

The Structure Feature of Essentially Disconnected Benzenoid Systems

Zheng Bo

Department of Mathematics and Computer Science, Fuqing Branch of Fujian Normal University, Fuqing, Fujian, 350300, P.R.China; e-mail: fiberic@163.com

Rongsi Chen ^{1,2}

Center for Discrete Mathematics and Theoretical Computer Science, Software College of Fuzhou University, Fuzhou, Fujian, 350002, P.R.China; e-mail: mathcrs@fzu.edu.cn

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Abstract: This paper deals with the structure of essentially disconnected benzenoid systems. The normal components induced digraph is introduced. It is proved that for an essentially disconnected benzenoid system, its normal components induced digraph is acyclic and connected. The lower bound for the number of normal components of an essentially disconnected benzenoid system is investigated. Moreover, the essentially disconnected benzenoid systems with two or three normal components are classified and constructed.

1. Introduction

A benzenoid system [1] is a finite 2-connected plane graph in which each interior face is bounded by a regular hexagon (cf. Fig.1). Since benzenoid systems aptly represent the skeleton of benzenoid hydrocarbons, in the study of benzenoid hydrocarbons [1-4], benzenoid systems are extensively used. Note that each benzenoid system is bipartite and 2-colorable. In the following, we use a convention that all the vertices of a benzenoid system H in question have been colored black and white so that the end vertices of any edge have different colors, and we denote H by $H = (W, B)$, where W and B are the sets of white vertices and black vertices of H , respectively. A perfect matching of H is an independent edge set such that each vertex of H is incident with one of the

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²Corresponding author.

edges of the independent edge set. For benzenoid systems perfect matchings correspond to the notion of Kekulé structures, which play a distinguished role in the theory of benzenoid hydrocarbons. A Kekuléan benzenoid system is a benzenoid system with Kekulé structures. An edge of a Kekuléan benzenoid system H is called a *fixed double* (*fixed single*) bond if it belongs to each (no) Kekulé structure of H . A *fixed bond* is either a fixed single bond or a fixed double bond.

A Kekuléan benzenoid system without (with) fixed bonds is said to be *normal* (*essentially disconnected*). Let H be an essentially disconnected Kekuléan benzenoid system. The *normal subgraph* of H , denoted by $N(H)$, is the subgraph induced by the non-fixed bonds of H . Each connected component of $N(H)$ is called a *normal component*. Similarly, we define the *fixed subgraph* $F(H)$ of H to be the subgraph induced by the fixed bonds of H , each connected component of $F(H)$ is called a *fixed component* (cf. Fig.1, the normal components are shown in shadow, while the fixed double bonds are shown by double lines.).

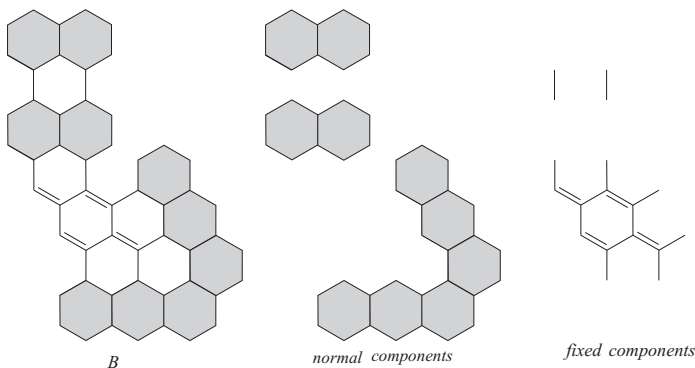


Fig. 1 A benzenoid system B and its normal components and fixed components

Clearly, $N(H)$ can be obtained by deleting the fixed double bonds together with their end vertices and deleting the fixed single bonds without their end vertices. The concepts “essentially disconnected” and “normal component” have proved to be very useful in certain enumeration techniques for Kekulé structures, and in the classification and enumeration of benzenoid hydrocarbons [6,7]. It is known that an essentially disconnected Kekuléan benzenoid system H has at least two normal components each of which is a normal benzenoid system [1], [2, p51]. P. Hansen and M. Zheng found that if an essentially disconnected benzenoid system has a single hexagon as one of its normal components,

then it has at least three normal components [8]. No more results about the structure of essentially disconnected benzenoid systems have been known.

In this paper we introduce the concept of normal components induced digraph (NC -induced digraph). Investigations are made for the structure feature of essentially disconnected benzenoid systems by means of NC -induced digraphs. It is proved that for an essentially disconnected benzenoid system G , its NC -induced digraph, denoted by $I_N(G)$, is acyclic and connected. A lower bound is given for the number of normal components of an essentially disconnected benzenoid system G which possesses a normal component without vertex lying on the boundary of G . The classification and construction of essentially disconnected benzenoid systems with 2 or 3 normal components are discussed.

2. Structure of essentially disconnected benzenoid systems

Let G be a graph. A *boundary* vertex (edge) of G is a (an) vertex (edge) that lies on the boundary of G . Let H a subgraph of G . $G - H$ denotes the subgraph of G obtained by deleting the vertices of H and their incident edges.

Definition 2.1 Let v a vertex of an essentially disconnected benzenoid system G . Vertex v is called a *spreading vertex* if it belongs to a normal component N of G , and is adjacent to a vertex of $G - N$.

Definition 2.2 Let N be a normal component of an essentially disconnected benzenoid system $G = (W, B)$. N is said to be of *type B* (W), if all the spreading vertices of N are black (white); N is said to be of *type M*, if N contains both white spreading vertices and black spreading vertices; N is said to be of *type I*, if none of the vertices of N is a boundary vertex of G .

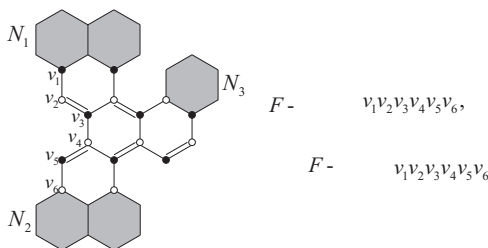


Fig.2 Illustrations for definition 2.2 and definition 2.4.

As depicted in Fig.2, N_1, N_2 and N_3 are of type B, W and M , respectively.

Definition 2.3 Denote by \mathcal{G}_n the set of essentially disconnected benzenoid systems with exactly n normal components. For $G \in \mathcal{G}_n$, denote by $n_W(G)$, $n_B(G)$ and $n_M(G)$ the number of normal components of type W , B and M , respectively.

Note that a normal component of type I is certainly a normal component of type M . For any $G \in \mathcal{G}_n$, we have $n_W(G) + n_B(G) + n_M(G) = n$.

Definition 2.4 Let $G = (W, B)$ be an essentially disconnected benzenoid system. A path P of G is said to be an F -path of G (cf. Fig.2) if it satisfies : 1. the edges of P are alternately fixed single bonds and fixed double bonds; 2. the end vertices of P are spreading vertices.

Definition 2.5 Let G be an essentially disconnected benzenoid system, N_1 and N_2 be two normal components of G . N_1 is said to be incident with an F -path P if one of the end vertices of P belongs to N_1 . We say N_1 connects to N_2 if N_1 and N_2 are incident with the same F -path. We say N_1 properly connects to N_2 if N_1 and N_2 are incident with the same F -path P ; and $N_1 \cap P$ is a black vertex, while $N_2 \cap P$ is a white vertex.

Let $G = (W, B) \in \mathcal{G}_n$, N_1, N_2, \dots, N_n the normal components of G . We construct the normal components induced digraph (NC -induced digraph) of G , denoted by $I_N(G)$, as follows (cf. Fig. 3):

1. the vertex set of $I_N(G)$ is $\{N_1, N_2, \dots, N_n\}$;
2. for any two vertices $N_i, N_j \in \{N_1, N_2, \dots, N_n\}$, there is an arc from N_i to N_j (N_i is said to be the tail of the arc and N_j is said to be the head of the arc) if and only if N_i is properly connected to N_j .

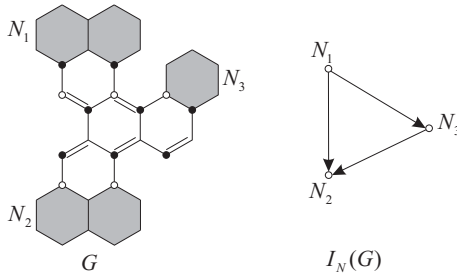


Fig.3 Benzenoid system G and its NC -induced digraph $I_N(G)$.

The indegree $d_{I_N(G)}^-(N)$ of a vertex N in $I_N(G)$ is the number of arcs with head N ; the outdegree $d_{I_N(G)}^+(N)$ of N in $I_N(G)$ is the number of arcs with tail N . We have:

Theorem 2.6 *Let G be an essentially disconnected benzenoid system, N a normal component of G . Then we have:*

1. $d_{I_N(G)}^+(N) = 0$ if and only if N is of type W ;
2. $d_{I_N(G)}^-(N) = 0$ if and only if N is of type B ;
3. $d_{I_N(G)}^+(N) > 0$ and $d_{I_N(G)}^-(N) > 0$ if and only if N is of type M .

Lemma 2.7 ([8]) *Each normal component of an essentially disconnected benzenoid system is a normal benzenoid system.*

Lemma 2.8 ([8]) *If a benzenoid system H with more than one hexagon has a normal component which is a single hexagon, then H has at least three normal components.*

Lemma 2.9 *Let G be an essentially disconnected benzenoid system, and v be a vertex of G . Then v is a spreading vertex if and only if v is incident with two non-fixed bonds and a fixed single bond.*

Proof. Suppose that vertex v is a spreading vertex. By the definition of spreading vertex, v belongs to a normal component N of G . By lemma 2.7, N is a normal benzenoid system. Thus v is incident with two edges in N which are non-fixed bonds. Note that any edge between N and $G - N$ is a fixed single bond. Hence v is incident with one fixed single bond.

Conversely, suppose that v is incident with two non-fixed bonds and a fixed single bond. Evidently, the two non-fixed bonds are adjacent and belong to a normal component N of G . Moreover, the other end vertex of the fixed single bond is in $G - N$. By the definition of spreading vertex, v is a spreading vertex. Therefore, the lemma holds. ■

Lemma 2.10 ([13]) *A hexagonal system H is normal if and only if H possesses a perfect matching M such that the boundary of H is an M -alternating cycle.*

Theorem 2.11 *For any $G \in \mathcal{G}_n$ ($n \geq 2$), $I_N(G)$ is acyclic.*

Proof. By contradiction. Assume that there is a directed cycle $C = N_{i_1}N_{i_2} \cdots N_{i_k}N_{i_1}$ in $I_N(G)$, where i_1, i_2, \dots, i_k are pairwise different. For any $1 \leq s \leq k$, by lemma 2.10, there is a Kekulé structure M_{i_s} of N_{i_s} such that the boundary of N_{i_s} is an M_{i_s} -alternating cycle since N_{i_s} is a normal benzenoid system. Let $M = \bigcup_{s=1}^k M_{i_s} \cup M^*$, where M^* is the set of fixed double bonds of G . No doubt, M is a Kekulé structure of G such that for each $1 \leq s \leq k$, the boundary of N_{i_s} is an M -alternating cycle. Note that i_1, i_2, \dots, i_k are pairwise different. One can check that there is an M -alternating cycle containing some

fixed bonds, a contradiction. The contradiction is caused by our assumption that there is a directed cycle in $I_N(G)$, so the assumption is false. Therefore, the theorem holds. ■

Corollary 2.12 *For any $G \in \mathcal{G}_n(n \geq 2)$, we have: $n_B(G) \geq 1, n_W(G) \geq 1$.*

Proof. By theorem 2.11, $I_N(G)$ is acyclic. So there are two vertices $N_i, N_j \in I_N(G)$ such that the indegree $d_{I_N(G)}^-(N_i) = 0$ and the outdegree $d_{I_N(G)}^+(N_j) = 0$. By theorem 2.6, the normal component N_i is of type B , and the normal component N_j is of type W . Therefore, $n_B(G) \geq 1, n_W(G) \geq 1$. ■

Corollary 2.13 *Let $G = (W, B)$ be an essentially disconnected benzenoid system. If G has a normal component of type M , then G has at least three normal components.*

Proof. By corollary 2.12, $n_B(G) \geq 1, n_W(G) \geq 1$. If $n_M(G) \geq 1$, then the number of normal components of G equals $n_W(G) + n_B(G) + n_M(G) \geq 3$. ■

The known theorem due to P. Hansen and M. Zheng [8] is a direct consequence of the above corollary:

Theorem 2.14 ([8]) *If an essentially disconnected benzenoid system H with more than one hexagon has a normal component which is a single hexagon, then H has at least three normal components.*

Proof. Let s be a single hexagon which is a normal component of G . Since G is a benzenoid system and s is a subgraph of G , there is another hexagon s' adjacent to s . Since s is a normal component of G , the two vertices belonging to both s and s' are spreading vertices. Note that these two vertices are adjacent to each other. Thus they are of different colors. Therefore, the normal component s is of type M . By corollary 2.13, G has at least three normal components. ■

Theorem 2.15 *For each positive integer triple (a, b, c) subject to*

$$\begin{cases} a \geq 1 \\ b \geq 1 \\ a + b + c = n \end{cases}$$

there is an essentially disconnected benzenoid system $G \in \mathcal{G}_n(n \geq 2)$ such that $(n_W(G), n_B(G), n_M(G)) = (a, b, c)$.

Proof. Case 1. $c = 0$. Without loss of generality, we may assume that $a \leq b$. Then we can construct as depicted in Fig. 4. There are b normal components of type B on the top, and there are $a = n - b$ normal components of type W on the bottom.

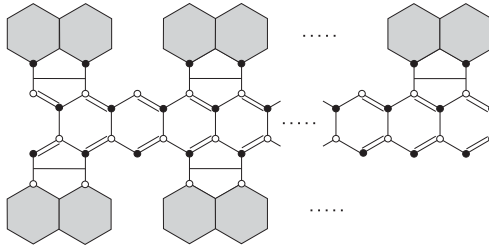


Fig. 4 An illustration for the construction for Case 1

Case 2. $c = n - 2$. Then we can construct as depicted in Fig. 5. The normal components with two hexagons are of type W and B , respectively; the normal components with only one hexagons are of type M .

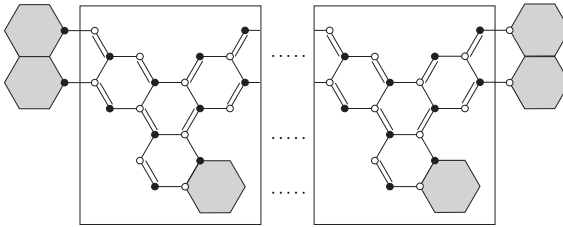


Fig. 5 An illustration for the construction for Case 2

Case 3. $0 < c < n - 2$. Then we can construct by combining the construction ways in Cases 1 and 2. For the essentially disconnected benzenoid system G depicted in Fig. 6, $(n_W(G), n_B(G), n_M(G)) = (a, b, c) = (1, 2, 3)$, ■

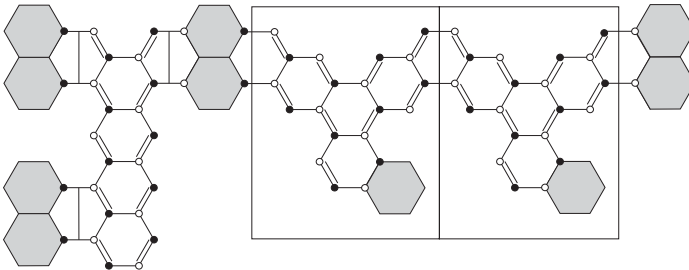


Fig. 6 An illustration for the construction for Case 3

Lemma 2.16 *Let G be an essentially disconnected benzenoid system. Then each fixed bond of G belongs to an F -path.*

Proof. Direct each fixed single (double) bond of G from its black (white) end vertex to its white (black) end vertex. It is not difficult to see that by our direction way, each fixed bond e is contained in a maximum directed path P such that the end vertices of P are spreading vertices (otherwise we can expand P at its end vertices). And the edges of P are alternately fixed single bonds and fixed double bonds. Therefore, by the definition of F -path, the lemma holds. ■

Lemma 2.17 *Let G be an essentially disconnected benzenoid system, and let P_1, P_2 be two F -paths. If there is a fixed single bond e such that one of its end vertices is on P_1 and the other one is on P_2 , then the normal components incident with P_1 or P_2 are connected in $I_N(G)$.*

Proof. Let N_1, N_2 (N_3, N_4) be the two normal components incident with P_1 (P_2). Clearly, N_1 (N_3) is connected to N_2 (N_4). Since e is a fixed single bond, e can not be incident with end vertices of P_1 or P_2 . In fact, the end vertices of e are incident with a fixed double bond of P_1 and a fixed double bond of P_2 , respectively. One can check that in the subgraph $P_1 \cup P_2 \cup \{e\}$, there is an F -path P_3 different from P_1, P_2 such that P_3 connects one of N_1, N_2 and one of N_3, N_4 (cf. Fig. 7). Therefore, N_1, N_2, N_3, N_4 are connected and the lemma holds. ■

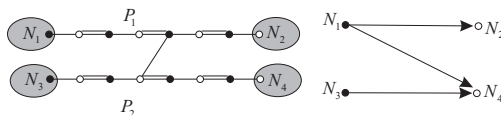


Fig. 7 Illustrations for the proof of lemma 2.17

Theorem 2.18 *Let G be an essentially disconnected benzenoid system. Then $I_N(G)$ is connected.*

Proof. Note that the normal components of G are connected by fixed components of G . It suffices to prove that for each fixed component F of G , the normal components $N_F^1, N_F^2, \dots, N_F^k$ incident with F are connected. For any $1 \leq t \leq k$, there is a fixed single bond e_t of F incident with a spreading vertex of N_F^t . By lemma 2.16, e_t belongs to an F -path P_t . Evidently, one of the components incident with P_t is N_F^t . Thus each normal component incident with F is connected to another one by an F -path which is a subgraph of F . Note that all the F -paths in the fixed component F are connected by fixed single bonds of F . By lemma 2.17, the theorem holds. ■

Lemma 2.19 ([9]) *For a benzenoid system G , the number of vertices of degree 2 is equal to the number of vertices of degree 3 on the boundary of G plus 6.*

Let N and N' be two normal components of a benzenoid system $G = (W, B)$, P and P' be two F -paths connecting N and N' , $P \cap N = u$, $P' \cap N = u'$, $P \cap N' = v$ and $P' \cap N' = v'$. Evidently, u and u' are spreading vertices of N ; while v and v' are spreading vertices of N' . The closed region bounded by N, P, N' and P' is a subgraph of G the boundary of which consists of F -paths P and P' ; the section of boundary of N between u and u' and the section of boundary of N' between v and v' .

Lemma 2.20 *Let N and N' be two normal components of a benzenoid system $G = (W, B)$, P and P' be two F -paths connecting N and N' , $P \cap N = u$, $P' \cap N = u'$. Let v be a spreading vertex of N in the closed region bounded by N, P, N' and P' . Then v, u and u' have the same color.*

Proof. By contradiction. Since $I_N(G)$ is acyclic, u and u' has the same color (Otherwise, in $I_N(G)$ there would be an arc from N to N' and an arc from N' to N , which make a directed cycle of $I_N(G)$). Assume that v has different color with u and u' . Without loss of generality, let u, u' be black and v white. By lemma 2.9 and lemma 2.16, v belongs to an F -path which connects N to another normal component N_1 . As argued above, $N_1 \neq N'$. One can check that N_1 must be inside the closed region bounded by N, N', P and P' , say R , otherwise there would be a direct loop on vertex N of $I_N(G)$, which contradicts theorem 2.11 (cf. Fig. 8).

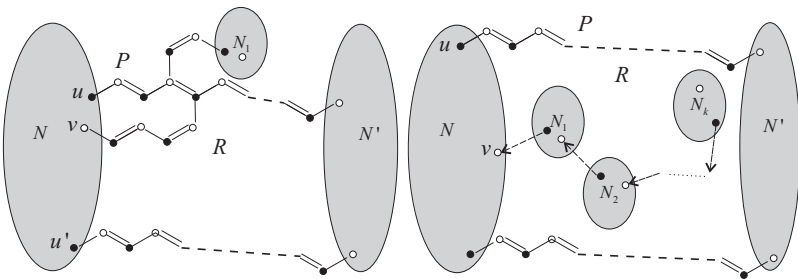


Fig. 8 Illustrations for the proof of lemma 2.20

Note that normal component N_1 has black and white vertices of degree 2 in N_1 on its boundary which are certainly spreading vertices in G . Thus the normal component N_1 in R is of type M . Hence there is another normal component N_2 in R such that N_2 properly connects to N_1 . Again N_2 is of type M . Continue this discussion, we can find in

R a series of normal components $N_1, N_2, \dots, N_k, \dots$ satisfying that N_{i+1} properly connects to $N_i, i = 1, 2, \dots$. Since R is finite, the number of different normal components in R is finite. Therefore, we can find two integers s and t such that $1 \leq s < t$ and $N_s = N_t$. One can check that there is a cycle in $I_N(G)$: $N_s = N_t \rightarrow N_{t-1} \rightarrow \dots \rightarrow N_{s+1} \rightarrow N_s$, a contradiction. This contradiction is caused by our assumption that v has different color with u and u' . Therefore, the assumption is false and the lemma holds. ■

By theorem 2.11 and the above lemma, we have the following immediately:

Lemma 2.21 *Let N be a normal component of type I of a benzenoid system $G = (W, B)$, w and b be two spreading vertices on the boundary of N such that w is white and b is black. Let N_w and N_b be normal components connecting N by F -paths with end vertices w and b , respectively. Then N_w and N_b are different.*

In the following we give a lower bound for the degree of a normal component of type I in $I_N(G)$.

Theorem 2.22 *Let N be a normal component of type I of a benzenoid system $G = (W, B)$. Then the degree of N is at least 6 in $I_N(G)$.*

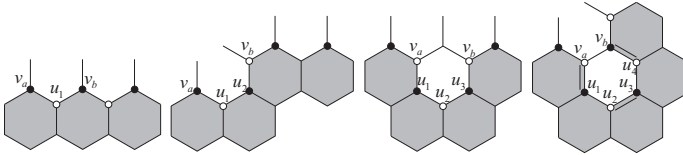


Fig. 9 Illustrations for the proof of theorem 2.22

Proof. We know that for normal component N of G there are black and white vertices of degree 2 in N on its boundary. Consider a section of the boundary of N : $v_a u_1 u_2 \dots u_j v_b$, where $d_N(v_a) = d_N(v_b) = 2$ and $d_N(u_i) = 3, i = 1, 2, \dots, j$. Clearly $0 \leq j \leq 4$ (when $j = 0$, the section is just two adjacent vertices $v_a v_b$). We claim that $j \leq 3$. In fact, if $j = 4$ (cf. Fig.9), then edge $v_a v_b$ belongs to G and is a fixed single bond of G . By lemma 2.10, N has a perfect matching M such that $v_a u_1, u_2 u_3$ and $u_4 v_b$ belong to M . Then $v_a u_1 u_2 u_3 u_4 v_b v_a$ is an M -alternating cycle containing fixed single bond $v_a v_b$, a contradiction.

It is obvious that all the vertices of degree 3 on the boundary of N are not spreading vertices (lemma 2.9), while each vertex of degree 2 in N on the boundary of N is a spreading vertex and is connected to a normal component of G by an F -path (lemma 2.16). Consider a section $v_a u_1 \dots u_j v_b$ on the boundary of N , where $d_N(v_a) = d_N(v_b) = 2$

and $d_N(u_t) = 3, t = 1, \dots, j$. For the cases $j = 1, 3$; it is clear that v_a and v_b are of the same color. Then the normal component incident with v_a need not be different from the normal component incident with v_b (lemma 2.21). While for the cases $j = 0, 2$, v_a and v_b have different colors. Then the normal component incident with v_a and the normal component incident with v_b are different (lemma 2.21).

Let $k_j (j = 1, 2, 3)$ be the number of the sections of type $v_a u_1 \dots u_j v_b$ on the boundary of N , where $d_N(v_a) = d_N(v_b) = 2$ and $d_N(u_t) = 3, t = 1, \dots, j$. Let m_i the number of vertices of degree i on the boundary of N , $i = 2, 3$. We have the following equalities:

$$m_2 = m_3 + 6 \text{ (by lemma 2.19)}, m_3 = k_1 + 2k_2 + 3k_3$$

Therefore, the lower bound for the degree of N in $I_N(G)$ is

$$d_{I_N(G)}(N) \geq m_2 - k_1 - k_3 = m_3 + 6 - k_1 - k_3 = 2k_2 + 2k_3 + 6$$

Consequently, the degree of N is at least 6 in $I_N(G)$. ■

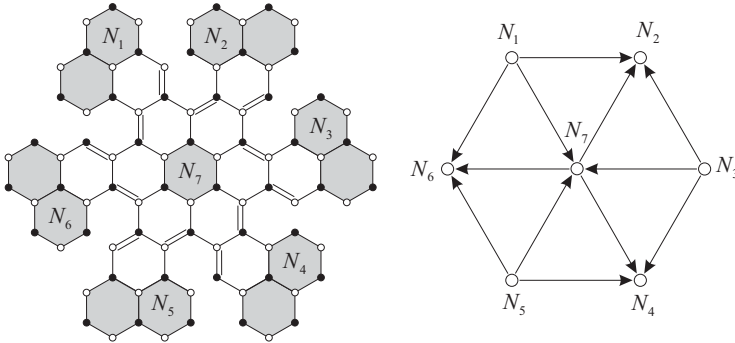


Fig. 10 The smallest benzenoid system G with a normal component of type I and the correspond $I_N(G)$

Corollary 2.23 *Let G be a benzenoid system. If G has a normal component of type I, then G has at least seven normal components.*

The smallest benzenoid system G with a normal component of type I is given in Fig. 10.

3. Classification and construction of \mathcal{G}_n

Let G be a benzenoid system with boundary C , E be a subset of the edge set $E(G)$ of G . E is said to be an *edge-cut* of G if $G - E$ is disconnected. In order to classify and construct \mathcal{G}_2 and \mathcal{G}_3 , we need the following definitions.

Definition 3.24 ([11]) A straight line segment P_1P_2 is called a cut segment if

1. P_i is the center of an edge e_i on C , $i = 1, 2$;
2. P_1P_2 is orthogonal to both e_1 and e_2 ;
3. any point of P_1P_2 is either an interior or a boundary point of some hexagon of G .

Definition 3.25 ([12]) A broken line segment P_1QP_2 is called a generalized cut (g -cut) segment if

1. P_i is the center of an edge e_i on C , $i = 1, 2$;
2. P_1Q and P_2Q are orthogonal to e_1 and e_2 , respectively;
3. Q is the center of a hexagon of G ; P_1Q and P_2Q form an angle of $\pi/3$ or $5\pi/3$;
4. Any point of P_1QP_2 is either an interior or a boundary point of some hexagon of G .

A special cut segment is either a cut segment or a g -cut segment. A special edge-cut E is the set of edges of G intersected by a special cut segment. In Fig. 11, $P_{1a}P_{2a}$ is a cut segment, while $P_{1d}Q_dP_{2d}$ is a g -cut segment.

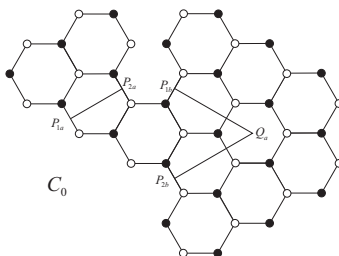


Fig. 11 An illustration for definitions 3.24 and 3.25

It is known [14] that an edge of an essentially disconnected benzenoid system is a fixed single bond if and only if it is contained in some special edge-cut. Based on the concept of special edge-cuts, a construction method for the benzenoid systems of $\mathcal{G}_n (n = 2, 3)$ is given in the following.

Let N be a normal component of a benzenoid system G . Denote by $G - N$ the subgraph of G obtained by deleting all the vertices of N together with their incident edges. Clearly, all the edges each of which has one end vertex in N and the other end vertex in $G - N$ form an edge cut of G , denoted by $(N, G - N)$.

Definition 3.26 Let N be a normal component of a benzenoid system $G \in \mathcal{G}_n$. An edge cut E incident with N is labeled by I (L) if the edges of E correspond to a cut segment (g -cut segment) of G ; otherwise, E is labeled by K .

One can check that if N is of type B or W , edge cuts incident with N can only be labeled by I or L . Then we classify and construct benzenoid systems of $\mathcal{G}_2, \mathcal{G}_3$ according to the labels of edge cuts.

1. For benzenoid systems of \mathcal{G}_2 :

By our results, each member of \mathcal{G}_2 has exactly two normal components N_1 and N_2 , one being of type W and the other being of type B . So benzenoid systems of \mathcal{G}_2 can be classified into three types : II, LL and IL , where XY means that the edge cut adjacent to N_1 is labeled by X , while the edge cut adjacent to N_2 is labeled by Y ; $X \in \{I, L\}, Y \in \{I, L\}$. It is easy to check that all the benzenoid systems of \mathcal{G}_2 have the same NC -induced digraph.

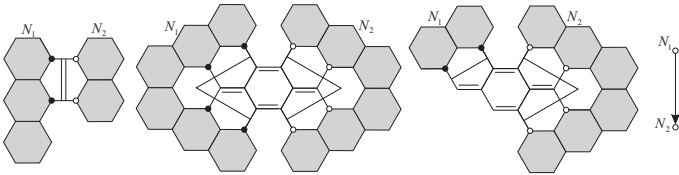


Fig. 12 Illustrations for benzenoid systems of \mathcal{G}_2 and their NC -induced digraph

2. For benzenoid systems of \mathcal{G}_3 :

For benzenoids of \mathcal{G}_3 with label K , they have only three types: IKI, IKL, LKL .

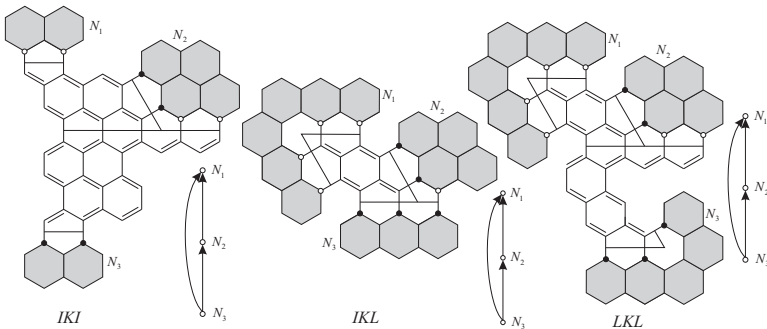


Fig. 13 Illustrations for benzenoid systems of \mathcal{G}_3 with label K and their NC -induced digraphs

Theorem 3.27 The NC -induced digraphs of benzenoids in \mathcal{G}_3 with label K are the same.

Proof. Evidently, for each benzenoid system G in \mathcal{G}_3 , $I_N(G)$ is a digraph with three vertices. By theorem 2.18, $I_N(G)$ is connected. Moreover, $I_N(G)$ is acyclic (theorem

2.11). Therefore, $I_N(G')$ is a digraph as shown in (cf. Fig. 13), the underlying graph of which is a cycle with three vertices. ■

For benzenoid systems of \mathcal{G}_3 without label K , they have ten types as follows:
 $IIII, IIIL, IILI, IILL, ILIL, ILLI, ILLL, LIIL, LILL, LLLL$.

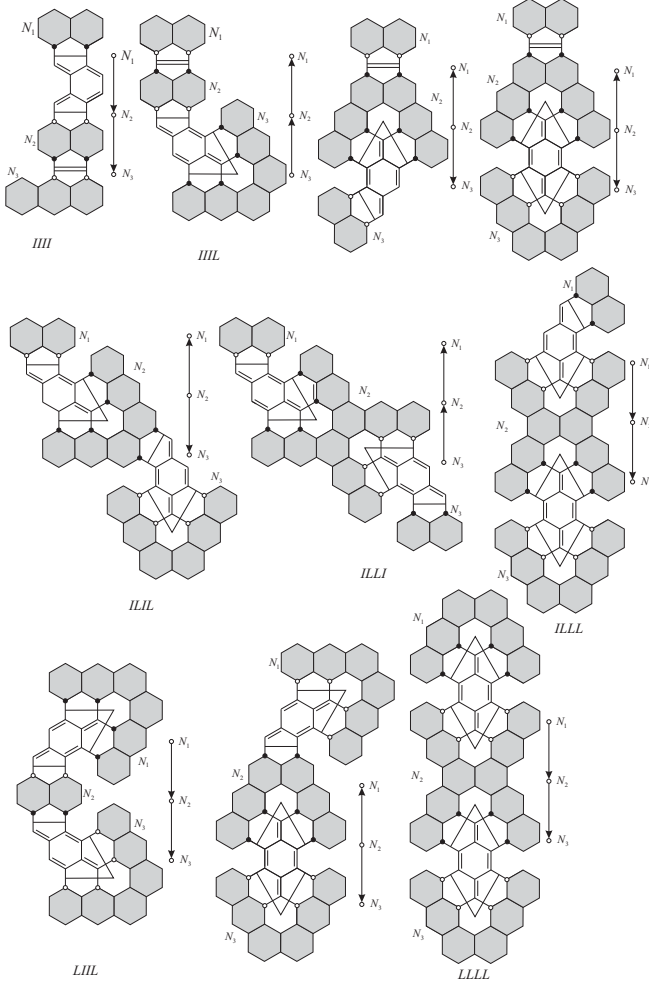


Fig. 14 Illustrations for benzenoid systems of \mathcal{G}_3 without label K and their NC -induced digraphs

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