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CHARACTERIZATION OF AN INVARIANT FOR BENZENOID SYSTEMS

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ABSTRACT

A new invariant T=(x,y,z) of benzenoid systems and some of its basic properties were given in [1]. In this paper we give the necessary and sufficient conditions for a positive integer triple T=(x,y,z) to correspond to a benzenoid system. Furthermore the necessary and sufficient conditions for T to correspond to a peri-condensed benzenoid system is also given.

Let B be a benzenoid system[2] which has at least one Kekulé structure. Let K be a Kekulé structure of B and let E(K) be the set of those edges of B which correspond to double bonds in K. The set $E(K)$ can be partitioned into three subsets, $E_1(K)$, $E_2(K)$ and $E_3(K)$, such that all edges from $E_i(K)$, $i=1,2,3$, are mutually parallel. The number of elements of $E_1(K)$, $E_2(K)$ and $E_3(K)$ is denoted by x, y, z, respectively, and by convention $x \leq y \leq z$. The non-decreasing positive integer triple (x,y,z) is written by T. In [1] we prove the following.

Theorem 1. For a benzenoid system B with a Kekulé structure K the triple T is independent of K. Therefore T is an invariant of B and we may write $T=T(B)$.

By theorem 1, any benzenoid system B with a Kekulé structure possesses a triple $T(B)=(x,y,z)$. But the inverse of this statement is not true, i.e., any positive integer triple $T=(x,y,z)$, needs not to correspond to a benzenoid system. For example, the triple $T=(2,2,2)$ does not correspond to any benzenoid system. It is natural to propose the following problem: What type of triples correspond to benzenoid systems?

For convenience, we define $\mathcal{T}$ as the set of those triples which each corresponds to a benzenoid system. Let $\mathcal{T}_1$ be the subset of $\mathcal{T}$ such that $T \in \mathcal{T}_1$ if and only if T corresponds to a catacondensed benzenoid system, and let $\mathcal{T}_2$ be the subset of $\mathcal{T}$ such that $T \in \mathcal{T}_2$ if and only if T corresponds a pericondensed benzenoid system. It is not difficult to see that $\mathcal{T}_1 \cup \mathcal{T}_2 = \mathcal{T}, \mathcal{T}_1 \cap \mathcal{T}_2 \neq \emptyset$. In (1) necessary and sufficient conditions for the triple $(x,y,z) \in \mathcal{T}_1$ were given as follows:

Theorem 2. (i) $T=(x,y,z)$ corresponds to a catacondensed benzenoid system if and only if $x+y+z$ is odd and $x+y \geqslant z+1$.

(ii) Let X, Y and Z be arbitrary non-negative integers. Then T corresponds to a catacondensed benzenoid system if and only if $x=Y+Z+1, y=Z+X+1, z=X+Y+1$.

In the present paper we give necessary and sufficient conditions for the triple $(x,y,z) \in \mathcal{T}$. Furthermore the necessary and sufficient conditions for the triple $(x,y,z) \in \mathcal{T}_2$ is given.

First we give the following lemmas.

Lemma 3. (1) The following two statements are equivalent:

(i) $x=1$;

(ii) B is the linear polyacene L_h (see Fig.1).

A benzenoid system is said to be of type I if it can be dissected by parallel horizontal lines L_i, $i=1, 2,\dots,t$, such that it decomposes into t+1 paths. The two top and the two bottom paths must be of even length and pairwise equal. All other paths must be of odd length. For illustration see Fig.2(1). The structure of the benzenoid system of type II is clear from Fig.2(2).

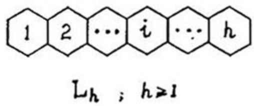
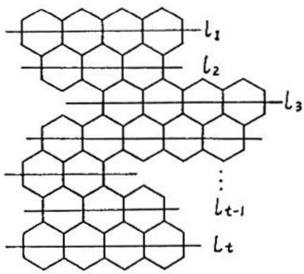
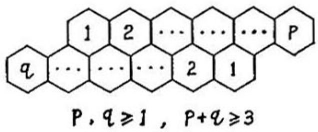


Fig.1



(1) Type I , $t \geq 3$



(2) Type II

Fig.2

Lemma 4. (1) The following two statements are equivalent:

(i) x=2;

(ii) B is a benzenoid system of type I or of type II.

Lemma 5. Let $T=(x,y,z)$, where $x+y-1 \leq z \leq xy$. Then $T \in \mathcal{T}$.

Proof. For any $T=(x,y,z)$, where $x+y-1 \leq z \leq xy$, we can find a subsystem B of the benzenoid system shown in Fig.3, such that $T(B)=(x,y,z)$.

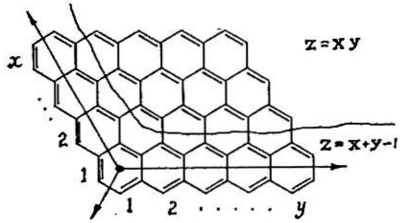


Fig.3

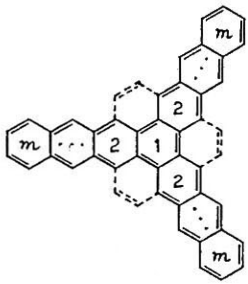


Fig.4

Lemma 6. Let $(x,y,z) \in \mathcal{T}$. Then $(x+1,y+1,z)$, $(x+1,y,z+1)$ $(x,y+1,z+1) \in \mathcal{T}$, where if $(x+1,y+1,z)$ and $(x+1,y,z+1)$ are not non-decreasing we will put it in order.

Proof. Let B be a benzenoid system corresponding to (x,y,z), where hexagons are drawn so that x counts the vertical double bonds. On the boundary of B we can find a vertical edge e_1 whose end vertices have degree 2 in B (see [2,P94]).

Let S_1 be the hexagon of B containing e_1, and let B' be the benzenoid system obtained from B by adding a hexagon S_1' such that $S_1' \cap S_1 = e_1$. Then $T(B')=(x,y+1,z+1)$, namely, $(x,y+1,z+1) \in \mathcal{T}$. By the same reason, we have $(x+1,y+1,z)$, $(x+1,y,z+1) \in \mathcal{T}$.

Lemma 7. (i) $(x,x,x) \in \mathcal{T}$, if and only if $x \neq 2$.

(ii) $T=(x,y,y) \in \mathcal{T}$ for $x<y$, if and only if $T \neq (2,3,3)$.

Proof. It follows from Fig.4 that $(x,x,x) \in \mathcal{T}$ for $x \neq 2$. Therefore, by lemma 6, we also have that $(x,y,y) \in \mathcal{T}$ for $x \neq 2, y>x$. For $T(B)=(2,y,z)$, by lemma 4, B can only be a benzenoid system of type I or of type II in Fig.2. It is not difficult to verify that $(2,2,2)$, $(2,3,3) \notin \mathcal{T}$, and $(2,4,4) \in \mathcal{T}$. So, from lemma 6, $(2,y,y) \in \mathcal{T}$ for $y \geq 4$.

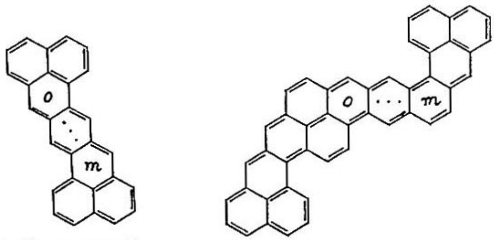
Lemma 8. (i) $(2,2,z) \in \mathcal{T}$ if and only if $2<z \leq 4$. (ii) $(2,3,z) \in \mathcal{T}$ if and only if $3<z \leq 6$. (iii) $(2,4,z) \in \mathcal{T}$ if and only if $z \neq 9,11$. (iv) $(2,5,z) \in \mathcal{T}$ if and only if $z \neq 12$. (v) $(2,y,z) \in \mathcal{T}$ for $y \geq 6$.

Proof. Since for $T(B)=(2,y,z)$, B can only be a benzenoid system of type I or of type II (see Fig.2), combining lemma 5 and 7, it is not difficult to verify that (i) and (ii) hold.

(iii) By lemma 5 and 7, $(2,4,z)\in\mathcal{T}$ for $4\leq z\leq 8$. For $z>8$, we construct two graphs (see Fig.5) which show that $(2,4,4+2m)\in\mathcal{T}$, and $(2,4,13+2m)\in\mathcal{T}$, $m\geq 0$. In other cases $z=9,11$. By lemma 4, it is easy to verify that $(2,4,9),(2,4,11)\notin\mathcal{T}$.

(iv) Since $(2,4,10)\in\mathcal{T}$ and $(2,4,12+m)\in\mathcal{T}$, $m\geq 0$, by lemma 6, $(2,5,11)$, $(2,5,13+m)\in\mathcal{T}$. For $5\leq z\leq 10$, $(2,5,z)$ $\in\mathcal{T}$, by lemma 5,7. The rest is $(2,5,12)$. By lemma 4, we have $(2,5,12)\notin\mathcal{T}$.

(v) By (iv) and lemma 6, $(2,6,z)\in\mathcal{T}$ for $z\neq 13$. Fig. 6 shows that $(2,6,13)\in\mathcal{T}$. So $(2,6,z)\in\mathcal{T}$ for all $z\geq 6$. Furthermore, by lemma 6, $(2,y,z)\in\mathcal{T}$ for $y\geq 6$.



$T(B)=(2,4,4+2m)$, $m\geq 0$ $T(B)=(2,4,13+2m)$, $m\geq 0$

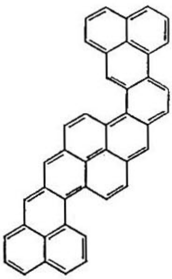
Fig. 5

<u>Lemma 9.</u> (i) $(3,3,z)\in\mathcal{T}$ if and only if $z\neq 11$;

(ii) $(3,y,z)\in\mathcal{T}$ for $y\geq 4$.

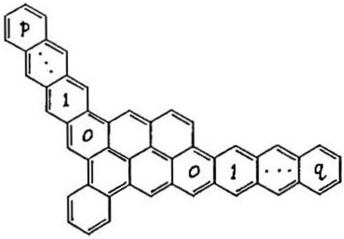
<u>Proof.</u> (i) By lemma 5,7, $(3,3,z)\in\mathcal{T}$ for $5\leq z\leq 9$. $(2,2,3)$, $(2,2,4)\in\mathcal{T}$ induce that $(3,3,3),(3,3,4)\in\mathcal{T}$. Fig.7 shows that $(3,3,13+2m)$, $(3,3,8+2m)\in\mathcal{T}, m\geq 0$. The rest is $(3,3,11)$. We prove that $(3,3,11)\notin\mathcal{T}$ in the Appendix.

(ii) By (i) and lemma 6, $(3,4,z)\in\mathcal{T}$ for $z\neq 12$. But $(3,4,12)\in\mathcal{T}$, by lemma 5. So $(3,4,z)\in\mathcal{T}$ for all $z\geq 4$. Furthermore, by lemma 6, $(3,y,z)\in\mathcal{T}$ for all $y\geq 4$.



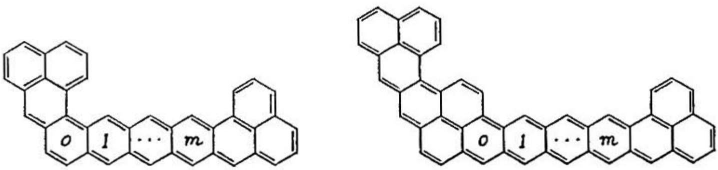
$T(B)=(2,6,13)$

Fig.6



$T(B)=(3+p, 4+q, 6+p+q)$,
$p\geq 0$, $q\geq 0$, $p\leq q+1$.

Fig.8



$T(B)=(3,3,8+2m)$, $m\geq 0$.

(1)

$T(B)=(3,3,13+2m)$, $m\geq 0$.

(2)

Fig.7

<u>Lemma 10.</u> $(x,y,z)\in\mathcal{T}$ for $x\geq 4$.

<u>Proof.</u> By $(4,4,4)$, $(3,4,z)\in\mathcal{T}$, we have $(4,4,z)\in\mathcal{T}$. Thus, by lemma 6, $(4,4+m,z+m)\in\mathcal{T}, m\geq 0$, that is, $(4,y,z)\in\mathcal{T}$

Now we get the following theorem.

<u>Theorem 11.</u> $T=(x,y,z)\in\mathcal{T}$ if and only if one of the following conditions holds:

$$\text{(i)}\begin{cases}x=1\\y=z\end{cases},\quad \text{(ii)}\begin{cases}x=2\\y=2\\2<z\leq 4\end{cases},\quad \text{or}\begin{cases}x=2\\y=3\\3<z\leq 6\end{cases},\quad \text{or}\begin{cases}x=2\\y=4\\z\neq 9,11\end{cases},$$

$$\text{or}\begin{cases}x=2\\y=5\\z\neq 12\end{cases},\quad \text{or}\begin{cases}x=2\\y\geq 6\end{cases}\quad \text{(iii)}\begin{cases}x=3\\y=3\\z\neq 11\end{cases},\quad \text{or}\begin{cases}x=3\\y\geq 4\end{cases}\quad \text{(iv)}\, x\geq 4$$

Now $\mathcal{T}_1$ and $\mathcal{T}$ have been determined, by theorem 2 and 11.

In order to get the necessary and sufficient conditions for $T=(x,y,z)$ to correspond to a pericondensed benzenoid system, we need only to determine the set $\mathcal{T}_1\setminus\mathcal{T}_2$, since $\mathcal{T}_2=\mathcal{T}\setminus\{\mathcal{T}_1\setminus\mathcal{T}_2\}$.

<u>Theorem 12.</u> $\mathcal{T}_1\setminus\mathcal{T}_2=\{(1,y,y)\}\cup\{(2,y,y+1)\}\cup\{(3,3,3),(3,3,5)\}$.

<u>Proof.</u> By lemma 3, $\{(1,y,y)\}\subset\mathcal{T}_1\setminus\mathcal{T}_2$.

In the proof of lemma 8,9 and 10, we can see that for $x\geq 2$, if $z\neq x+y-1$ and $(x,y,z)\neq(3,3,3)$, then $(x,y,z)\in\mathcal{T}_2$. It is easy to verify that $\{(3,3,3),(3,3,5)\}\subset\mathcal{T}_1\setminus\mathcal{T}_2$. Fig.8 shows that $(x,y,x+y-1)\in\mathcal{T}_2$ for $x\geq 3$,

$y \geq 4$. The rest is $\{(2,y,y+1)\}$. By lemma 4, it also is not difficult to verify that $\{(2,y,y+1)\} \subset \mathcal{T}_1 \setminus \mathcal{T}_2$.

Finally, we have the following theorem.

Theorem 13. $T=(x,y,z) \in \mathcal{T}$ if and only if one of the following conditions holds:

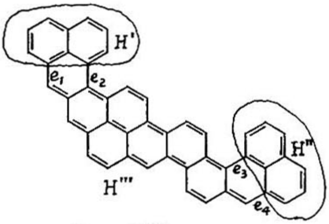
$$\text{(i)} \begin{cases} x=2 \\ y=2 \\ z=4 \end{cases}, \quad \text{or} \begin{cases} x=2 \\ y=3 \\ z=5,6 \end{cases}, \quad \text{or} \begin{cases} x=2 \\ y=4 \\ z\neq 5,9,11 \end{cases}, \quad \text{or} \begin{cases} x=2 \\ y=5 \\ z\neq 6,12 \end{cases},$$

$$\text{or} \begin{cases} x=2 \\ y\geq 6 \\ z\neq y+1 \end{cases}, \quad \text{(ii)} \begin{cases} x=3 \\ y=3 \\ z\neq 3,5,11 \end{cases}, \quad \text{or} \begin{cases} x=3 \\ y=4 \end{cases}, \quad \text{(iii)} \quad x\geq 4 .$$

Appendix

In order to prove that $(3,3,11) \notin \mathcal{T}$, we need to define a class of benzenoid systems.

A benzenoid system B is said to be of type III, as shown in Fig.9, if $B-\{e_1,e_2,e_3,e_4\}$ has three components H', H'', H''', where H' and H'' are two linear polyacenes each containing two hexagons, and by deleting all vertical edges H''' can be decomposed into r paths ($r\geq 2$) of odd length whose intial edges in the left have the same direction as shown in Fig.9.



Type III

Fig.9

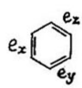


Fig.10

Lemma 14. For a benzenoid system B with a Kekulé structure K, $T(B)=(3,3,10+m), m\geqslant 0$, only if B is a benzenoid system of type III.

Proof. We put B on a plane so that the edges in $E_1(K)$ are parallel to the vertical line, and the edges in $E_2(K)$ are parallel to the edge e_y in Fig.10.

Let $l_i, i=1,\ldots,t$, be the horizontal lines passing through the centers of hexagons of B, and let T_i be the set of vertical edges of B which are intersected by l_i. Let H^* be the subgraph of B obtained by deleting all vertical edges from B. Then the subgraph of H^* lying at the upper bank of l_1 is denoted by H_o, the subgraph lying between l_i and l_{i+1} is denoted by H_i for $i=1,\ldots,t-1$, and the subgraph lying at the lower bank of l_t is denoted by H_t. Clearly, any component of $H_j, j=0,1,\ldots,t$, is a path. Suppose a path P_{jk} in H_j is on the perimeter of B. When the region above(below) P_{jk} is the exterior face of B, we call P_{jk} the top(bottom)-path of B. Obviously a top-path P_{jk} of B must be of even length. Therefore, it is not difficult to see that $|T_{j+1} \cap E_1(K)|=1$ (see Fig.11). If P_{jk} is a bottom-path, then $|T_j \cap E_1(K)|=1$. Since $x=|E_1(K)|=3$, the number of top-paths and bottom-paths of B are at most three. Thus for any j, H_j has at most two components.

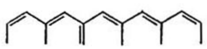


Fig.11

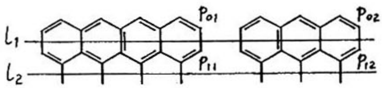


Fig.12

If H_o has exactly two components P_{o1} and P_{o2}, then $|T_2 \cap E_1(K)|=1$. Otherwise H_1 also has exactly two components P_{11} and P_{12}, and P_{o1} and P_{11} have the same length, so do P_{o2} and P_{12} (see Fig.12). Clearly, then $y>3$, a contradiction. Therefore, B can only be a graph shown in Fig.13. But, if $p=q=r=1$, $T(B)=(3,3,3)$, $z<10$, and otherwise $y>3$. So we have that both H_o and H_t have exactly one component each.

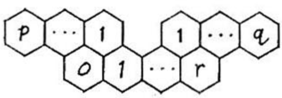


Fig.13

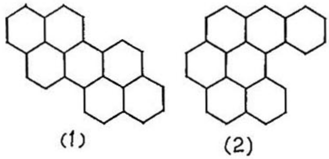


Fig.14

Suppose that B contains exactly a top-path and a bottom-path. If $t=3$, B can only be a graph shown in Fig.14. It is easy to see that if $y=3$, then $z\leq 9$, and otherwise $y>3$. If $t>3$, B can only be a graph shown in Fig.15. Clearly, $y>3$.

Now we can say that B has exactly three top-paths and bottom-paths. Without loss of generality, we assume that B has two top-paths and one bottom-path. It is not difficult to see that the upper bank of l_2 is a linear polyacene with two hexagons, and $|T_1 \cap E_1(K)|=1$, $|\{H_0 \cup H_1\} \cap E_2(K)|=2$, $|\{H_0 \cup H_1\} \cap E_3(K)|=2$. Thus $|T_t \cap E_1(K)|=1$ and $|\{H_2 \cup \ldots \cup H_t\} \cap E_2(K)|=1$. Let $T_t=\{e_1, e_2, \ldots, e_r\}$ (see Fig.16). $T_t \cap E_1(K)$ can only be e_{r-1} or e_r, otherwise $|H_t \cap E_2(K)| > 1$.

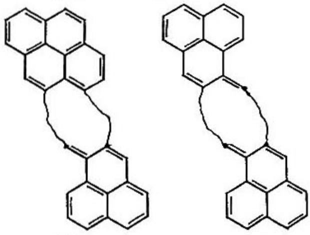

(1) (2)

Fig.15

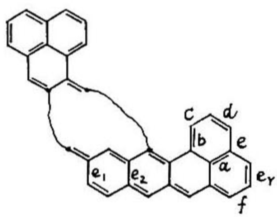


Fig.16

If $e_r \in E_1(K)$, $a \in E_2(K)$, then $b \in E_1(K)$, and $\{c,d\}$ forms a top-path of B, so B indeed is of type III. For the other cases it is also not difficult to verify that the conclusion is true.

Now, by lemma 14 and Fig.7, we can assert that $(3,3,11) \notin \mathcal{T}$.

Acknowledgement.

We would like to thank the referees for their helpful suggestions.

References

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