' passing through the centre of $s_1$ will satisfy that

$$p(H/U(C'))-v(H/U(C'))=w(U(C'))-b(U(C'))+|C'|=[w(U(C))-2]-[b(U(C))-2]+|C_{12}|=p(H/U(C))-v(H/U(C))>|C_{12}|=|C''|,$$

contradicting that H is of type I (see Fig.4(2)). Moreover, the hexagon $s_3$ must belong to H. Otherwise there is a cut segment C" as shown in Fig.4(3). Put C" in horizontal position, then $v(H/U(C''))-p(H/U(C''))=w(U(C''))-b(U(C''))-|C''|=[w(U(C))-1]-[b(U(C))-3]-|C_{12}|=w(U(C))-b(U(C))=p(H/U(C))-v(H/U(C))-|C_{12}|>0$. This contradicts that H is of type I, too.

Now, since $p(H/U(C))-v(H/U(C))=v(H/L(C))-p(H/L(C))\geq |C_{12}|+1=3$, it is easy to see that $U(C)$ contains at least seven hexagons, and if $U(C)$ contains exactly seven hexagons, U($\mathbb{C}$) can only be as shown in Fig.4(1).

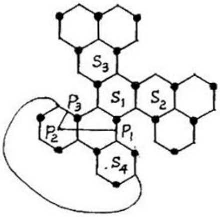


Fig.4(1)

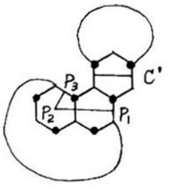


Fig.4(2)

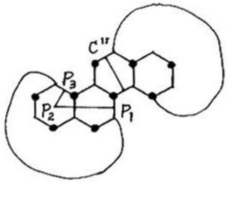


Fig.4(3)

By the same reason the hexagon $s_4$ (see Fig.4(1)) must belong to H, and L($\mathbb{C}$) and H can only be as shown in Fig.3.

It is easy to verify that H is of type I.

In the other cases, $|\mathbb{C}_{12}|+|\mathbb{C}_{23}|\geq 4$. We shall prove that $h>14$.

Let X (Y) be the set of the hexagons in U($\mathbb{C}$) (L($\mathbb{C}$)), and let H[X] be the benzenoid system induced by X.

If $|\mathbb{C}_{23}|=1$, $|\mathbb{C}_{12}|\geq 3$, then $v(H/L(\mathbb{C}))-p(H/L(\mathbb{C}))=p(H/U(\mathbb{C}))-v(H/U(\mathbb{C}))\geq|\mathbb{C}_{12}|+1\geq 4$. We can see that $|Y|\geq 5$. If $h\leq 14$, then $|X|=h-|Y|-|\mathbb{C}|+1\leq 6$. On the other hand $p(H[X])-v(H[X])$ must be greater than one, so $|X|\geq 6$. Hence we have that $|X|=6$, $|Y|=5$ and $|\mathbb{C}_{12}|=3$. Then H[X] consists of either one triangulene or two phenalenes (see Fig.5), and H can only be as shown in Fig.6. But in H there is a horizontal cut $\mathbb{C}'$ such that $p(H/U(\mathbb{C}'))-v(H/U(\mathbb{C}'))>|\mathbb{C}'|$, contradicting that H is of type I.

If $|\mathbb{C}_{12}|\geq 2$, $|\mathbb{C}_{23}|\geq 2$, and $h\leq 14$, it is easy to see that $|Y|\geq 6$, so $|X|\leq 5$. Clearly, this is impossible.

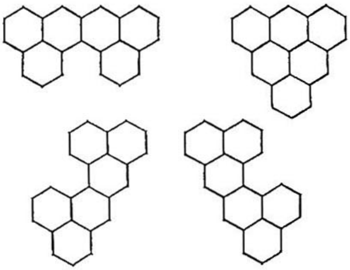

Fig.5

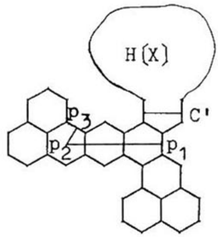


Fig.6

Now it follows that the benzenoid system shown in Fig.3 is the unique smallest concealed non-Kekuléan benzenoid system of type I.

By theorem 3, for a benzenoid system with $h<14$, the necessary conditions in lemma 1 is alao sufficient. In fact, we have the stronger result.

Theorem 4. Let H be a benzenoid system with $h<14$. Then H has a Kekulé pattern if and only if, for each of its six possible positions and every horizontal cut $\mathbb{C}$,

(i) $p(H)=v(H)$,

(ii) $p(H/U(\mathbb{C}))-v(H/U(\mathbb{C}))\leq|\mathbb{C}|$.

Proof. The necessity is clear. We only need prove the sufficiency.

Suppose that the conditions (i) and (ii) are satisfied, but H has no Kekulé pattern.

Since $h<14$, by theorem 3, H is not of type I. So there is a horizontal cut $\mathbb{C}$ in H that does not satisfy the conditions in lemma 1. But H satisfies the conditions (i) and (ii), by our assumption. Hence $p(H/U(\mathbb{C}))-v(H/U(\mathbb{C}))<0$.

Let X (Y) be the set of the hexagons in $U(\mathbb{C})$ $(L(\mathbb{C}))$, and let $H[X]$ be the benzenoid system induced by X.

If $|\mathbb{C}|=2$, then $v(U(\mathbb{C}))-p(U(\mathbb{C}))\geq 3$, and $v(H[X])-p(H[X])\geqslant 2$. So $|X|\geqslant 6$. Similarly, $|Y|\geqslant 6$. From $h\leq 13$, we have that $|X|=|Y|=6$. Thus $v(H[X])-p(H[X])=2$, $v(H/U(\mathbb{C}))-p(H/U(\mathbb{C}))=1$, and $U(\mathbb{C})$ can only be one of the benzenoid systems as shown in Fig.7. Put the cut segment C' in horizontal position, then $p(H/U(\mathbb{C}'))-v(H/U(\mathbb{C}'))=3>|\mathbb{C}'|$. This contradicts our assumption.

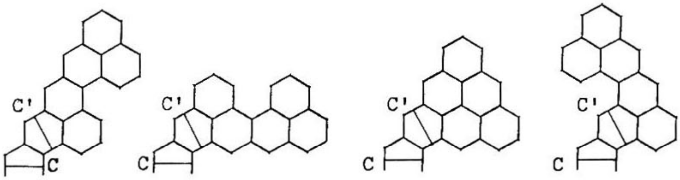


Fig.7

If $|\mathbb{C}|>2$, then either $|X|$ or $|Y|$, say $|X|$, is less than six. So $v(H[X])-p(H[X])\leq 1$, and $p(H/U(\mathbb{C}))-v(H/U(\mathbb{C}))\geqslant 0$. This is also a contradiction.

The theorem now is proved.

In addition, [3] gave the result that a smallest concealed non-Kekuléan benzenoid system contains exactly 11 hexagons. It can be stated as the following theorem.

Theorem 5[3]. Let H be a benzenoid system with $h<11$. Then H has a Kekulé pattern if and only if, for each of its six possible positions, $p(H)=v(H)$.

Furthermore, by the computer-generation, [8] asserted that there exist only eight smallest concealed non-Kekuléan benzenoid system.

Using theorem 4 in this paper, we can give it a simple proof which does not depend on the computer-generation.

Theorem 6. The eight benzenoid systems which have been found in [8] are the only smallest concealed non-Kekuléan benzenoid systems.

Proof. Let H be a smallest concealed non-Kekuléan benzenoid system with h hexagons. From the examples in [8], we have that $h \leq 11 < 14$. Thus, by theorem 4, there is a horizontal cut $\mathbb{C}$ in H such that $p(H/U(\mathbb{C}))-v(H/U(\mathbb{C})) \geq |\mathbb{C}|+1$.

Let Z be the set of all the hexagons in H, and let X (Y) be the set of the hexagons in $U(\mathbb{C})$ $(L(\mathbb{C}))$. Then

$$p(H[Z\setminus Y])-v(H[Z\setminus Y])=v(H[Z\setminus X])-p(H[Z\setminus X])=p(H/U(\mathbb{C}))-v(H/U(\mathbb{C}))-|\mathbb{C}|+1 \geq 2. \qquad \ldots\ldots (1)$$

If $|\mathbb{C}| \geq 3$, then $|X| + |Y| \leq 9$, and either $|X|$ or $|Y|$, say $|X|$, is less than or equal to 4. Clearly, this is impossible. Hence $|\mathbb{C}|=2$. By the inequality (1), we have that $|X| \geq 5$, $|Y| \geq 5$ and $h \geq 11$. It implies that $|X|=|Y|=5$ and $h=11$. Furthermore, $H[Z\setminus Y]$ can only be one of the benzenoid systems as shown in Fig.5. The cases of $H[Z\setminus X]$ are similar to $H[Z\setminus Y]$. It is not difficult to see that they can only make the eight smallest concealed non-Kekuléan benzenoid systems which have been found in [8].

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