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A CONSTRUCTION METHOD FOR CONCEALED NON-KEKULÉAN BENZENOID SYSTEMS WITH h = 12,13

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ABSTRACT. In this paper we give a construction method for concealed non-Kekuléan benzenoid systems with h = 12,13, and prove that there are exactly 98 concealed non-Kekuléan benzenoid systems with h = 12 and 1097 such benzenoid systems with h = 13.

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Eight concealed non-Kekuléan benzenoid systems with eleven hexagons have been found by I.Gutman, A.T.Balaban, H.Hosoya, S.J.Cyvin (see [1]-[5]). I.Gutman also stated that no such systems exist for $h<11$. In [6], by the computer-generation, it was **claimed** that there are exactly 8 smallest concealed non-Kekuléan benzenoid systems (h=11). Recently we gave a rigorous proof of this fact [7]. In addition, by the computer-aided generation, He Wenchen et al. found that there are exactly 98 such benzenoid systems with h=12 [8].

In this paper, we attempt to give a construction method for concealed non-Kekuléan benzenoid systems with h = 12,13, and prove that there are exactly 98 such benzenoid systems with h = 12, and 1097 such benzenoid systems with h = 13.

Let H be a benzenoid system drawn in the plane such that one of the three edge directions is vertical. The concepts of a horizontal cut segment C, a horizontal cut $\mathbb{C}$, $U(\mathbb{C})$, $L(\mathbb{C})$, and the numbers of peaks (valleys), p(H) (v(H)), $p(H/U(\mathbb{C}))$ $(v(H/U(\mathbb{C}))$, were intruduced in [9]. For convenience, we denote by X, Y and Z the sets of the hexagons in $U(\mathbb{C})$, $L(\mathbb{C})$ and H, respectively, and, for $S \subset Z$, we denote by H[S] the induced subgraph in H of S.

In [7] we proved the following theorem.

Theorem 1 [7]. 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) $p(H/U(\mathbb{C}))-v(H/U(\mathbb{C}))\leq|\mathbb{C}|$.

From this theorem, we can give the following theorem .

Theorem 2. Let H be a concealed non-Kekuléan benzenoid system with $h<14$. Then there is a horizontal cut $\mathbb{C}$ in H such that (i) $p(H/U(\mathbb{C}))-v(H/U(\mathbb{C}))>|\mathbb{C}|$, and (ii) $|\mathbb{C}|= 2$.

Proof. By theorem 1, there is a horizontal cut $\mathbb{C}$ in H such that (i) follows. We need only to prove that $|\mathbb{C}|= 2$.

Suppose that $|\mathbb{C}| \geq 3$. By $h < 14$, we have $|X| + |Y| < 12$. Thus either $|X|$ or $|Y|$, say $|X|$, is less than or equal to 5, hence $p(H[X]) - v(H[X]) \leq 1$. On the other hand, $p(H[Z \setminus Y]) - v(H[Z \setminus Y]) = p(H/U(\mathbb{C})) - v(H/U(\mathbb{C})) - (|\mathbb{C}| - 1) \geq 2$. So $H[Z \setminus Y]$ must be as shown in Fig.1, that is, there are $|\mathbb{C}|$ hexagons in $H[X]$ each of which has one vertex incident with an edge in $\mathbb{C}$. The number of the other hexagons in $H[X]$ is equal to $|X| - |\mathbb{C}| \leq 5 - |\mathbb{C}| \leq 2$. Clearly, then $p(H[X]) - v(H[X]) \leq 0$, and $p(H/U(\mathbb{C})) - v(H/U(\mathbb{C})) \leq |\mathbb{C}|$. This contradicts (i).

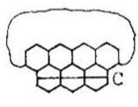


Fig.1

Now we can give a construction method for concealed non-Kekuléan benzenoid systems with $h < 14$.

Definition 3. A concealed non-Kekuléan benzenoid system H is said to be reducible if there is a hexagon in H, say a reducible hexagon of H, which contains four vertices of valency 2 of H, otherwise H is said to be irreducible.

Obviously, a reducible hexagon of H corresponds to a vertex of valency one of the characteristic graph of H.

Let N_h $(\overline{N}_h)$ denote the set of all reducible (irreducible) concealed non-Kekuléan benzenoid systems with h hexagons. Since the smallest concealed non-Kekuléan benzenoid system contains eleven hexagons, $\overline{N}_h = \emptyset$ for $h < 11$, and $N_h = \emptyset$ for $h < 12$.

Let $H \in N_h$, and let s be a reducible hexagon. We denote by H-s the benzenoid system $H[Z \setminus \{s\}]$. Clearly, $H - s \in N_{h-1} \cup \overline{N}_{h-1}$. Conversely, we also say that $H = (H-s)+s$ is generated from $H'=H-s$ by adding the hexagon s. The common edge of s and $H'=H-s$ is called an attachable edge of H'. For $H \in N_h \cup \overline{N}_h$, let $E^*(H)$ be the set of all attachable edges of H. $E^*(H)$ can be divided as the union of equivalence classes $\bigcup_{i=1}^{r} E_i^*(H)$ such that $e_j, e_k \in E_i^*(H)$ if e_j and e_k lie on the symmetric positions in H. The number of equivalence classes of $E^*(H)$ is denoted by $r(E^*(H))=r$.

The below theorem follows evidently.

Theorem 4. Let $H \in N_h$. Then there is unique $H' \in \overline{N}_{h-i}$, $1 \leq i \leq h-11$, such that H is generated from H' by adding i hexagons one by one.

From theorem 4, the benzenoid systems in N_{12} can be generated from the benzenoid systems in $\overline{N}_{11}$ by adding one hexagon, and the benzenoid systems in N_{13} can be generated from the systems in $\overline{N}_{11}$ ($\overline{N}_{12}$) by adding two (one) hexagons.

Lemma 5. Let $H_1' \in \overline{N}_{h_1}$ and $H_2' \in \overline{N}_{h_2}$ be two distinct benzenoid systems, and let H_1 and H_2 be benzenoid systems in N_h which are generated from H_1' and H_2', respectively. Then H_1 and H_2 are not isomorphic.

Lemma 6. Let $H \in N_h \cup \overline{N}_h$, and let $N_{h+1}(H) \subset N_{h+1}$ be the set of all the benzenoid systems which are generated from H by adding one hexagon. Then $|N_{h+1}(H)| = r(E^*(H))$.

Lemma 7. Let $H \in N_h$, and let $N_{h+2}(H) \subset N_{h+2}$ be the set of all the benzenoid systems which are generated from H by addinng two hexagons s_1, s_2, and in $H+s_1+s_2 \subset N_{h+2}(H)$ s_1 and s_2 are not adjacent. Then $N_{h+2}(H)$ can be divided as the union of disjoint subsets $\bigcup_{i=1}^{r} N_{h+2}^i(H)$ such that $H' \in N_{h+2}^i(H)$ if at least one edge in $E_i^*(H)$ is not on the boundary of H', and each edge in $E_j^*(H)$, $j < i$, is on the boundary of H'.

In the following, we give a construction method for the benzenoid systems in $\overline{N}_h$, h=12,13.

By theorem 2, for a benzenoid system H in $\overline{N}_h$, $h < 14$, there is a horizontal cut $\mathbb{C}$ such that $|\mathbb{C}|=2$, and $p(H/U(\mathbb{C}))-v(H/U(\mathbb{C})) \geq |\mathbb{C}|+1=3$. Let s* be the unique hexagon in $Z \setminus X \cup Y$. Then $|X|+|Y|<13$, and $5 \leq |X| \leq 7$, $5 \leq |Y| = h-|X|-1 \leq 7$. Thus the construction of H depends on the construction of $U(\mathbb{C})$ and $L(\mathbb{C})$ (or $H[X \cup \{s^*\}]$ and $H[Y \cup \{s^*\}]$) with $|\mathbb{C}|=2$, $5 \leq |X| \leq 7$, $5 \leq |Y| = h-|X|-1 \leq 7$, and $p(H/U(\mathbb{C}))-v(H/U(\mathbb{C}))= v(H/L(\mathbb{C}))-p(H/L(\mathbb{C})) \geq 3$. By symmetry, we need only to investigate the construction of $U(\mathbb{C})$ or $H[X \cup \{s^*\}]$.

<u>Lemma 8.</u> Let $H \in \overline{N}_h$, $h < 14$, and let $\mathbb{C}$ be a horizontal cut of H which satisfies that (i) $|\mathbb{C}|=2$, (ii) $p(H/U(\mathbb{C}))-v(H/U(\mathbb{C})) \geq 3$. Then $H[X \cup \{s^*\}]$ must be isomorphic to one of the benzenoid systems as shown in Fig.2.

<u>Proof.</u> Since $p(H/U(\mathbb{C}))-v(H/U(\mathbb{C})) \geq 3$ and $|X| \leq 7$, we have that

$$p(H[X \cup \{s^*\}])-v(H[X \cup \{s^*\}]) \geq 2, \quad \cdots (1)$$

and

$$1 \leq p(H[X])-v(H[X]) \leq 2. \quad \cdots (2)$$

Case 1. $|X|=5$.

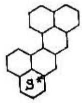
Clearly, by inequality (1), $H[X \cup \{s^*\}]$ must be isomorphic to one of the three benzenoid systems A_1, A_2 and A_3 in Fig.2.

Case 2. $|X|=6$.

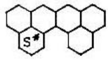
Subcase 2.1. $p(H[X])-v(H[X])=2$.

Then $H[X]$ must be isomorphic to one of A_1, A_2, and A_3.

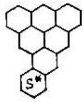
A_1



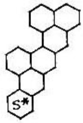
A_2



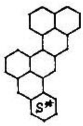
A_3



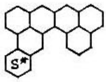
B_1



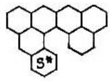
B_2



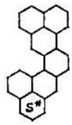
B_3



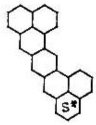
B_4



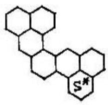
B_5



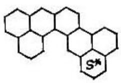
C_1



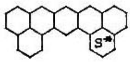
C_2



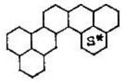
C_3



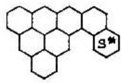
C_4



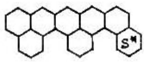
C_5



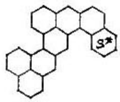
C_6



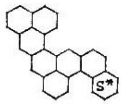
D_1



D_2



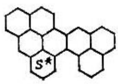
D_3



D_4

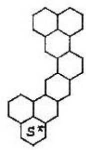
D_5

E_1

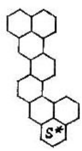


E_2

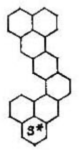
E_3



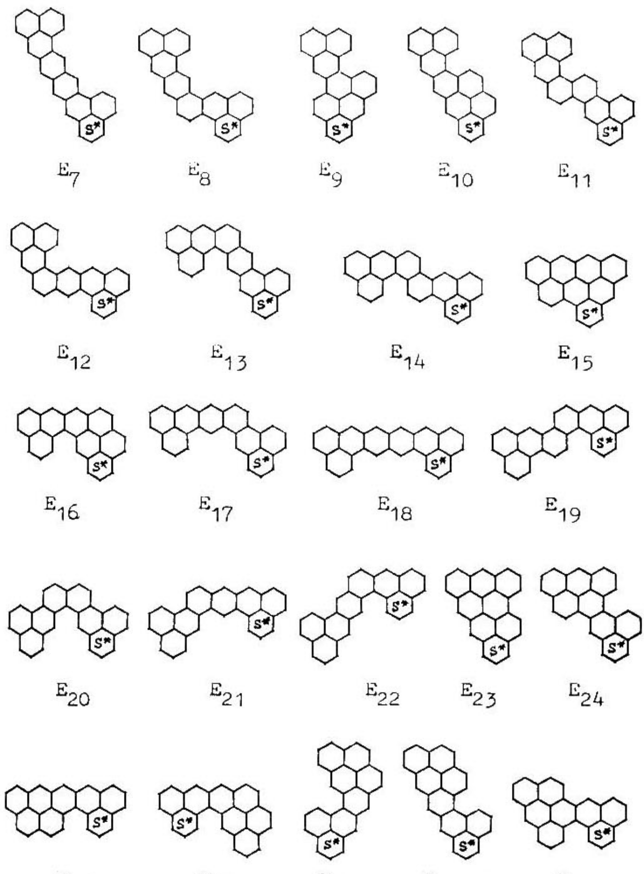
E_4



E_5



E_6


S*
E7
E8
E9
E10
E11
E12
E13
E14
E15
E16
E17
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E26
E27
E28
E29

Fig.2

So $H[X\cup\{s^*\}]$ must be isomorphic to one of the five benzenoid systems B_1, B_2, B_3, B_4, B_5 in Fig.2.

Subcase 2.2. $p(H[X])-v(H[X])=1$.

Then, by inequality (1), s^* must be adjacent to two hexagons s_1, s_2 in $H[X]$. So $|X\setminus\{s_1,s_2\}|=4$, and $p(H[X\setminus\{s_1,s_2\}])-v(H[X\setminus\{s_1,s_2\}])\leq 1$. Note that $H\in\overline{N}_h$, there is no reducible hexagon in H. Thus $H[X\setminus\{s_1,s_2\}]$ is connected. Otherwise each component of $H[X\setminus\{s_1,s_2\}]$ contains at least two hexagons, then $H[X\cup\{s^*\}]$ can only be the benzenoid system as shown in Fig.3. But then $p(H[X])-v(H[X])=-2$, a contradiction.

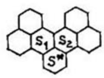


Fig.3

In addition, by inequality (1), we have that $p(H[X\setminus\{s_1,s_2\}])-v(H[X\setminus\{s_1,s_2\}])=1$. Otherwise there are three hexagons s_3, s_4 and s_5 in $H[X\setminus\{s_1,s_2\}]$ each of which is adjacent to s_1 or s_2, and lies above s_1 and s_2, the other hexagon s_6 in X would be a reducible hexagon in H, again a contradiction. Hence $H[X\setminus\{s_1,s_2\}]$ consists of a phenalene together with another hexagon s_3, and s_3 is adjacent to s_1 or s_2. Now it is not difficult to see that $H[X\cup\{s^*\}]$ must be isomorphic to one of the six benzenoid systems $C_1,C_2,\cdots,C_6$ in Fig.2.

Case 3. $|X|=7$.

Subcase 3.1. $p(H[X])-v(H[X])=2$.

Then s^* is adjacent only to one hexagon in $H[X]$. Otherwise, let s_1 and s_2 be adjacent to s^*. Since $|X\setminus\{s_1,s_2\}|=5$, $p(H[X\setminus\{s_1,s_2\}])-v(H[X\setminus\{s_1,s_2\}])\leq 1$. But $p(H[X])-v(H[X])=2$. So, if $H[X\setminus\{s_1,s_2\}]$ is connected, there are three hexagons in $H[X\setminus\{s_1,s_2\}]$ each of which is adjacent to s_1 or s_2 and lies above s_1 and s_2. Then it is easy to see that $p(H[X])-v(H[X])\leq 1$, a contradiction. If $H[X\setminus\{s_1,s_2\}]$ is not connected , it has exactly two components, where one contains two hexagons, another contains three hexagons. Obviously, then $p(H[X])-v(H[X])\leq 0$. This is also a contradiction.

Let $s_1\in X$ be the hexagon adjacent to s^*.

If two vertical edges of s_1 are both on the boundary of $H[X\cup\{s^*\}]$, there is another horizontal cut $\mathfrak{C}'$ which satisfies the conditions of theorem 2(see Fig.4). Then $|X'|=6$, and we reduce it to case 2. Hence a vertical edge of s_1 is not on the boundary of $H[X\cup\{s^*\}]$.

Let s_2 be the other hexagon in $H[X\cup\{s^*\}]$ which contains the vertical edge of s_1(see Fig.5).

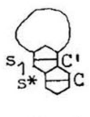


Fig.4

Fig.5

If s_2, s_3 and s_4 are all in $H[X\cup\{s^*\}]$, then $H[X\setminus\{s_1\}]$ is connected, and $p(H[X\setminus\{s_1\}])-v(H[X\setminus\{s_2\}])=p(H[X])-v(H[X])$ $=2$. Combining $|X\setminus\{s_1\}|=6$, $H[X\setminus\{s_1\}]$ must be one of A_1, A_2 and A_3 in Fig.2. This is a contradiction.

If s_2, $s_3\in X$, $s_4\notin X$, then $p(H[X\setminus\{s_1\}])-v(H[X\setminus\{s_2\}])=3$. This is also impossible.

Hence the following two cases can only happen.

(i) $s_2\in X$, s_3, $s_4\notin X$. Then $H[X\setminus\{s_1\}]$ is connected, and $p(H[X\setminus\{s_1\}])-v(H[X\setminus\{s_1\}])=2$. So $H[X\setminus\{s_1\}]$ must be isomorphic to one of A_1, A_2 and A_3 in Fig.2, and $H[X\cup\{s^*\}]$ must be isomorphic to one of D_1, D_2, D_3, D_4 in fig.2.

(ii) $s_2, s_4 \in X$, $s_3 \notin X$. Clearly, $H[X \cup \{s^*\}]$ must be isomorphic to D_5 in Fig.2.

Subcase 3.2. $p(H[X]) - v(H[X]) = 1$.

Then there are two hexagons s_1, s_2 in $H[X]$ which are adjacent to s^*, $|X \setminus \{s_1, s_2\}| = 5$, and $0 \leq p(H[X \setminus \{s_1, s_2\}]) - v(H[X \setminus \{s_1, s_2\}]) \leq 1$.

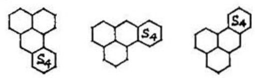
If $p(H[X \setminus \{s_1, s_2\}]) - v(H[X \setminus \{s_1, s_2\}]) = 0$, there are three hexagons each of which is adjacent to s_1 or s_2, and lies above s_1 and s_2. Then , since H is irreducible, $H[X \cup \{s^*\}]$ must be isomorphic to E_1 in Fig.2.

Hence $p(H[X \setminus \{s_1, s_2\}]) - v(H[X \setminus \{s_1, s_2\}]) = 1$.

If $H[X \setminus \{s_1, s_2\}]$ is not connected, then each component of $H[X \setminus \{s_1, s_2\}]$ contains at least two hexagons, so there are exactly two components where one possesses two hexagons, and another possesses three hexagons. Since H is irreducible, $H[X \setminus \{s_1, s_2\}]$ must be isomorphic to E_2 in Fig.2.

Now we suppose $H[X \setminus \{s_1, s_2\}]$ is connected.

If $H[X \setminus \{s_1, s_2\}]$ is reducible, then its reducible hexagon, say s_3, must be adjacent to s_1 or s_2 in $H[X \cup \{s^*\}]$, and $p(H[X \setminus \{s_1, s_2, s_3\}]) - v(H[X \setminus \{s_1, s_2, s_3\}]) = 1$. Obviously, $H(H[X \setminus \{s_1, s_2, s_3\}]$ can only be isomorphic to one of the three benzenoid systems as shown in Fig.6. Let s_4 be the reducible hexagon of $H[X \setminus \{s_1, s_2, s_3\}]$. Then s_4 and s_3 are adjacent in $H[X \setminus \{s_1, s_2\}]$.



(1) (2) (3)

Fig. 6

Otherwise, both s_3 and s_4 would be reducible hexagons of $H[X \setminus \{s_1, s_2\}]$, and s_4 is also adjacent to s_1 or s_2. Clearly, this is impossible. Thus $H[X \setminus \{s_1, s_2\}]$ must be isomorphic to one of the eight benzenoid systems as shown in Fig.7(1)-(8). It is also evident that $H[X\setminus\{s_1,s_2\}]$ cannot be isomorphic to the benzenoid system as shown in Fig.7(9).

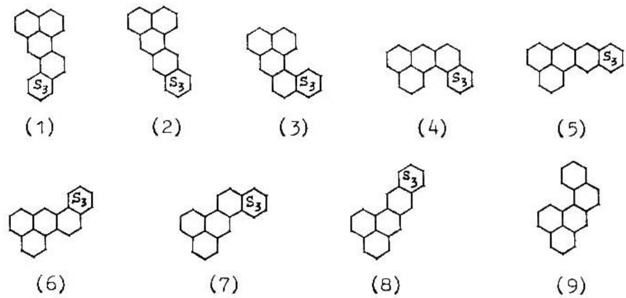
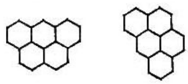


Fig.7

Now it is easy to verify that $H[X \cup \{s^*\}]$ must be isomorphic to one of the twenty benzenoid systems $E_3, E_4, \cdots, E_{22}$ in Fig.2.

If $H[X\setminus\{s_1,s_2\}]$ is irreducible, then $H[X\setminus\{s_1,s_2\}]$ must be isomorphic to one of the two benzenoid systems in Fig.8. Similarly, $H[X \cup \{s^*\}]$ must be isomorphic to one of the seven benzenoid systems $E_{23}, E_{24}, \cdots, E_{29}$ in Fig.2.



(1) (2)

Fig.8

Before continuing, we define some notations.

Let $H(11,i)$, $i=1,2,\cdots,8$, denote the eight benzenoid systems in $\widetilde{N}_{11}$ as shown in Fig.9, and let $N_{12}(11,i)$ ($N_{13}(11,i)$) denote the set of all the reducible concealed non-Kekuléan benzenoid systems generated from $H(11,i)$ by adding one (two) hexagon(s).

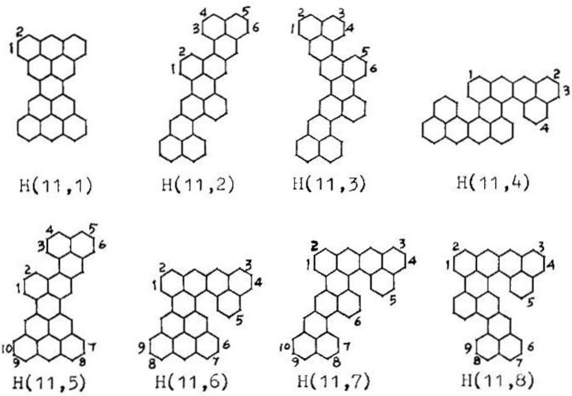


Fig.9. The number j on the boundary of H(11,i) indicates an edge in $E_j^*(H(11,i))$.

Let $A=\{A_1, A_2, A_3\}$, $B=\{B_1, B_2, \cdots, B_5\}$, $C=\{C_1, C_2, \cdots, C_6\}$, $D=\{D_1, D_2, \cdots, D_5\}$, $E=\{E_1, E_2, \cdots, E_{29}\}$. Let $P, Q \in \{A, B, C, D, E\}$, $N' \in P$, $N'' \in Q$, and let $\overline{N}_h(N', N'') \subset \overline{N}_h$, $h > 11$, be the set of all the benzenoid systems such that $H \in \overline{N}_h(N', N'')$ if $H[X \cup \{s^*\}]$ ($H[Y \cup \{s^*\}]$) is isomorphic to one benzenoid system in N' (N''). In particular, for $H', H'' \in A \cup B \cup C \cup D \cup E$, we denote $\overline{N}_h(\{H'\}, N'') = \overline{N}_h(H', N'')$, $\overline{N}_h(\{H'\}, \{H''\}) = \overline{N}_h(H', H'')$.

Now we can give the following theorems.

<u>Theorem 9.</u> There are exactly 98 concealed non-Kekuléan benzenoid systems with $h=12$.

<u>Proof.</u> For $H \in N_{12}$, by theorem 4, H can be generated from a benzenoid system in N_{11} by adding one hexagon. By lemmas 5, 6, it is not difficult to see that

$N_{12}(11,1) = r(E^*(H(11,1))) = 2$, $N_{12}(11,2) = 6$, $N_{12}(11,3) = 6$,

$N_{12}(11,4)=4$, $N_{12}(11,5)=10$, $N_{12}(11,6)=9$, $N_{12}(11,7)=10$, $N_{12}(11,8)=11$, and $|N_{12}|=\left|\bigcup_{i=1}^{8} N_{12}(11,i)\right|=\sum_{i=1}^{8}|N_{12}(11,i)|=58$.

In Fig.9, by attaching one hexagon to an indicated edge of $H(11,i)$, it is not difficult to obtain all the benzenoid systems in N_{12} (see Fig.10(1)-(58)).

For $H\in\overline{N}_{12}$, $|X|+|Y|=11$, and $5\le|X|\le 6$, $5\le|Y|\le 6$. Without loss of generality, let $|X|=5$, $|Y|=6$. Thus, by lemma 8, $H[X\cup\{s^*\}]$ $(H[Y\cup\{s^*\}])$ must be isomorphic to one benzenoid system in A $(B\cup C)$.

It is not difficult to verify that

$|\overline{N}_{12}(A_1,B)|=5$, $|\overline{N}_{12}(A_2,\{B_2,B_3\})|=3$, $|\overline{N}_{12}(A_2,\{B_4,B_5\})|=4$, $|\overline{N}_{12}(A_3,\{B_4,B_5\})|=2$; and $\overline{N}_{12}(A_2,B_1)=\overline{N}_{12}(A_1,\{B_2,B_3\})$, $\overline{N}_{12}(A_3,\{B_1,B_2,B_3\})=\overline{N}_{12}(\{A_1,A_2\},\{B_4,B_5\})$.

Furthermore, $\overline{N}_{12}(A_1,B)$, $\overline{N}_{12}(A_2,\{B_2,B_3\})$, $\overline{N}_{12}(A_2,\{B_4,B_5\})$, and $\overline{N}_{12}(A_3,\{B_4,B_5\})$ are pairwise disjoint. So

$$|\overline{N}_{12}(A,B)|=|\overline{N}_{12}(A_1,B)|+|\overline{N}_{12}(A_2,\{B_2,B_3\})|+|\overline{N}_{12}(A_2,\{B_4,B_5\})|+|\overline{N}_{12}(A_3,\{B_4,B_5\})|=14.$$

Similarly, we have that

$|\overline{N}_{12}(A_1,C)|=6$, $|\overline{N}_{12}(A_2,C)|=12$, $|\overline{N}_{12}(A_3,C)|=8$, and the above three sets are pairwise disjoint. So

$$|\overline{N}_{12}(A,C)|=\left|\bigcup_{i=1}^{3}\overline{N}_{12}(A_i,C)\right|=\sum_{i=1}^{3}|\overline{N}_{12}(A_i,C)|=26.$$

Clearly, $\overline{N}_{12}(A,B)$ and $\overline{N}_{12}(A,C)$ are also disjoint. Thus

$$|\overline{N}_{12}|=|\overline{N}_{12}(A,B\cup C)|=|\overline{N}_{12}(A,B)|+|\overline{N}_{12}(A,C)|=40.$$

Finally, it follows that $|N_{12}\cup\overline{N}_{12}|=98$.

The forty benzenoid systems in $\overline{N}_{12}$ are shown in Fig.10 (59)-(98).

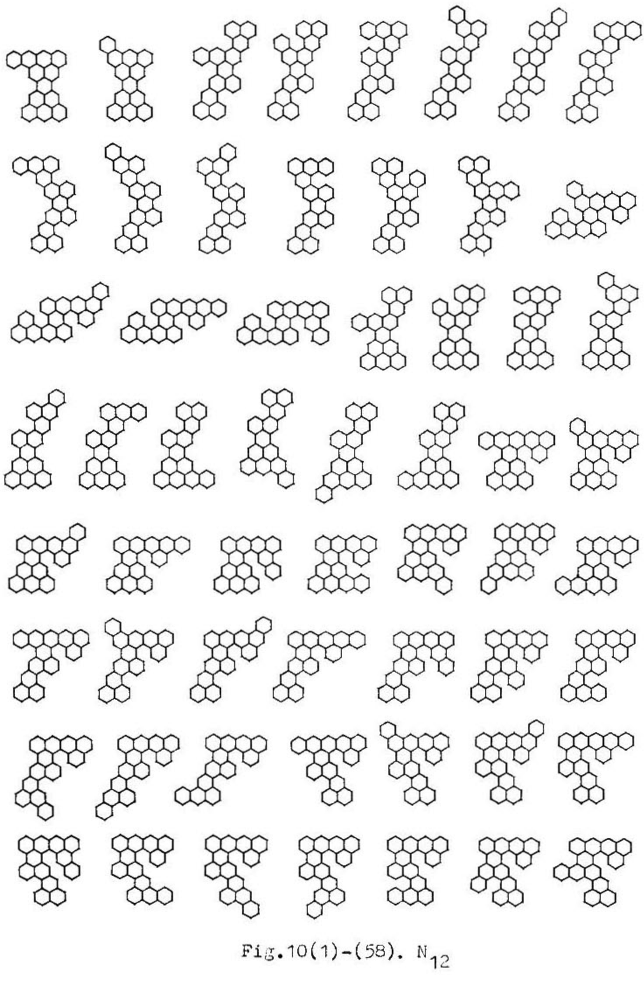
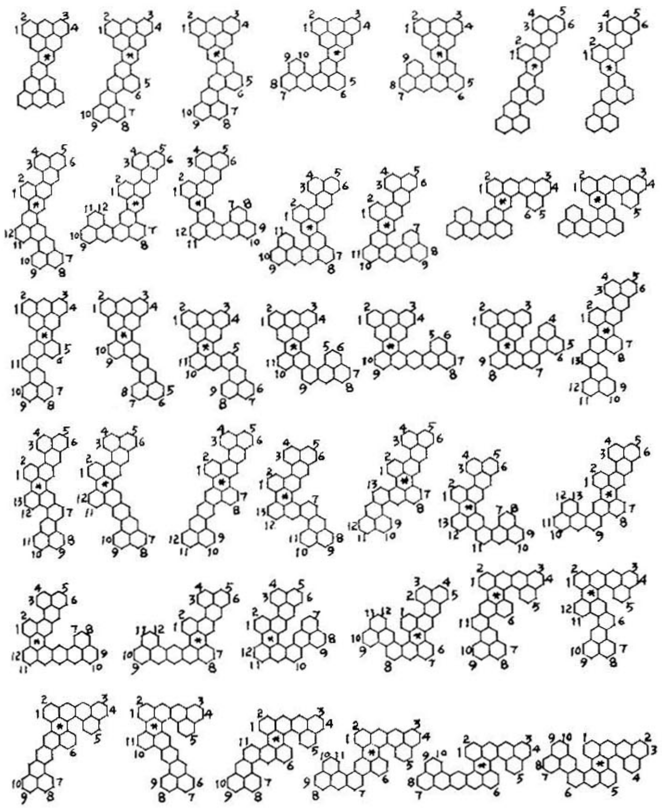


Fig.10(1)-(58). N_{12}



The number j on the boundary of $H \in \widetilde{N}_{12}$ indicates an edge in $E_j^*(H)$.

Fig.10(59)-(98). $\widetilde{N}_{12}$

Let $H(12,j)$, $j=1, 2, \cdots, 40$, denote the forty benzenoid systems in $\overline{K}_{12}$, and let $N_{13}(12,j)$ denote the set of all the benzenoid systems generated from $H(12,j)$ by adding one hexagon.

Theorem 10. There are exactly 1097 concealed non-Kekuléan benzenoid systems with $h = 13$.

Proof. For $H \in N_{13}(12,j)$, $j=1,2,\cdots,40$, from lemma 5 and Fig.10, we can see that

$$\left|\bigcup_{j=1}^{40} N_{13}(12,j)\right| = \sum_{j=1}^{40}\left|N_{13}(12,j)\right| = 422.$$

For $H \in N_{13}(11,i)$, $i=1,2,\cdots,8$, H is generated from $H(11,i)$ by adding two hexagons, say s_1 and s_2.

If s_1 and s_2 are adjacent in H, let $H \in N_{13,1}(11,i)$, otherwise let $H \in N_{13,2}(11,i)$. So $N_{13}(11,i) = N_{13,1}(11,i) \cup N_{13,2}(11,i)$, and $N_{13,1}(11,i) \cap N_{13,2}(11,i) = \emptyset$.

By lemma 7, $\left|N_{13,1}(11,i)\right| = \left|\bigcup_{j=1}^{r} N_{13,1}^{j}(11,i)\right| = \sum_{j=1}^{r}\left|N_{13,1}^{j}(11,i)\right|$.

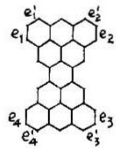


Fig.11

For $H(11,1)$, $r = r(E^*(H(11,1))) = 2$,
$E_1^*(H(11,1)) = \{e_1, e_2, e_3, e_4\}$,
$E_2^*(H(11,1)) = \{e_1', e_2', e_3', e_4'\}$ (see Fig.11).

If s_1 contains one of e_1, e_2, e_3 and e_4, say e_1, then s_2 has six possible positions. They correspond to six benzenoid systems in $N_{13,1}(11,1)$, that is, $\left|N_{13,1}^{1}(11,1)\right| = 6$. If both s_1 and s_2 do not contain any edge in $E_1^*(H(11,1))$, then s_1 must contain one of e_1', e_2', e_3' and e_4', say e_1', and then s_2 has three possible positions, that is, $\left|N_{13,1}^{2}(11,1)\right| = 3$. So $\left|N_{13,1}(11,1)\right| = 9$.

Similarly, from Fig.9, we have that

$\left|N_{13,1}(11,2)\right| = \sum_{j=1}^{6}\left|N^{j}_{13,1}(11,2)\right| = 10+8+6+5+2+1=32,$

$\left|N_{13,1}(11,3)\right| = \sum_{j=1}^{6}\left|N^{j}_{13,1}(11,3)\right| = 10+9+6+4+2+1=32,$

$\left|N_{13,1}(11,4)\right| = \sum_{j=1}^{4}\left|N^{j}_{13,1}(11,4)\right| = 7+4+3+1=15,$

$\left|N_{13,1}(11,5)\right| = \sum_{j=1}^{10}\left|N^{j}_{13,1}(11,5)\right| = 8+7+6+6+4+4+2+2+0+0=39,$

$\left|N_{13,1}(11,6)\right| = \sum_{j=1}^{9}\left|N^{j}_{13,1}(11,6)\right| = 7+7+5+5+3+2+2+0+0=31,$

$\left|N_{13,1}(11,7)\right| = \sum_{j=1}^{10}\left|N^{j}_{13,1}(11,7)\right| = 8+8+6+6+5+3+2+2+0+0=40,$

$\left|N_{13,1}(11,8)\right| = \sum_{j=1}^{11}\left|N^{j}_{13,1}(11,8)\right| = 9+9+7+7+6+4+4+2+1+0+0=49,$

and $\left|\bigcup_{i=1}^{8} N_{13,1}(11,i)\right| = 247.$

For $H \in N_{13,2}(11,i)$, H can be generated from $H(11,i)+s_1 \in N_{12}$ by adding one hexagon s_2 such that s_2 is adjacent to s_1.

From Fig.9,10, it is easy to verify that

$\left|N_{13,2}(11,1)\right| = 6$, $\left|N_{13,2}(11,2)\right| = 16$, $\left|N_{13,2}(11,3)\right| = 16$,
$\left|N_{13,2}(11,4)\right| = 12$, $\left|N_{13,2}(11,5)\right| = 28$, $\left|N_{13,2}(11,6)\right| = 25$,
$\left|N_{13,2}(11,7)\right| = 28$, $\left|N_{13,2}(11,8)\right| = 30$, and $\left|\bigcup_{i=1}^{8} N_{13,2}(11,i)\right| = 161.$

Now we have that

$\left|N_{13}\right| = 422+247+161=830.$

For $H \in \overline{N}_{13}$, $|X|+|Y|=12$, and $5 \le |X| \le 7$, $5 \le |Y| \le 7$. Without loss of generality, we need only to consider the following two cases.

Case 1. $|X|=5$, $|Y|=7$. Then $H[X \cup \{s^*\}]$ $(H[Y \cup \{s^*\}])$ must be isomorphic to one in A (D∪E), by lemma 8.

It is easy to verify that:

(i) $\left|\overline{N}_{13}(A_1, D)\right| = 5$, $\left|\overline{N}_{13}(A_2, \{D_2, D_3\})\right| = 3$,

$|\overline{N}_{13}(A_2,\{D_4,D_5\})|=4$, $|\overline{N}_{13}(A_3,\{D_4,D_5\})|=2$, $\overline{N}_{13}(A_2,D_1)=\overline{N}_{13}(A_1,\{D_2,D_3\})$, $\overline{N}_{13}(A_3,\{D_1,D_2,D_3\})=\overline{N}_{13}(\{A_1,A_2\},D_4)$; furthermore, $\overline{N}_{13}(A_1,D)$, $\overline{N}_{13}(A_2,\{D_2,D_3\})$, $\overline{N}_{13}(A_2,\{D_4,D_5\})$, and $\overline{N}_{13}(A_3,\{D_4,D_5\})$ are pairwise disjoint, so $|\overline{N}_{13}(A,D)|=5+3+4+2=14$.

(ii) $|\overline{N}_{13}(A,E_i)|=5$, for $i=1,4,5,6,7,9,10,11,13,17,23,24,27,28$,

$|\overline{N}_{13}(A,E_i)|=4$, for $i=2,3,8,12,14,15,16,18,19,20,21,22,25,26,29$,

and $\overline{N}_{13}(A,E_i)\cap\overline{N}_{13}(A,E_j)=\emptyset$, for $i\neq j$, $i,j\in\{1,2,\cdots,29\}$, so $|\overline{N}_{13}(A,E)|=130$.

Case 2. $|X|=|Y|=6$. Then $H[X\cup\{s^*\}]$ ($H[Y\cup\{s^*\}]$) must be isomorphic to one in BUC, by lemma 8.

Similarly, we have that:

(i) $|\overline{N}_{13}(B,B)|=\left|\bigcup_{i=1}^{5}\overline{N}_{13}(B_i,\{B_i,\cdots,B_5\})\right|=\sum_{i=1}^{5}|\overline{N}_{13}(B_i,\{B_i,\cdots,B_5\})|=10+8+6+4+2=30.$

(ii) $|\overline{N}_{13}(C,C)|=\left|\bigcup_{i=1}^{6}\overline{N}_{13}(C_i,\{C_i,\cdots,C_6\})\right|=\sum_{i=1}^{6}|\overline{N}_{13}(C_i,\{C_i,\cdots,C_6\})|=12+10+7+4+2+1=36.$

(iii) $\overline{N}_{13}(B_i,C_j)\cap\overline{N}_{13}(B_k,C_l)=\emptyset$, for $(i,j)\neq(k,l)$, $i,k\in\{1,2,\cdots,5\}$, $j,l\in\{1,2,\cdots,6\}$,

and $|\overline{N}_{13}(B,C)|=\left|\bigcup_{i=1}^{5}\overline{N}_{13}(B_i,C)\right|=\sum_{i=1}^{5}|\overline{N}_{13}(B_i,C)|=12+12+12+10+11=57.$

Clearly, $\overline{N}_{13}(A,D)$, $\overline{N}_{13}(A,E)$, $\overline{N}_{13}(B,B)$, $\overline{N}_{13}(C,C)$, and $\overline{N}_{13}(B,C)$ are pairwise disjoint.

Now we conclude that

$|\overline{N}_{13}|=|\overline{N}_{13}(A,D)|+|\overline{N}_{13}(A,E)|+|\overline{N}_{13}(B,B)|+|\overline{N}_{13}(C,C)|+|\overline{N}_{13}(B,C)|=$

$= 14+130+30+36+57=267$, and $|N_{13} \cup \widetilde{N}_{13}| = 830+267=1097$.

CONCLUSION

In a previous work [7] we have proved analytically that there are exactly 8 concealed non-Kekuléan benzenoid systems with h = 11, after this fact had been established by computer programming [6]. In the present work we deduce that there are 98 concealed non-Kekuléan benzenoid systems with h = 12, but again this number had been derived by computers in a very recently published work [8]. The corresponding number 1097 for h = 13 was obtained by the analytical methods in the present work for the first time. It would be interesting to compare this number to a result obtained eventually by computer programming.

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