

# Global Forcing Number of Some Chemical Graphs\*

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## Abstract

A global forcing set  $S$  of a simple connected graph  $G$  with a perfect matching is a set of edges such that no two different perfect matchings of  $G$  coincide on  $S$ . The minimum size of global forcing sets of  $G$  is called the global forcing number of  $G$ . In this paper we give two characterizations for a set of edges to be a global forcing set of a graph. As their applications, we obtain explicit formulas for the global forcing numbers of two kinds of hexagonal systems, parallelogram  $B_{p,q}$  and zigzag multiple chain  $Z(k,l)$ , and we prove that the global forcing number of a catafused coronoid with  $n$  hexagons is  $n$  or  $n - 1$ , correcting the mistake of a known result. Finally, we obtain a sharp lower bound  $\lceil \frac{2f}{3} \rceil$  on the global forcing number of a boron-nitrogen fullerene graph  $B$  by showing that any two adjacent faces of  $B$  form a nice subgraph, where  $f$  is the face number of  $B$ .

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# 1 Introduction

The concept of innate degree of freedom of a Kekulé structure was introduced by Klein and Randić [8], which coincides with the concept of forcing number of a perfect matching introduced by Harary et al. in [6]. The forcing number of a perfect matching is the smallest cardinality of edge sets that is contained only in this perfect matching. Later, there are some research papers concerning forcing number, see [1, 2, 7, 9, 10, 12, 13, 19].

In [15, 16], Vukičević et al. classified all the Kekulé structures of  $C_{60}$  into six classes according to their innate degree of freedom. But there are still considerable different structures among the Kekulé structures with the same innate degree of freedom. In order to deal with so many Kekulé structures in fullerene graphs, Vukičević [17] recently introduced a further forcing concept under the name “global (or total) forcing set”. Let  $G$  be a graph with a perfect matching. A global forcing set of  $G$  is a set of edges  $S \subseteq E(G)$  that can distinguish all perfect matchings of  $G$  completely, *i.e.*, no two different matchings of  $G$  coincide on  $S$ . Different from forcing set, global forcing set is defined globally in a graph, *i.e.*, without reference to a particular perfect matching. Hence studying global forcing set is a significant problem. In [14, 17], Vukičević gave an explicit formula for the global forcing number of the grid graphs and established a bound on the global forcing number of the triangular grid with equal number of vertices in each row and column. Došlić [5] proved that the global forcing number of all cata-condensed benzenoids with  $n$  hexagons is  $n$ . Vukičević and Došlić provided a method to study global forcing set of a graph in terms of nice cycles of the graph.

In this paper we shall characterize global forcing sets of a graph, and then as applications, we obtain the global forcing numbers of some chemical graphs. The paper is organized as follows. In Section 2, we give two characterizations for a set of edges to be a global forcing set. Accordingly, we provide a way to find a global forcing set of a graph. In Section 3, we give explicit formulas for the global forcing numbers of two kinds of hexagonal systems, parallalogram  $B_{p,q}$  and zigzag multiple chain  $Z(k, l)$ . Došlić [5] obtained that the global forcing number of any catafused coronoid  $CC_n$  with  $n$  hexagons is  $n$ . In Section 4, however we found that it is wrong and show that the global forcing number of  $CC_n$  is  $n - 1$  if  $CC_n$  has two adjacent  $L_2$  mode hexagons on its main ring, and  $n$  otherwise. In Section 5, we obtain a sharp lower bound  $\lceil \frac{2f}{3} \rceil$  on the global forcing number of a boron-nitrogen fullerene graph  $B$  by showing that any two adjacent faces of

$B$  form a nice subgraph, where  $f$  is the face number of  $B$ . Furthermore, we point out that the lower bound can be achieved by any 3-resonant  $BN$ -fullerene graph.

## 2 Definitions and some results

We use [11] for terminology and notation not defined here. Let  $G$  be a graph. A set of independent edges of a graph  $G$  is called a *matching* of  $G$ . A *perfect matching* (or *Kekulé structure* in chemical literature)  $M$  of  $G$  is a matching such that every vertex is incident with exactly one edge in  $M$ . An edge of  $G$  is *allowed* if it lies in some perfect matching of  $G$  and *forbidden* otherwise. A graph is said to be *elementary* if its allowed lines form a connected subgraph of  $G$ . For a connected bipartite graph, the elementary property is equivalent to the property that all edges are allowed [11].

A subgraph  $H$  of  $G$  is said to be *nice* if  $G - V(H)$  has a perfect matching. Let  $G$  be a bipartite graph with a perfect matching  $M$  and  $C$  a cycle of  $G$ . We call  $C$  an  $M$ -*alternating* cycle if the edges of  $C$  appear alternately in  $M$  and  $E(G) \setminus M$ . It is obvious that an even cycle  $C$  of  $G$  is nice if and only if there is a perfect matching  $M$  of  $G$  such that  $C$  is  $M$ -alternating. Let  $G$  be a plane bipartite graph and  $C$  the boundary of a face  $f$  of  $G$ . If  $G$  has a perfect matching  $M$  such that  $C$  is an  $M$ -alternating cycle, then  $f$  is called a *resonant face*. It is obvious that a face is resonant if and only if the boundary of it is a nice cycle.

The *symmetric difference* of two sets  $A$  and  $B$  is the set of elements belonging to exactly one of  $A$  and  $B$ , denoted by  $A\Delta B$ .

Let  $G = (V, E)$  be a graph with a perfect matching and  $\mathcal{M}(G)$  the set of all perfect matchings in  $G$ . Let  $S \subseteq E(G)$  and  $S = \{e_1, e_2, \dots, e_{|S|}\}$ . Let  $\mathcal{M}(G)|_S = \{M|_S : M \in \mathcal{M}(G)\}$ , where  $M|_S$  denotes the restriction of  $M$  on  $S$ , i.e.,  $M|_S = M \cap S$ . Define  $f_S: \mathcal{M}(G)|_S \rightarrow \{0, 1\}^{|S|}$  by

$$[f_S(M|_S)]_i = \begin{cases} 1, & \text{if } e_i \in M|_S, \\ 0, & \text{otherwise.} \end{cases}$$

If  $f_S$  is an injection, then  $S$  is called a *global forcing set* of  $G$ . The smallest cardinality of global forcing sets of  $G$  is called the *global forcing number* of  $G$ , denoted by  $\gamma(G)$ . If  $G$  has no perfect matchings, then we regard  $\emptyset$  as its global forcing set. Hence, all the graphs we considered in this paper have a perfect matching.

For example, we consider the graph Naphthalene shown in Fig. 1. Naphthalene contains three different perfect matchings,  $M_1 = \{e_1, e_4, e_6, e_9, e_{11}\}$ ,  $M_2 = \{e_2, e_4, e_6, e_8, e_{10}\}$ ,  $M_3 = \{e_1, e_3, e_5, e_7, e_9\}$ . Let  $S = \{e_6, e_9\}$ . Since  $M_1 \cap S = \{e_6, e_9\}$ ,  $M_2 \cap S = \{e_6\}$ ,  $M_3 \cap S = \{e_9\}$ , we know that  $f_S$  is an injection. Hence  $S$  is a global forcing set of Naphthalene.

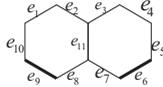


Fig. 1.  $\{e_6, e_9\}$  is a global forcing set.

Let  $G$  be a simple connected graph with the cyclomatic number  $c(G) = |E(G)| - |V(G)| + 1$ . In [5], Došlić established the following bounds on the global forcing number of a graph.

**Proposition 2.1.** [5] *Let  $G$  be a simple connected graph with a perfect matching. Then  $\lceil \log_2 K(G) \rceil \leq \gamma(G) \leq c(G)$ , where  $K(G) = |\mathcal{M}(G)|$ . Moreover,  $\gamma(G) = c(G)$  if and only if all cycles of  $G$  are nice.*

Since the global forcing number of a general graph may not equal the bounds, and since the enumeration of perfect matchings in general graphs is a #P-complete problem, it makes sense to search for an approach to determine the global forcing number of  $G$ . In the following theorem, we give a characterization for a global forcing set of a graph.

**Theorem 2.2.** *Let  $G$  be a graph with a perfect matching. Then  $S \subseteq E(G)$  is a global forcing set of  $G$  if and only if  $S$  intersects each nice cycle of  $G$ .*

*Proof.* Let  $C$  be any nice cycle of  $G$ . Then  $G - V(C)$  has a perfect matching. Therefore, we can find two perfect matchings  $M_1, M_2$  of  $G$  such that  $M_1 \Delta M_2 = C$ . If  $S$  is a global forcing set of  $G$ , then  $M_1|_S \neq M_2|_S$ . Since  $M_1$  and  $M_2$  have the same restriction on  $E(G) \setminus E(C)$ , we know that  $S \not\subseteq E(G) \setminus E(C)$ . That implies that  $S \cap C \neq \emptyset$ .

Conversely, suppose that  $S$  intersects each nice cycle of  $G$ . If  $S$  is not a global forcing set of  $G$ , then  $G$  has two different perfect matchings  $M_1$  and  $M_2$  such that  $M_1|_S = M_2|_S$ . Then  $S \cap (M_1 \Delta M_2) = \emptyset$ . Note that  $M_1 \Delta M_2$  consists of at least one  $M_1$  and  $M_2$  alternating cycle. Let  $C$  be any such cycle. Then  $C$  is a nice cycle. Hence  $S \cap C \neq \emptyset$ . But  $C \subseteq (M_1 \Delta M_2)$ , a contradiction.  $\square$

The following corollary is of fundamental importance. It will play a crucial role in determining the global forcing number of a graph.

**Corollary 2.3.** *Let  $G$  be a connected graph with a perfect matching, and  $\mathbf{T} = \{T \mid T \text{ is a connected spanning subgraph of } G \text{ without any nice cycle of } G\}$ . Then*

$$\gamma(G) = c(G) - \max_{T \in \mathbf{T}} \{c(T)\}$$

*Proof.* For each  $T \in \mathbf{T}$ , since  $T$  is a connected spanning subgraph of  $G$  without any nice cycle of  $G$ ,  $E(G) \setminus E(T)$  intersects each nice cycle of  $G$ . Since  $V(G) = V(T)$ , by Theorem 2.2, we know that

$$\gamma(G) = |E(G)| - \max_{T \in \mathbf{T}} \{|E(T)|\} = c(G) - \max_{T \in \mathbf{T}} \{c(T)\}$$

□

Corollary 2.3 shows that one can always demonstrate a minimum global forcing set by exhibiting a maximum connected spanning subgraph without any nice cycle of  $G$ . In the following, we always assume that  $T$  is a connected spanning subgraph without any nice cycle of a graph.

**Theorem 2.4.**  *$S$  is a global forcing set of  $G$  if and only if for each nice subgraph  $H$ ,  $S|_H$  is a global forcing set of  $H$ .*

*Proof.* Suppose for each nice subgraph  $H$  of  $G$ ,  $S|_H$  is a global forcing set of  $H$ . In particular, since  $G$  is a nice subgraph of itself,  $S$  is a global forcing set of  $G$ .

Conversely, suppose  $S$  is a global forcing set of  $G$  and  $H$  is any nice subgraph of  $G$ . Let  $S' := S|_H$ . If  $H$  has at most one perfect matching, then  $\emptyset$  is a global forcing set of  $H$ . Since  $\emptyset \subseteq S'$ ,  $S'$  is also a global forcing set of  $H$ . If  $H$  has at least two perfect matchings, let  $M'_1, M'_2$  be any two perfect matchings of  $H$ . Since  $H$  is a nice subgraph,  $G - V(H)$  has a perfect matching  $M_0$ . Let  $M_1 = M'_1 \cup M_0, M_2 = M'_2 \cup M_0$ . Then  $M_1$  and  $M_2$  are perfect matchings of  $G$ . Because  $S$  is a global forcing set of  $G$ , we have  $M_1|_S \neq M_2|_S$ . Hence  $M'_1|_{S'} \neq M'_2|_{S'}$  and  $S|_H$  is a global forcing set of  $H$ . □

The following corollary is a direct consequence of Theorem 2.4.

**Corollary 2.5.** *Let  $G$  be a simple connected graph with a perfect matching. If  $G_1, G_2, \dots, G_k$  are nice subgraphs of  $G$  which are pairwise disjoint, then  $\gamma(G) \geq \gamma(G_1) + \dots + \gamma(G_k)$ .*

### 3 Hexagonal systems

A *hexagonal* (or *benzenoid*) *system* is a finite connected planar graph without cut vertices in which every interior region is bounded by a regular hexagon of unit side length. A hexagonal system (*HS*)  $H$  is said to be *cata-condensed* if every vertex of  $H$  is on the boundary of  $H$ . Otherwise, the graph is *peri-condensed*.

**Theorem 3.1.** [5] *Let  $H$  be a cata-condensed HS with  $n$  hexagons. Then  $\gamma(H) = n$ .*

**Lemma 3.2.** [5] *Let  $H$  be an elementary peri-condensed HS with  $n$  hexagons. Then  $\gamma(H) \leq n - 1$ .*

It can be seen that the global forcing number of a cata-condensed *HS* can be obtained by Theorem 3.1. For a peri-condensed *HS*, there are few results. In this section, we will consider two kinds of peri-condensed hexagonal systems and give explicit formulas for the global forcing numbers of them.

A straight line segment  $C$  with end points  $P_1, P_2$  is called a *cut segment* of a hexagonal system  $H$  if

- (a)  $C$  is orthogonal to one of the three edge directions ,
- (b) each of  $P_1, P_2$  is the center of an edge lying on the contour of  $H$ ,
- (c) the graph obtained from  $H$  by deleting all edges intersected by  $C$  has exactly two components.

As an illustrative example,  $P_1P_2$  is a cut segment of the hexagonal system shown in Fig. 2.

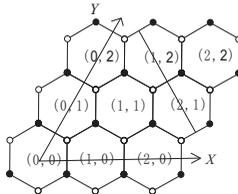


Fig. 2. Labels for the hexagons of  $B_{3,3}$  and a cut segment  $P_1P_2$  of  $B_{3,3}$ .

Let  $\mathbf{C}$  denote the set of edges of  $H$  intersected by  $C$ . Then  $\mathbf{C}$  is called an (*elementary, orthogonal*) cut of  $H$ . Color the vertices of  $H$  with black and white. As indicated in Fig. 2, every cut  $\mathbf{C}$  has the property that all vertices next to the cut segment on the one side

of the segment are black and on the other side are white. Therefore, the components of  $H - C$  will be called the *black bank*  $B(\mathbf{C})$  and the *white bank*  $W(\mathbf{C})$ , respectively.

*Benzenoid parallelogram*  $B_{p,q}$  is a hexagonal system which consists of  $p \times q$  hexagons, arranged in  $q$  rows, each row consisting of  $p$  hexagons. For convenience, the hexagons of  $B_{p,q}$  ( $p, q \geq 2$ ) are labeled as followed. Firstly, we establish an affine coordinate system  $XOY$  (see Fig. 2): take the bottom side as the  $x$ -axis, a lateral side as  $y$ -axis, their intersection as the origin  $O$  such that both sides form an angle of  $60^\circ$ . For any positive integer  $n$ , let  $Z_n$  be the finite set  $\{0, 1, \dots, n - 1\}$ . The distance between a pair of parallel edges in a hexagon is a unit length. Each hexagon is labeled by the coordinates  $(x, y)$  of its center, where  $x \in Z_p, y \in Z_q$ . Hence such a hexagon is denoted by  $h_{x,y}$ ,  $H_y = \bigcup_{x=0}^{p-1} h_{x,y}$  is called the  $y$ th layer ( $0 \leq y \leq q - 1$ ).

For a bipartite graph  $G=(B, W)$ , we use  $B(G)$  and  $W(G)$  to denote the sets of black vertices and white vertices of  $G$  respectively. Let  $b(G)=|B(G)|$  and  $w(G)=|W(G)|$ . For  $Q \subseteq V(G)$ , denote its neighborhood by  $N_G(Q)$ . The following is the famous Hall's Theorem.

**Theorem 3.3.** (*Hall's Theorem*) *A bipartite graph  $G=(B, W)$  has a matching that saturates  $B$  if and only if for all  $Q \subseteq B$ ,  $|N_G(Q)| \geq |Q|$ .*

We call two cycles *tangent* if they share exactly one path. We call a cycle a  $k$ -face cycle if the interior region surrounded by the cycle contains  $k$  faces. A  $k$ -face cycle of  $H$  is *skew* if the line connected the centers of the  $k$  faces is a straight line which is not parallel to  $x$ -axis and  $y$ -axis.

**Lemma 3.4.** *Let  $\mathcal{S}$  be any set of skew 2-face cycles of  $B_{p,q}$  which are pairwise tangent or disjoint. Then the union  $U$  of the cycles of  $\mathcal{S}$  does not contain any nice cycle of  $B_{p,q}$ .*

*Proof.* Suppose, to the contrary, that  $U$  contains a nice cycle  $C_0$  of  $B_{p,q}$ . Then the interior region of  $C_0$  is composed of several skew 2-faces. Suppose  $C$  is the leftmost cut segment of  $B_{p,q}$  such that  $C_0$  is on the left bank of the corresponding elementary cut of  $C$ , say  $\mathbf{C}$  (see Fig. 3). Such a segment must exist, since  $h_{p-1,q-1}$  is not contained in any skew 2-face cycle. Let  $B(\mathbf{C})$  be the upper component. If  $|\mathbf{C}| = l + 1$ , we claim that  $b(B(\mathbf{C})) - w(B(\mathbf{C})) = l$ . In fact, let  $\{x_1, \dots, x_{l+1}\}$  be the set of all the black vertices of  $\mathbf{C}$ , where  $x_1$  is the upmost vertex. Then for  $x_1$ , there is a zigzag path with  $x_1$  and a white vertex as its two end vertices along the upper side of  $H_{q-1}$ . For each other vertex  $x_i$  ( $i = 2, \dots, l + 1$ ), there is

a zigzag path with  $x_i$  and a black vertex as its two end vertices along the lower side of  $H_{q+1-i}$  (see Fig. 3). Those paths are disjoint and cover all the vertices of  $B(\mathbf{C})$ . Then  $b(B(\mathbf{C})) - w(B(\mathbf{C})) = l$ . Hence the claim holds.

Since  $C_0$  is a nice cycle of  $B_{p,q}$ ,  $G := B_{p,q} - V(C_0)$  has a perfect matching. Let  $Q$  be the set of all the black vertices of  $B(\mathbf{C})$ . Since  $l + 1 \geq 2$ , removing  $C_0$  from  $B_{p,q}$  will reduce at least two neighbor vertices of  $Q$ . Thus  $|N_G(Q)| \leq |N_{B_{p,q}}(Q)| - 2 = w(B(\mathbf{C})) + |\mathbf{C}| - 2 = b(B(\mathbf{C})) - 1 = |Q| - 1$ . By Hall's Theorem,  $B_{p,q} - V(C_0)$  has no perfect matchings, a contradiction.  $\square$

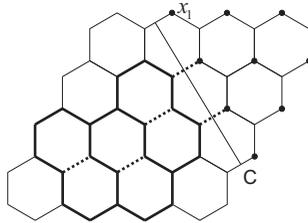


Fig. 3. Illustration for the proof of Lemma 3.4.

**Theorem 3.5.** *Let  $q \leq p$ . Then*

$$\gamma(B_{p,q}) = \begin{cases} \frac{pq+q}{2}, & \text{if } q \text{ is even,} \\ \frac{pq+p}{2}, & \text{otherwise.} \end{cases}$$

*Proof.* We first consider even  $q$ . A hexagonal chain is called a  $k$ -chain if it consists of  $k$  hexagons. Then  $B_{p,q}$  is composed of  $p - q + 1$  skew  $q$ -chains, 2 skew  $(q - i)$ -chains for  $i = 1, \dots, q - 1$  (see Fig. 4(a)). Every  $k$ -chain ( $k = 1, \dots, q$ ) contains  $\lfloor \frac{k}{2} \rfloor$  pairwise tangent or disjoint skew 2-face cycles. Since  $\lfloor \frac{q}{2} \rfloor \times (p - q + 1) + 2 \times (\lfloor \frac{q-1}{2} \rfloor + \lfloor \frac{q-2}{2} \rfloor + \dots + \lfloor \frac{2}{2} \rfloor + \lfloor \frac{1}{2} \rfloor) = \frac{q}{2} \times (p - q + 1) + 4 \times [(\frac{q-1}{2} - 1) + \dots + 1] = \frac{pq-q}{2}$ , it follows that  $B_{p,q}$  has  $\frac{pq-q}{2}$  pairwise tangent or disjoint skew 2-face cycles. By Lemma 3.4, the union  $U$  of those cycles does not contain any nice cycle of  $B_{p,q}$ . By adding as many edges as possible to  $U$  on condition that they cannot generate a new cycle, we can obtain a spanning subgraph  $T$  of  $B_{p,q}$  (see Fig. 4(b)). By Corollary 2.3, we know that  $E(B_{p,q}) \setminus E(T)$  is a global forcing set of  $B_{p,q}$ . Therefore,  $\gamma(B_{p,q}) \leq |E(B_{p,q})| - |E(T)| = c(B_{p,q}) - c(T) = pq - \frac{pq-q}{2} = \frac{pq+q}{2}$ .

On the other hand, let  $G_i = (\bigcup_{y=0}^{q-1-i} h_{i,y}) \cup (\bigcup_{x=i+1}^{p-1} h_{x,q-1-i})$  ( $i = 0, \dots, q - 1$ ). We claim that each  $G_i$  is a nice subgraph of  $B_{p,q}$ . In fact, for any  $G_i$ ,  $B_{p,q} - G_i$  has one or two components. Let the upper component be  $K_1$  (when  $i = 0, K_1 = \emptyset$ ), the other one

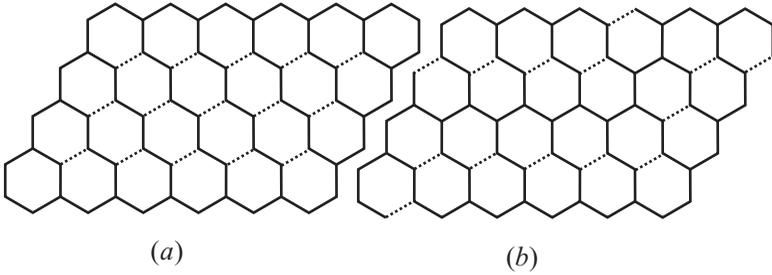


Fig. 4.(a) The skew chains in  $B_{6,4}$ ;(b) A connected spanning subgraph  $T$  without any nice cycle of  $B_{6,4}$ .

$K_2$  (when  $i = q - 1, K_2 = \emptyset$ ). As illustrated in Fig. 5,  $V(K_1), V(K_2)$  can be covered by some disjoint odd paths. Then  $K_1$  and  $K_2$  have perfect matchings. Hence each  $G_i$  is a nice subgraph of  $B_{p,q}$ .

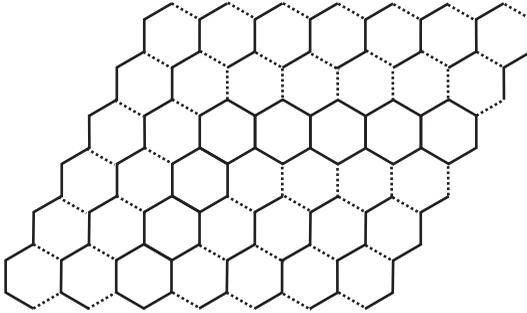


Fig. 5.  $G_2$  in  $B_{7,6}$  and the covered odd paths in  $B_{7,6} - G_2$ .

In particular,  $G_0, G_2, \dots, G_{q-2}$  are disjoint nice subgraphs of  $B_{p,q}$ ,  $\gamma(G_i) = p + q - 1 - 2i$ , for  $i = 0, 2, \dots, q - 2$ . By Corollary 2.5,  $\gamma(B_{p,q}) \geq \gamma(G_0) + \gamma(G_2) + \dots + \gamma(G_{q-2}) = (p + q - 1) + (p + q - 5) + \dots + (p - q + 3) = \frac{pq+q}{2}$ . So we have that  $\gamma(B_{p,q}) = \frac{pq+q}{2}$ .

If  $q$  is odd, then  $\lfloor \frac{q}{2} \rfloor \times (p - q + 1) + 2 \times (\lfloor \frac{q-1}{2} \rfloor + \lfloor \frac{q-2}{2} \rfloor + \dots + \lfloor \frac{2}{2} \rfloor + \lfloor \frac{1}{2} \rfloor) = \frac{q-1}{2} \times (p - q + 3) + 4 \times [\lfloor \frac{q-1}{2} \rfloor - 1) + \dots + 1] = \frac{pq-p}{2}$ . By the similar discussion, we have  $\gamma(B_{p,q}) \leq \frac{pq+p}{2}$ . On the other hand, since  $G_0, G_2, \dots, G_{q-1}$  are disjoint nice subgraphs, it follows that  $\gamma(B_{p,q}) \geq \gamma(G_0) + \gamma(G_2) + \dots + \gamma(G_{q-1}) = (p + q - 1) + (p + q - 5) + \dots + (p - q + 1) = \frac{pq+p}{2}$ . Hence  $\gamma(B_{p,q}) = \frac{pq+p}{2}$ .  $\square$

In the following, we consider the global forcing number of zigzag multiple chain  $Z(k, l)$

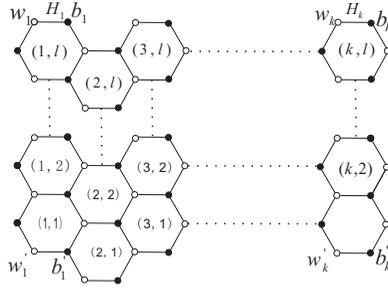


Fig. 6. Label the center of each hexagon of zigzag multiple chain  $Z(k, l)$ .

[3] which is illustrated in Fig. 6. For convenience, we label the center of each hexagon of  $Z(k, l)$  with an ordered pair  $(x, y)$  (see Fig. 6) and denote each hexagon of  $Z(k, l)$  by  $h_{x,y}$  ( $x = 1, 2, \dots, k, y = 1, 2, \dots, l$ ). Color the vertices of  $Z(k, l)$  with white and black. Let  $H_i = \bigcup_{j=1}^l h_{i,j}$ ,  $P_i$  ( $Q_i$ ) be the zigzag path along the left (right) side of  $H_i$  ( $i = 1, \dots, k$ ). Denote the end vertices of  $P_i$  (resp.  $Q_i$ ) by  $w_i, w'_i$  (resp.  $b_i, b'_i$ ) (see Fig. 6).

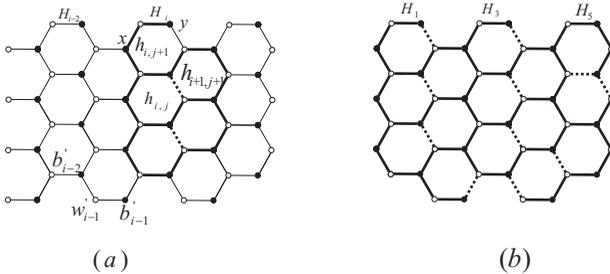


Fig. 7. Illustration for the proof of Theorem 3.6.

**Theorem 3.6.**  $\gamma(Z(k, l)) = l \lceil \frac{k}{2} \rceil + \lfloor \frac{k}{2} \rfloor$ .

*Proof.* The argument is similar to the proof of Theorem 3.5. We only prove the situation of odd  $k$  here.

Without loss of generality, we always assume that  $w_1 b_1$  is higher than  $w_2 b_2$ . Let  $H = H_1 \cup h_{2,1} \cup H_3 \cup \dots \cup h_{k-1,1} \cup H_k$ . Then  $H$  is a cata subgraph of  $Z(k, l)$  covering all the vertices of  $Z(k, l)$ . Therefore  $H$  is a nice subgraph of  $Z(k, l)$ . By Theorems 2.4 and 3.1,  $\gamma(Z(k, l)) \geq \gamma(H) = l \lceil \frac{k}{2} \rceil + \lfloor \frac{k}{2} \rfloor$ .

On the other hand, let  $\mathcal{C} = \{C_{i,j} | C_{i,j} = \partial(h_{i,j} \cup h_{i+1,j+1}), i = 1, 3, 5, \dots, k-4, k-2, 1 \leq j \leq l-1\}$ . Clearly, any two cycles of  $\mathcal{C}$  are pairwise tangent or disjoint.

**Claim.** The union  $U$  of all the cycles in  $\mathcal{C}$  does not contain any nice cycle of  $Z(k, l)$ .

Suppose, to the contrary, that  $U$  contains a nice cycle  $C_0$  of  $Z(k, l)$ . Let  $P_i$  be the rightmost zigzag path such that the region surrounded by  $C_0$  is on the right side of  $P_i$ . Let  $J$  denote the subgraph of  $Z(k, l)$  induced by the edge set of  $C_0 \cap P_i$ . Then  $J$  is bipartite and we have  $|W(J)| - |B(J)| \geq 1$ . Since  $Z(k, l)$  is a plane graph, the interior region of  $C_0$  is composed of several 2-faces. Suppose  $C_{i,j}$  is the upmost 2-face cycle which is in the interior region of  $C_0$  and intersects  $P_i$ . There are two neighbor vertices of  $C_{i,j}$  in  $h_{i,j+1}$ , say  $x$  and  $y$ . Without loss of generality, let  $x \in P_i, y \in Q_i$ . It is easy to see that  $x, y$  are black vertices (see Fig. 7(a)).

Let  $P = P_i \cup \{w_i b_i\} \cup Q_{b_i y}$ , where  $Q_{b_i y}$  is a part of  $Q_i$  with  $b_i$  and  $y$  as its two end vertices. Since  $P$  is an odd path, we have  $|W(P)| = |B(P)|$ .  $Z(k, l) - V(P)$  has two components, say  $K_1, K_2$ , where  $K_1$  is the left component. If  $i \neq 1$ , then  $K_1 = H_1 \cup \dots \cup H_{i-2} \cup \{b'_{i-2} w'_{i-1}, w'_{i-1} b'_{i-1}\}$ . If  $i = 1$ , then  $K_1 = \emptyset$ . In either case,  $|B(K_1)| = |W(K_1)|$ .

For convenience, let  $G' = Z(k, l) - V(C_0)$ . Let  $S$  be the set of all the black vertices of  $K_1$  and  $P$  in graph  $G'$ , i.e.,  $S = B(K_1) \cup B(P) \setminus B(J)$ . Since  $N_{G'}(S) = W(K_1) \cup W(P) \setminus W(J)$ , we have  $|N_{G'}(S)| = |W(K_1)| + |W(P)| - |W(J)| = |B(K_1)| + |B(P)| - |W(J)| \leq |B(K_1)| + |B(P)| - |B(J)| - 1 = |S| - 1$ . By Hall's Theorem,  $G'$  has no perfect matchings. Then  $C_0$  is not a nice cycle of  $Z(k, l)$ , a contradiction. Consequently, the claim holds. By adding as many edges as possible to  $U$  on condition that they cannot generate a new cycle, we can obtain a spanning subgraph  $T$  of  $Z(k, l)$  (see Fig. 7(b)). Therefore,  $\gamma(Z(k, l)) \leq |E(Z(k, l))| - |E(T)| = c(Z(k, l)) - c(T) = l \lceil \frac{k}{2} \rceil + \lfloor \frac{k}{2} \rfloor$ .  $\square$

## 4 Catafused coronoids

In this section, we shall consider the global forcing number of catafused coronoid graphs. A *coronoid graph* is a graph obtained from a peri-condensed benzenoid by deleting some internal vertices and/or edges in such a way that any remaining edge belongs to at least one hexagon and the remaining graph has only one bounded non-hexagonal face. A coronoid graph is *catafused* if it has no vertices shared between three hexagons. The *inner dual* of a coronoid graph  $G$  is obtained from its standard dual by deleting the vertices corresponding to the non-hexagonal faces and all incident edges (indicated in Fig. 8). A coronoid graph

is catafused if and only if its inner dual is a unicyclic graph.

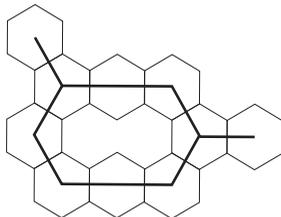


Fig. 8. Illustration for the inner dual of a catafused coronoid.

Let  $CC_n$  denote a catafused coronoid with  $n$  hexagons. The hexagons that correspond to the vertices of the unique cycle in its inner dual graph form a ring in  $CC_n$ , which is called the *main ring* of  $CC_n$ . Some modes of hexagons are presented in Fig. 9, the reader may refer to [3] for the more concrete definition of modes of hexagons. It is obvious that a catafused coronoid may possess the modes  $L_1$ ,  $L_2$ ,  $A_2$  and  $A_3$ . The  $A_2$  and  $A_3$  mode hexagons on the main ring are called *key* hexagons of  $CC_n$ . Let  $H$  be a subgraph of  $CC_n$ . Let  $CC_n \ominus H$  be the remaining subgraph of  $CC_n$  after deleting all the vertices which belong only to  $H$ .

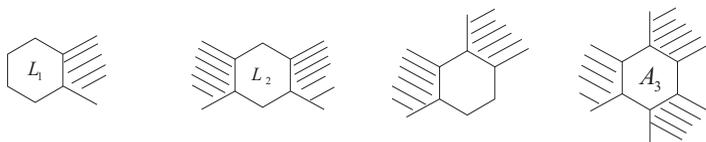


Fig. 9. Some modes of hexagons in a benzenoid.

In [5], Došlić obtained that  $\gamma(CC_n) = n$ . However, we have found a counterexample (see Fig. 10). Since the spanning subgraph  $T$  of the graph  $CC_{10}$  shown in bold has no nice cycles of  $CC_{10}$ , by Corollary 2.3, we have  $\gamma(CC_{10}) \leq c(CC_{10}) - c(T) = 10 + 1 - 2 = 9$ .

**Lemma 4.1.** [5]  $CC_n$  is Kekuléan and elementary.

**Lemma 4.2.** Let  $C$  be a cycle of  $CC_n$  which does not contain the non-hexagonal face in its interior region. Then  $C$  is a nice cycle of  $CC_n$  if and only if  $C$  does not contain all the key hexagons in its interior region.

*Proof.* Suppose that  $C$  contains all the key hexagons of  $CC_n$  in its interior region. Since  $C$  does not contain the non-hexagonal face in its interior region, there must be some  $L_2$

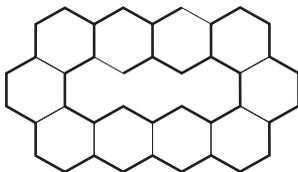


Fig. 10. A catafused coronoid  $CC_{10}$  whose global forcing number is not 10.

mode hexagons on the main ring of  $CC_n$  which are not contained in the interior region of  $C$  and form a linear hexagonal chain, say  $G_0$  (see Fig. 11(a)).  $G_0$  intersects  $C$  at two edges. Embed  $CC_n$  in the plane with the two edges vertical. Since  $G_0$  is a linear hexagonal chain, any perfect matching of  $G_0$  cannot contain two vertical edges. Hence  $G_0 - V(G_0 \cap C)$  has no perfect matchings. Since  $G_0 - V(G_0 \cap C)$  is a component of  $CC_n - V(C)$ , it follows that  $CC_n - V(C)$  has no perfect matchings. This means that  $C$  is not a nice cycle.

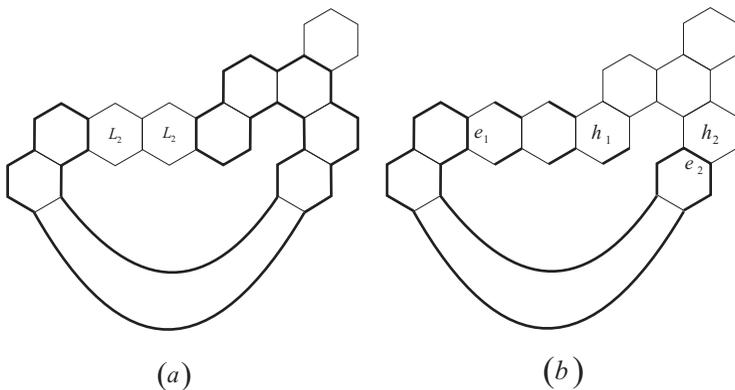


Fig. 11. Illustration for the proof of Lemma 4.2.

Conversely, suppose that  $C$  does not contain all the key hexagons in its interior region. If  $C$  does not contain any hexagon of the main ring in its interior region, then one component of  $CC_n \ominus C$  is a catafused coronoid with less hexagons, and the other possible components are cata-condensed hexagonal systems, which are elementary. Hence  $C$  intersects each component of  $CC_n \ominus C$  at only one edge, which belongs to a perfect matching of the component. Then each component contains a matching covering all the vertices of the component except the two endpoints of the joining edge. The union of

such matchings in every components of  $CC_n \ominus C$  is a perfect matching of  $CC_n - V(C)$ . Hence,  $C$  is a nice cycle. If  $C$  contains at least one hexagon of the main ring in its interior region, then each component of  $CC_n \ominus C$  is a cata-condensed hexagonal system. There is only one component, say  $G_0$ , containing some hexagons of the main ring. Then  $G_0$  intersects  $C$  at two edges, say  $e_1$  and  $e_2$ . Since  $G_0$  is a cata-condensed hexagonal system with at least one  $A_2$  or  $A_3$  mode hexagon,  $e_1$  and  $e_2$  are contained in a perfect matching of  $G_0$ . In fact, let  $h_1$  ( $h_2$ ) be the key hexagon of  $G_0$  which is nearest to  $e_1$  ( $e_2$ ). Since  $G_0$  contains at least one key hexagon,  $h_1$  and  $h_2$  must exist. Let  $e_1$  (resp.  $e_2$ ) be a matching edge. Then it determines a perfect matching in a linear sub-hexagonal chain of  $G_0$  except  $h_1$  (resp.  $h_2$ ) (see Fig. 11(b)). But since  $h_1$  and  $h_2$  are  $A_2$  or  $A_3$  mode,  $e_1$  and  $e_2$  cannot force the edges of other hexagons to be matching edges. Hence the degree of all remaining vertices are at least two after deleting all the matching edges and their incident vertices. Thus the remaining subgraph is still a cata-condensed hexagonal system. Hence  $G_0$  has a perfect matching containing  $e_1$  and  $e_2$ . Note that the other components of  $CC_n \ominus C$  are cata-condensed hexagonal systems intersecting  $C$  at only one edge. Then each component of  $CC_n - V(C)$  has a perfect matching. Hence  $C$  is a nice cycle.  $\square$

**Lemma 4.3.** *Let  $G$  be a plane connected graph. If  $G$  has exactly  $k$  interior faces, then  $c(G) = k$ .*

*Proof.* Let  $T_0$  be a spanning tree of  $G$ . Once we delete an edge  $e \in E(G) \setminus E(T_0)$  from  $G$ , the number of interior faces of  $G - e$  decreases by one. Note that  $T_0$  has no interior faces. Hence when  $G$  turns into  $T_0$ , the number of interior faces decreases by  $k$ . That means that we need to delete  $k$  edges from  $G$ . Thus  $c(G) = k$ .  $\square$

**Theorem 4.4.**

$$\gamma(CC_n) = \begin{cases} n - 1, & \text{if } CC_n \text{ has two adjacent } L_2 \text{ mode hexagons on its main ring,} \\ n, & \text{otherwise.} \end{cases}$$

*Proof.* Let  $f$  be the bounded non-hexagonal face of  $CC_n$ . If  $CC_n$  has an  $L_2$  mode hexagon  $f_1$  on its main ring, then  $\partial(f \cup f_1)$  isolates one vertex in its interior region. If  $CC_n$  has no  $L_2$  mode hexagons on its main ring, it still has two adjacent key hexagons  $f_2$  and  $f_3$  on its main ring, then  $\partial(f \cup f_2 \cup f_3)$  isolates odd vertices in its interior region. In either case,  $CC_n$  has at least one non-nice cycle. Then  $\gamma(CC_n) \leq n$ .

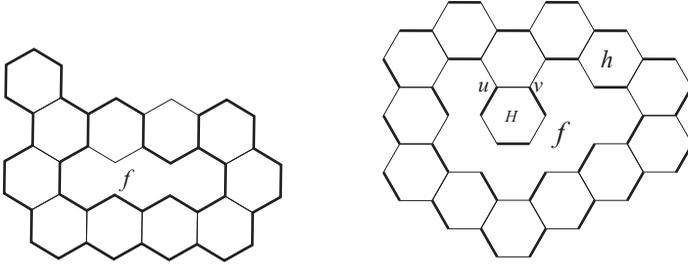


Fig. 12. Illustration for the proof of Theorem 4.4.

To form the main ring,  $CC_n$  has at least one key hexagon. Let  $h_0$  be a key hexagon of  $CC_n$ . Then by Lemma 4.2,  $CC_n \ominus h_0$  is a nice subgraph of  $CC_n$ . By Theorems 2.4 and 3.1,  $\gamma(CC_n) \geq \gamma(CC_n \ominus h_0) = n - 1$ .

**Case 1.**  $CC_n$  has two adjacent  $L_2$  mode hexagons on its main ring, say  $h_1, h_2$ .

$\partial(f \cup h_1)$  is a non-nice cycle of  $CC_n$ , since it isolates a vertex of  $CC_n$ . On the other hand, by Lemma 4.2,  $\partial(CC_n \ominus (h_1 \cup h_2))$  is a non-nice cycle. The union  $U$  of the two cycles generates a new cycle which is non-nice since it isolates a vertex of  $h_2$  (see Fig. 12(a)). Hence,  $U$  does not contain any nice cycle of  $CC_n$ . By adding as many edges as possible to  $U$  on condition that they cannot generate a new cycle, we can obtain a spanning subgraph  $T$  with  $c(T) = 2$ . By Corollary 2.3,  $\gamma(CC_n) \leq n + 1 - 2 = n - 1$ .

**Case 2.**  $CC_n$  does not have two adjacent  $L_2$  mode hexagons on its main ring.

It suffices to show that every global forcing set contains at least  $n$  edges. By Corollary 2.3, it is equivalent to prove that  $c(T) \leq 1$  for any spanning subgraph  $T$  without any nice cycle of  $CC_n$ . Suppose, to the contrary, that  $c(T) \geq 2$ . By Lemma 4.3,  $T$  has at least two interior faces. Let  $F_1, F_2, \dots, F_k$  ( $k \geq 2$ ) be the interior faces of  $T$ . If all the interior faces do not contain  $f$ , then by Lemma 4.2, every interior face of  $T$  contains all the key hexagons. Since such faces are mutually disjoint except for their boundaries, we know that  $k = 1$ , a contradiction. Consequently, there is one interior face, say  $F_1$ , containing  $f$ , and one interior face, say  $F_2$ , containing all the key hexagons.

We claim that  $F_1$  contains at least one hexagon of the main ring. Suppose, to the contrary, that  $F_1$  does not contain any hexagon of the main ring. Since  $V(CC_n)$  is covered by  $\partial(f)$  and the other even cycle,  $\partial(f)$  is a nice cycle. Then there is a perfect matching

$M$  of  $CC_n$  such that  $\partial(f)$  is an  $M$ -alternating cycle. If  $\partial(F_1) = \partial(f)$ , then  $\partial(F_1)$  is a nice cycle, a contradiction. Hence, there are some cata-condensed sub-hexagonal systems in the interior region of  $\partial(F_1)$ . For any such cata-condensed sub-hexagonal system  $H$ , since  $F_1$  does not contain any hexagon of the main ring,  $H$  intersects  $\partial(F_1)$  at only one edge, say  $uv$ . If  $u$  and  $v$  are not covered by the edges of  $M|_{F_1}$ , then both of them must be covered by edges of  $M|_H$ . Consequently,  $M\Delta\partial(H)$  is a perfect matching of  $CC_n$  containing  $uv$  (see Fig. 12(b)). Carry out the above procedure for each cata-condensed sub-hexagonal system in the interior region of  $\partial(F_1)$ , we can get a perfect matching  $M'$  of  $CC_n$  such that  $\partial(F_1)$  is an  $M'$ -alternating cycle. Then  $\partial(F_1)$  is a nice cycle, a contradiction. Hence  $F_1$  contains at least one hexagon on the main ring. Let  $h$  be such a hexagon. Since  $F_2$  contains all the key hexagons on the main ring, the hexagons of the main ring contained in  $F_1$  are all  $L_2$  mode. Hence  $h$  is  $L_2$  mode. Since  $CC_n$  does not have two adjacent  $L_2$  mode hexagons on its main ring, the two hexagons adjacent to  $h$  are key hexagons, which are thus contained in  $F_2$ . Since all the hexagons of the main ring not contained in  $F_2$  are in a component of  $CC_n \ominus F_2$ ,  $F_2$  contains all the hexagons of the main ring except  $h$ . Since  $h$  is contained in  $F_1$ ,  $F_1 \cup F_2$  contains the main ring. Then all the hexagons contained in the interior region of  $F_1$  and  $F_2$  form a catafused coronoid whose boundary is a nice cycle. Hence  $F_1 \cup F_2$  contains a nice cycle, a contradiction. Therefore  $c(T) \leq 1$ .  $\square$

## 5 $BN$ -fullerene graphs

In this section, we shall establish a sharp lower bound on the global forcing number of boron-nitrogen fullerenes. Boron-nitrogen fullerenes (or  $BN$ -fullerene graphs) are cubic plane graphs with only square and hexagonal faces. By a simple calculation using Euler's formula, we have that there are exactly 6 square faces and others hexagonal. Among all  $BN$ -fullerene graphs, there is a class of graphs, we denote it by  $\mathcal{T} = \bigcup_{n \geq 1} \{T_n\}$ , where  $T_n$  consists of  $n$  concentric layers of hexagons, capped on each end by a cap formed by three squares. In the degenerate case  $n = 0$ , we get the ordinary cube.

A graph  $G$  is *cyclically  $k$ -edge connected* if  $G$  cannot be separated into two components, each of which contains a cycle, by deleting fewer than  $k$  edges. The *cyclical edge-connectivity* of  $G$ , denoted by  $c\lambda(G)$ , is the greatest number  $k$  such that  $G$  is cyclically  $k$ -edge connected. Let  $\mathcal{H}$  be a set of disjoint faces of  $G$ . If  $G$  has a perfect matching  $M$  such that the boundary of each face of  $\mathcal{H}$  is an  $M$ -alternating cycle, then  $\mathcal{H}$  is called

a resonant pattern of  $G$ . For a positive integer  $k$ , if every  $i$  ( $1 \leq i \leq k$ ) disjoint faces of  $G$  form a resonant pattern, then  $G$  is called  $k$ -resonant.

In the following, we present some properties of  $BN$ -fullerene graphs.

**Lemma 5.1.** [4] For every  $BN$ -fullerene graph  $B$ . If  $B \in \mathcal{T}$ , then  $c\lambda(B) = 3$ ; otherwise,  $c\lambda(B) = 4$ .

**Lemma 5.2.** [18] If  $G$  is a cyclically 4-edge connected 3-regular plane graph, then there are neither three faces which are pairwise adjacent but do not share a common vertex, nor two faces sharing at least two disjoint edges in  $G$ .

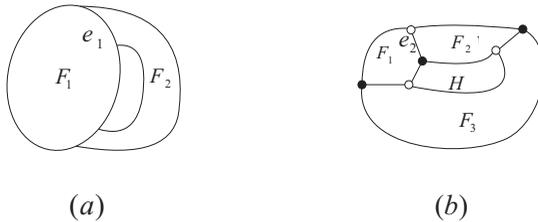


Fig. 13. Illustration for the proof of Corollary 5.3.

Let  $C = v_1v_2 \dots v_nv_1$  be a cycle. Let  $d_C(v_i, v_j)$  denote the distance between  $v_i$  and  $v_j$  on  $C$ . Two edges  $v_iv_{i+1}$  and  $v_jv_{j+1}$  of  $C$  with  $1 \leq i, j \leq k$  are *opposite* if  $d_C(v_i, v_j) = d_C(v_{i+1}, v_{j+1})$  and equals half of the length of  $C$ , where  $v_{k+1} = v_1$ . We say the distance between  $v_iv_{i+1}$  and  $v_jv_{j+1}$  is 1 if  $d_C(v_i, v_{j+1}) = 1$  or  $d_C(v_{i+1}, v_j) = 1$ .

**Corollary 5.3.** Let  $B$  be a  $BN$ -fullerene graph. Then there are no two faces sharing at least two disjoint edges in  $B$ . Moreover, if  $F_1, F_2, F_3$  are three different faces of  $B$  and the distance between  $F_1 \cap F_2$  and  $F_1 \cap F_3$  is 1 in  $F_1$ , then  $F_2 \cap F_3 = \emptyset$ .

*Proof.* By Lemma 5.1,  $c\lambda(B) = 3$  or 4.

If  $c\lambda(B) = 4$ , by Lemma 5.2, we can draw the conclusion.

If  $c\lambda(B) = 3$ , then  $B \in \mathcal{T}$ . If there are two faces sharing at least two disjoint edges, then two such edges form a cyclically 2-edge cut (see Fig. 13(a)). This is a contradiction. Consequently, any two faces share at most one edge. Moreover, consider the three faces  $F_1, F_2, F_3$  of  $B$ . Let  $F_1 \cap F_3 = \{e_1\}$ ,  $F_1 \cap F_2 = \{e_2\}$ , where  $e_i = b_iw_i$  ( $i = 1, 2$ ). Suppose to the contrary, that  $F_2 \cap F_3 \neq \emptyset$ . Since  $F_2$  and  $F_3$  share at most one edge, we suppose

that  $F_2 \cap F_3 = \{e_3\}$ , where  $e_3 = b_3w_3$ . Since the distance between  $e_1, e_2$  is 1, it follows that  $w_1b_2 \in E(B)$  or  $w_2b_1 \in E(B)$ . Without loss of generality, suppose  $w_1b_2 \in E(B)$ . Note that  $\{e_1, e_2, e_3\}$  is a cut. Suppose  $w_3$  is in the component of  $B - \{e_1, e_2, e_3\}$  which contains  $w_1, b_2$  (see Fig. 13(b)). The boundary of the component is a cycle, denoted by  $C$ . Let the subgraph induced by the vertices in the interior region of  $C$  be  $H$ . Since  $C$  is an even cycle, it follows that  $b(C) = w(C)$ . Note that  $b(C) - 1$  black vertices on  $C$  are connected to white vertices of  $H$  and  $w(C) - 2$  white vertices on  $C$  are connected to black vertices of  $H$ . Hence  $3b(H) - (w(C) - 2) = 3w(H) - (b(C) - 1)$ . Thus  $3b(H) + 1 = 3w(H)$ . This is impossible. Hence,  $F_2 \cap F_3 = \emptyset$ .  $\square$

**Theorem 5.4.** [18] *Every BN-fullerene graph is 2-resonant.*

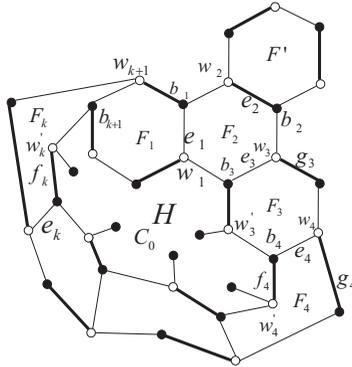


Fig. 14. Illustration for the proof of Lemma 5.5.

Basing on the above results, we have the following interesting property of *BN*-fullerene graphs.

**Lemma 5.5.** *For a BN-fullerene graph  $B$ , any two adjacent faces form a nice subgraph of  $B$ .*

*Proof.* Let  $F_1, F_2$  be any two adjacent faces of  $B$ . If one of the two faces, say  $F_2$ , is a square, by Corollary 5.3, there is another face  $F_3$  adjacent to  $F_2$ , but disjoint with  $F_1$ . By Theorem 5.4,  $\{F_1, F_3\}$  is a resonant pattern. Thus we can find a perfect matching  $M$  such that  $\partial(F_1 \cup F_2)$  is an  $M$ -alternating cycle. That is,  $\partial(F_1 \cup F_2)$  is a nice cycle of  $B$ .

Suppose that both of  $F_1$  and  $F_2$  are hexagons. By Corollary 5.3, there is another face  $F'$  adjacent to  $F_2$ , but disjoint with  $F_1$ . Let  $F_1 \cap F_2 = \{e_1\}$ ,  $F' \cap F_2 = \{e_2\}$ . Since  $\{F_1, F'\}$  is a resonant pattern, we can get a perfect matching  $M$  of  $B$  such that  $F_1$  and  $F'$  are  $M$ -alternating,  $e_1 \notin M$  and  $e_2 \in M$ .

Color the vertices of  $B$  with white and black. Let  $e_1 = b_1 w_1$ ,  $e_2 = b_2 w_2$ . If  $e_3 = b_3 w_3 \in M$ , then  $\partial(F_1 \cup F_2)$  is an  $M$ -alternating cycle. If not, we claim that  $e_3$  is contained in an  $M$ -alternating cycle  $C$  such that  $C \cap \partial(F_1) = \emptyset$  and  $C \cap \partial(F') = \emptyset$ . Suppose, to the contrary, that any  $M$ -alternating cycle passing through  $e_3$  intersects  $\partial(F_1)$  or  $\partial(F')$ . Since  $e_3 \notin M$ ,  $b_3$  and  $w_3$  are incident with other matching edges, say  $f_3, g_3$  respectively. Note that  $f_3, g_3$  and  $e_3$  are on the boundary of a face, say  $F_3$ . If  $F_3$  is a square, then we obtain an  $M$ -alternating cycle  $\partial(F_3)$  passing through  $e_3$  and by Corollary 5.3,  $\partial(F_3) \cap \partial(F_1) = \emptyset$ ,  $\partial(F_3) \cap \partial(F') = \emptyset$ , a contradiction. Hence,  $F_3$  is a hexagon. The opposite edge of  $e_3$  in  $F_3$ , denoted by  $e_4 = b_4 w_4$ , is not a matching edge, otherwise it contradicts the hypothesis. So  $b_4, w_4$  are incident with other matching edges, say  $f_4, g_4$  respectively. Clearly,  $e_4, f_4, g_4$  are on the boundary of a face, say  $F_4$ . By the similar discussion,  $F_4$  is a hexagon. Go on with this procedure, we finally obtain a sequence of hexagonal faces  $F_3, F_4, \dots, F_k$  ( $k \geq 4$ ).

Let  $G_i = \partial(F_1) \cup \partial(F_2) \cup \partial(F') \cup \partial(F_3) \cup \dots \cup \partial(F_i)$  ( $i = 3, \dots, k$ ). Suppose  $F_k$  is the first hexagon which intersects its former graph at not only one edge. Since  $b_k w_k \notin M$ ,  $b_k$  and  $w_k$  are incident with other matching edges, say  $f_k, g_k$  respectively. Let  $f_i = b_i w'_i$  ( $i = 3, \dots, k$ ). Since  $F_k$  is a hexagon and intersects  $G_{k-1}$  at not only the edge  $b_k w_k$ ,  $w'_k$  is adjacent to a black vertex of  $G_{k-1}$  other than  $b_k$ . Note that all the black vertices of  $f_i$  ( $i = 3, \dots, k-1$ ) are full degree,  $w'_k$  is not adjacent to any  $b_i$ . Since  $B$  is a plane graph,  $w'_k$  is not adjacent to any black endpoint of  $g_i$ . Hence,  $w'_k$  is adjacent to exactly one black vertex of  $F_1$  and  $F'$ . In either case, we can get an  $M$ -alternating cycle  $C_0 \subset E(G)$  passing through all the matching edges  $f_3, \dots, f_k$  (see Fig. 14). Let  $H$  be the subgraph induced by the vertices in the interior region of  $C_0$ . Since  $M|_H$  is a perfect matching of  $H$ , we have  $b(H) = w(H)$ . On the other hand, since  $B$  is a 3-regular bipartite graph, some vertices on  $C_0$  are connected to some vertices of  $H$ . Let  $A$  be the set of all such vertices of  $C_0$ . If  $w'_k$  is adjacent to a black vertex of  $F_1$ , then  $A = \{w'_3, \dots, w'_k\} \cup (A \cap F_1)$ . Suppose  $A$  has  $w$  white vertices and  $b$  black vertices. Since there are equal white vertices and black vertices in  $A \cap F_1$ ,  $w > b$ . On the other hand, since  $H$  is a bipartite graph,

$|E(H)| = 3b(H) - w = 3w(H) - b$ , which yields  $w = b$ , a contradiction. If  $w'_k$  is adjacent to a black vertex of  $F'$ , then we can also draw a contradiction by the similar discussion. Consequently,  $e_3$  is contained in an  $M$ -alternating cycle  $C_0$  such that  $C_0 \cap \partial(F_1) = \emptyset$  and  $C_0 \cap \partial(F') = \emptyset$ . Hence, we can obtain a perfect matching such that  $\partial(F_1 \cup F_2)$  is an  $M$ -alternating cycle by switching the matching edges of  $C_0$ . Thus,  $\partial(F_1 \cup F_2)$  is a nice cycle of  $B$ . □

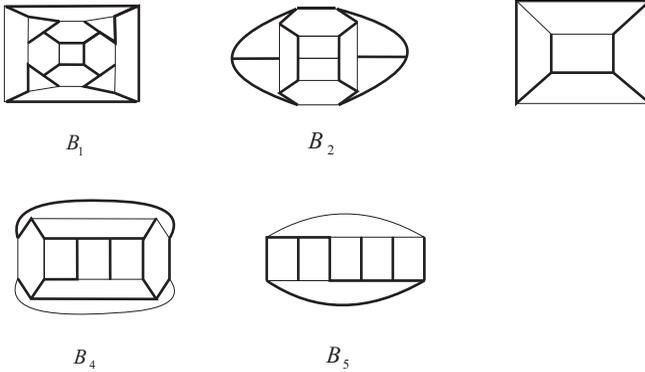


Fig. 15. The 3-resonant  $BN$ -fullerene graphs with cyclical edge connectivity 4.

**Theorem 5.6.** [18] *A cyclically 4-edge connected  $BN$ -fullerene graph  $B$  is  $k$ -resonant ( $k \geq 3$ ) if and only if  $B$  is one of  $B_1, B_2, B_3, B_4, B_5$  in Fig. 15.*

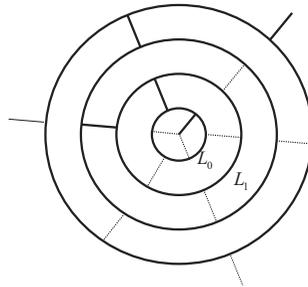


Fig. 16. A maximum spanning subgraph of  $T_n$  without any nice cycle of  $T_n$ .

**Theorem 5.7.** For any BN-fullerene graph  $B$  with  $f$  faces, we have

$$\gamma(B) \geq \lceil \frac{2f}{3} \rceil$$

and the bound can be achieved by the 3-resonant BN-fullerene graphs.

*Proof.* Since  $B$  is elementary, each face of  $B$  is resonant and any 2-face cycle is a nice cycle of  $B$ . Consequently, for any spanning subgraph  $T$  of  $B$ , each face of  $T$  must contain at least 3 faces of  $B$ . Since  $B$  has  $f$  faces,  $T$  has at most  $\lfloor \frac{f}{3} \rfloor$  faces. By Lemma 4.3,  $c(T) \leq \lfloor \frac{f}{3} \rfloor - 1$ . Hence we have  $\gamma(B) \geq f - 1 - (\lfloor \frac{f}{3} \rfloor - 1) = \lceil \frac{2f}{3} \rceil$ .

We now show that this lower bound can be achieved when  $B$  is 3-resonant. If  $c\lambda(B) = 4$ , by Theorem 5.6,  $B$  is one of  $B_1, B_2, B_3, B_4, B_5$  shown in Fig. 16. Their subgraphs  $T$  are all shown in bold in Fig. 16, which implies that  $c(T) \geq \lfloor \frac{f}{3} \rfloor - 1$  for each  $B_i$  ( $i = 1, \dots, 5$ ). Hence  $\gamma(B) \leq \lceil \frac{2f}{3} \rceil$ . If  $B = T_n \in \mathcal{T}$ , since there are three faces in each layer, the total face number of  $T_n$  is  $3n+6$ . Denote the boundary of the  $i$ th layer by  $L_i$  ( $0 \leq i \leq n$ ). There are odd vertices in the interior region of each  $L_i$ . Then  $L_i$  is not a nice cycle. Choose an arbitrary traverse edge  $e_j$  (the traverse edge is defined as the edge whose endpoints are on two layers) in each layer ( $0 \leq j \leq n+1$ ). Let  $T' = \bigcup_{i=0}^n (L_i \cup \{e_i\}) \cup \{e_{n+1}\}$ . All  $L_i$  ( $0 \leq i \leq n$ ) are pairwise disjoint, then  $T'$  is a connected spanning subgraph of  $T_n$  without any nice cycle of  $T_n$  (see Fig. 16). By Corollary 2.3, we have

$$\gamma(T_n) \leq |c(T_n)| - |c(T')| = 3n + 6 - 1 - (n + 1) = 2n + 4 = \lceil \frac{2f}{3} \rceil$$

By the first statement of the theorem, we know that  $\gamma(B) = \lceil \frac{2f}{3} \rceil$  for any 3-resonant BN-fullerene graph. □

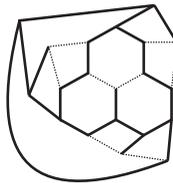


Fig. 17.  $G_1$  with a spanning subgraph (in bold).

**Remark 5.8.** For non-3-resonant BN-fullerene graphs  $B$ ,  $\gamma(B)$  may be equal to or strictly larger than  $\lceil \frac{2f}{3} \rceil$ .

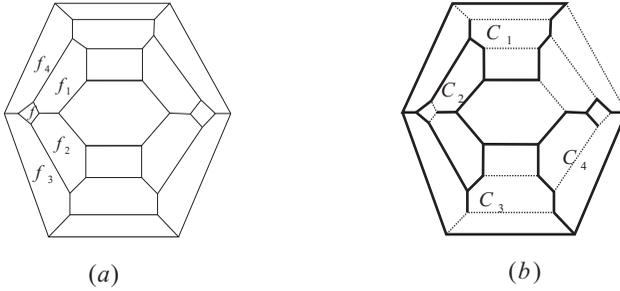


Fig. 18. (a) Labels for some faces of  $G_2$ ; (b) A subgraph  $T_2$  of  $G_2$ .

For example, we consider two non-3-resonant  $BN$ -fullerene graphs. For the graph  $G_1$  shown in Fig. 17, a subgraph  $T$  is shown in bold. Since  $c(T) = 3 = \lfloor \frac{f}{3} \rfloor - 1$ , by Corollary 2.3,  $\gamma(G_1) \leq c(G_1) - c(T) = 11 - 3 = 8$ . By Theorem 5.7, we have  $\gamma(G_1) = 8 = \lceil \frac{2f}{3} \rceil$ . For the graph  $G_2$  shown in Fig. 18(a) which has 18 faces, we have

**Proposition 5.9.**  $\gamma(G_2) = \lceil \frac{2f}{3} \rceil + 1 = 13$ .

*Proof.* By Theorem 5.7,  $\gamma(G_2) \geq \lceil \frac{2f}{3} \rceil = 12$ . We can show that the spanning subgraph  $T_1$  of  $G_2$  shown in bold in Fig. 18(b) does not contain any nice cycle of  $G_2$ . Since  $c(T_1) = 4$ , by Corollary 2.3,  $\gamma(G_2) \leq 17 - 4 = 13$ .

We now show that  $\gamma(G_2) \neq 12$ , which will establish the proposition. If  $\gamma(G_2) = 12$ , then by Corollary 2.3, we know that for any maximum spanning subgraph  $T_2$  without any nice cycle of  $G_2$ ,  $c(T_2) = 5$ . This implies that  $T_2$  has 6 faces and each face contains exactly 3 faces of  $G_2$ . Since any two squares are disjoint, the face cycle of  $T_2$  which contains a square in its interior region can only be the boundary of one of  $K_1, K_2, K_3, K_4$  shown in Fig. 19. We can show that any 3-face cycle as one of  $\partial(K_1), \partial(K_2)$  and  $\partial(K_3)$  is a nice cycle. Hence any face cycle of  $T_2$  which contains a square in its interior region can only be as  $\partial(K_4)$ . Since  $G_2$  has 6 pairwise disjoint squares, and since  $T_2$  has 6 faces, we know that each face cycle of  $T_2$  can only be as  $\partial(K_4)$ . Hence the square  $f$  of  $G_2$  indicated in Fig. 18(a) is contained in the interior region of one of the four possible 3-face cycles:  $\partial(f \cup f_1 \cup f_2), \partial(f \cup f_2 \cup f_3), \partial(f \cup f_3 \cup f_4)$  and  $\partial(f \cup f_4 \cup f_1)$ . We can deduce that  $T_2$  contains a nice cycle of  $G_2$  if  $f$  is contained in the interior region of any of the above four cycles, a contradiction. Hence  $\gamma(G_2) \neq 12$ .  $\square$

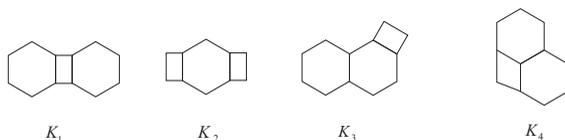


Fig. 19. 3-face cycles which contain a square in their interior regions.

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