

# ***k*-Resonance in Benzenoid Systems, Open-ended Carbon Nanotubes, Toroidal Polyhexes; and *k*-Cycle Resonant Graphs \***

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(Received March 23, 2006)

Dedicated to Prof. Fuji Zhang on the occasion of his 70th birthday

## **Abstract.**

Let  $G$  be either a benzenoid system (hexagonal system) or an open-ended carbon nanotube (tubule) or a toroidal polyhex.  $G$  is said to be  $k$ -resonant if, for  $1 \leq t \leq k$ , any  $t$  disjoint hexagons of  $G$  are mutually resonant, that is, there is a Kekule structure (or perfect matching)  $K$  of  $G$  such that each of the  $k$  hexagons is an  $K$ -alternating hexagon. A connected graph  $G$  is said to be  $k$ -cycle resonant if, for  $1 \leq t \leq k$ , any  $t$  disjoint cycles in  $G$  are mutually resonant. The concept of  $k$ -resonant graphs is closely related to Clar's aromatic sextet theory, and the concept of  $k$ -cycle resonant graphs is a natural generalization of  $k$ -resonant graphs. Some necessary and sufficient conditions for a benzenoid system or a tubule or a toroidal polyhex (resp. a graph) to be  $k$ -resonant (resp.  $k$ -cycle resonant) have been established. In this paper, we will give a survey on investigations of  $k$ -resonant benzenoid systems,  $k$ -resonant tubules,  $k$ -resonant toroidal polyhexes, and  $k$ -cycle resonant graphs.

\*The Project Supported by NSFC.

## 1. Introduction.

A *benzenoid system* (or *hexagonal system*) denotes the carbon atom skeleton graph of a benzenoid hydrocarbon, which is a 2-connected plane graph whose every interior face is bounded by a regular hexagon. An *open-ended carbon nanotube* or a *tubule* is a part of some regular hexagonal tessellation of a cylinder. A *toroidal polyhex* (or *toroidal graphitoid*, *torene*) is a toroidal fullerene which can be regarded as a tessellation of entire hexagons on the torus. A Kekule structure  $K$  of a graph  $G$  corresponds to a perfect matching (1-factor) of  $G$ . An edge of a graph  $G$  is said to be *allowed* if it is in some perfect matching of  $G$  and *forbidden*, otherwise. A connected graph  $G$  is *elementary*, if all the allowed edges of  $G$  induce a connected spanning subgraph of  $G$ . A cycle (or circuit)  $C$  in  $G$  is said to be *conjugated* or *resonant* if there is a Kekule structure  $K$  of  $G$  such that  $C$  is a  $K$ -alternating cycle. In conjugated circuit model<sup>[1-12]</sup>, conjugated circuits with different sizes have different resonant energies. If the size of a conjugated circuit is equal to  $4n+2$ , then the smaller  $n$  the larger resonant energy. So the conjugated hexagon has the largest energy. On the other hand, from a purely empirical standpoint, Clar found that various electronic properties of polycyclic aromatic hydrocarbons can be predicted by appropriately defining an aromatic sextet for their Kekule structures<sup>[13-23]</sup>. According to Clar's aromatic sextet theory, a *Clar formula* of a benzenoid system  $G$  is a set of mutually resonant sextets with the maximum cardinal number, where sextets mean resonant hexagons and a set of mutually resonant sextets means a set of disjoint hexagons for which there is a Kekule structure  $K$  so that all of the disjoint hexagons are  $K$ -alternating hexagons. The number of sextets in a Clar formula of  $G$  is called the Clar number of  $G$ .

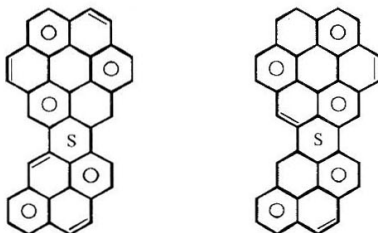


Fig. 1. A benzenoid system  $G$  with Clar number 5 and with two Clar formulae.

For a benzenoid system  $G$  with Clar number  $c$ , Clar formulae of  $G$  may be not unique, and, for  $1 \leq k \leq c$ , any  $k$  disjoint hexagons of  $G$  are not certainly mutually resonant. Fig. 1 shows a benzenoid system  $G$  with Clar number 5, which have two Clar formulae, and the hexagon  $s$  is not resonant.

An interesting problem arises: under what conditions any  $k$  disjoint hexagons of a benzenoid system  $G$  are mutually resonant? The same problem arises for a tubule and a toroidal polyhex.

Let  $G$  be either a benzenoid system or a tubule or a toroidal polyhex. If  $G$  satisfies such property, that is, for a positive integer  $k$  and  $1 \leq t \leq k$ , any  $t$  disjoint hexagons of  $G$  are mutually resonant, that is, there is a Kekule structure  $K$  of  $G$  such that each of the  $k$  hexagons is an  $K$ -alternating hexagon, then  $G$  is said to be  $k$ -resonant or  $k$ -coverable.

1-resonant benzenoid systems are first introduced by I. Gutman<sup>[24]</sup>, and a sufficient condition for a benzenoid system to be 1-resonant was also given. Some necessary and sufficient conditions for a benzenoid system to be 1-resonant was given by F. Zhang and R. Chen<sup>[25]</sup>. Later F. Zhang and M. Zheng<sup>[26]</sup> gave a similar characterization for 1-resonant generalized benzenoid systems, where a generalized benzenoid system is a 2-connected subgraph of a benzenoid system, which may have some holes. F. Zhang proposed the concept of  $k$ -resonant benzenoid systems, and then M. Zheng<sup>[27]</sup> further gave some pretty results for  $k$ -resonant benzenoid systems with  $k \geq 2$ , and gave the lower bound of the Clar number of  $k$ -resonant benzenoid system ( $k \geq 3$ ). Chen and Guo<sup>[29]</sup>, Lin and Chen<sup>[30]</sup> generalized Zheng's results to generalized benzenoid systems.

F. Zhang and L. Wang<sup>[31]</sup> first investigated  $k$ -resonance of tubules. They gave the construction method of  $k$ -resonant tubules for  $k=1$  and  $k \geq 3$ , where the construction method of 1-resonant tubules is due to a construction method of 1-resonant plane graphs given by H. Zhang and F. Zhang<sup>[32]</sup>. In addition, F. Zhang and L. Wang<sup>[31]</sup> gave the lower bound of Clar number of  $k(\geq 3)$ -resonant tubules.

For  $k$ -resonant toroidal polyhexes, W. Shiu, P. Lam, and H. Zhang<sup>[33]</sup> gave a sufficient condition for some disjoint hexagons of a toroidal polyhex to be mutually resonant, and characterized  $k$ -resonant toroidal polyhexes for  $k=1,2,3$ .

The concept of  $k$ -cycle resonant graphs was first introduced by X. Guo and F. Zhang<sup>[34]</sup>, which is a natural generalization of the concept of

$k$ -resonant benzenoid systems. Some properties and necessary and sufficient conditions of  $k$ -cycle resonant graphs and planar  $k$ -cycle resonant graphs were given <sup>[34-39, 42]</sup>.

In the paper, we will give a survey and review on investigations of  $k$ -resonant benzenoid systems,  $k$ -resonant tubules,  $k$ -resonant toroidal polyhexes, and  $k$ -cycle resonant graphs.

## 2. $k$ -Resonant (or $k$ -Coverable) Benzenoid Systems.

$k$ -resonant benzenoid systems are also called  $k$ -coverable benzenoid systems. A **cover** of a benzenoid system  $G$  is a set of disjoint hexagons of  $G$  such that after deleting all the vertices on these hexagons the remainder of  $G$  has a Kekule structure or is empty. A maximum cover of  $G$  is a cover with maximum cardinal number, which is also called a Clar formula. In other words, a cover of  $G$  is a set of mutually resonant hexagons of  $G$ , and a maximum cover is a set of mutually resonant hexagons with the maximum cardinal number.

For 1-coverable benzenoid systems, Zhang and Chen gave the following theorem.

**Theorem 1** <sup>[25]</sup>. Let  $H$  be an hexagonal system. Then each hexagon of  $H$  covers  $H$  iff either (1)  $H$  contains no fixed bond, or (2) there exist a perfect matching  $M$  of  $H$  such that the contour of  $H$  is an  $M$ -alternating cycle.

A generalized benzenoid system  $G$  is said to be complete if each edge of  $G$  is contained on a hexagon. For a complete generalized benzenoid system  $H$ , Zhang and Zheng <sup>[26]</sup> gave a similar necessary and sufficient condition for  $H$  to be  $k$ -resonant.

**Theorem 2** <sup>[26]</sup>. Every hexagon of a complete generalized hexagonal system  $H$  is resonant if and only if the boundaries of the infinite face and non-hexagon faces of  $H$  are resonant.

A sufficient condition for a benzenoid system to be 2-resonant was given by M. Zheng <sup>[27]</sup>.

**Theorem 3** <sup>[27]</sup>. A benzenoid system  $H$  is 2-resonant if  $H$  is 1-resonant and any pair of two disjoint hexagons of  $H$  with at least one boundary hexagon are mutually resonant.

In a draft of a book <sup>[28]</sup>, the above sufficient condition is improved as the following theorem.

**Theorem 4** <sup>[28]</sup>. A benzenoid system  $H$  is 2-coverable if and only if  $H$  is 1-coverable and any two disjoint side hexagons of  $H$  form a cover of  $H$ .

A complete characterization of  $k(\geq 3)$ -resonant benzenoid systems was given by M. Zheng <sup>[27]</sup>.

**Theorem 5** <sup>[27]</sup>. A benzenoid system is  $k(\geq 3)$ -resonant if and only if it is 3-resonant.

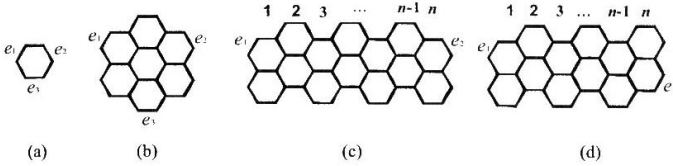


Figure 2. Four  $k(\geq 3)$ -resonant bricks: (a) A single hexagon; (b) a crown; (c)  $T_n$ ,  $n \geq 1$ ,  $n$  is odd; (d)  $T_n$ ,  $n \geq 2$ ,  $n$  is even. The edges in  $\{e_1, e_2, e_3\}$  in a crown or a single hexagon are attachable edges. The edges  $e_1, e_2$  in  $T_n$  are attachable edges.

Zheng defined four  $k(\geq 3)$ -resonant-bricks as shown in Fig. 2. If a benzenoid system  $H$  can be constructed from the four types of bricks by affixing them in attachable edges successively,  $H$  is said to have a  $k$ - $r$ -brick decomposition. A series of lemmas in ref. [27] imply the following theorem.

**Theorem 6** <sup>[27]</sup>. A benzenoid system  $H$  is  $k(\geq 3)$ -resonant if and only if  $H$  has a  $k$ - $r$ -brick decomposition.

Chen and Guo <sup>[29]</sup>, Lin and Chen <sup>[30]</sup> proved that the results of theorems 5 and 6 are also valid for generalized benzenoid systems (see Fig. 3).

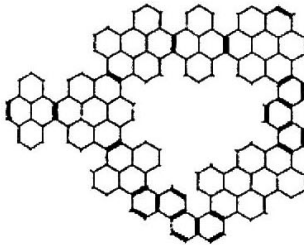


Fig. 3. A  $k$ -coverable generalized benzenoid system with  $k \geq 3$ .

### 3. $k$ -resonance of open-ended carbon nanotubes

Using the language of graph theory, a *Tubule*  $T$  is defined to be a finite section of a hexagonally tessellated cylinder produced by deleting two disjoint edge cuts such that each edge of  $T$  belongs to at least one hexagon of  $T$ .

In the following, a tubule  $T$  is drawn in such a way that its axis is vertical. Denote the top and bottom perimeter of  $T$  by  $c_1$  and  $c_2$ , respectively.

For a graph  $G$  with perfect matchings, a cycle  $c$  of  $G$  is *nice* if  $G - c$  has a perfect matching.

Let  $G$  be a graph, and let  $x$  and  $y$  be two distinct vertices in  $G$ . Let  $P$  be a path disjoint from  $G$ . Let  $(G + P)_{(x,y)}$  denote the graph obtained from  $G$  by identifying the two end vertices of  $P$  with vertices  $x$  and  $y$  in  $G$ , respectively. We also say that  $(G + P)_{(x,y)}$  is obtained from  $G$  by adding an ear or a handle. If the attachment vertices of  $P$  in  $(G + P)_{(x,y)}$  may not be mentioned,  $(G + P)_{(x,y)}$  may be simply denoted by  $G + P$ .

Let  $x$  be an edge. Let  $G_r = x + P_1 + P_2 + \cdots + P_r$  be the graph obtained from  $x$  by adding ears of odd length,  $P_1, P_2, \cdots, P_r$ , such that  $G_i = x + P_1 + P_2 + \cdots + P_i$ ,  $i = 1, 2, \cdots, r$ , is bipartite. The decomposition  $G_r = x + P_1 + P_2 + \cdots + P_r$  is called an (bipartite) *ear decomposition* of  $G_r$ .

H. Zhang and F. Zhang<sup>[32]</sup> investigated reducible face decomposition and face resonance of plane elementary bipartite graphs.

An ear decomposition  $(G_1, G_2, \dots, G_r = G)$  (equivalently,  $G = x + P_1 + P_2 + \cdots + P_r$ ) of a planar elementary bipartite graph  $G$  is called a reducible face decomposition, if  $G_1$  is the boundary of an interior face of  $G$  and the  $i$ th ear  $P_i$  is exterior to  $G_{i-1}$  such that  $P_i$  and a part of the periphery of  $G_{i-1}$  surround an interior face of  $G$  for all  $2 \leq i \leq r$ .

**Theorem 7**<sup>[32]</sup>. Let  $G$  be a planar elementary bipartite graph other than  $K_2$ . Then  $G$  has a reducible face decomposition starting with the boundary of any interior face of  $G$ .

**Corollary 8**<sup>[32]</sup>. Let  $G$  be a planar bipartite graph other than  $K_2$ . Then  $G$  is

elementary if and only if  $G$  has a reducible face decomposition.

**Theorem 9** <sup>[32]</sup>. Let  $G$  be a planar bipartite graph with more than two vertices. Then each face (including the infinite face) of  $G$  is 1-resonant iff  $G$  is elementary.

Zhang and Wang <sup>[31]</sup> first investigated  $k$ -resonant tubules. They first gave necessary and sufficient condition for a 1-resonant tubule to be 1-resonant, based on the above results.

**Corollary 10** <sup>[31]</sup>. A tubule  $T$  is 1-resonant iff  $T$  is elementary.

The above results can be also used to construct 1-resonant tubules.

For 2-resonant tubules, up to now, there is no simple procedure to recognize them and the constructive procedure has not been found, either. It seems to be a very challenging problem in the study of 2-resonant tubules as well as for benzenoid systems.

For  $k(k \geq 3)$ -resonant tubules, Zhang and Wang <sup>[31]</sup> gave the following results. Three small tubules are showed in Fig. 4.

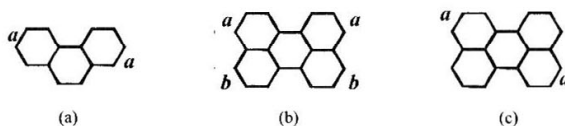


Figure 4. Three small tubules: (a)  $A_3$ , (b)  $\bar{T}_3$ , and (c)  $\bar{T}_4$ , where the edges or dangling edges with the same label are identified.

The smallest armchair tubule  $A_3$  has no disjoint hexagon and each hexagon is resonant. Thus  $A_3$  is  $k(k \geq 1)$ -resonant.  $\bar{T}_3$  and  $\bar{T}_4$  are also  $k(k \geq 1)$ -resonant tubules. In fact, each hexagon and each pair of disjoint hexagons of  $\bar{T}_3$  and  $\bar{T}_4$  are resonant, and  $\bar{T}_3$  and  $\bar{T}_4$  have at most two disjoint hexagons.



Figure 5. Three types of tubules formed by identifying the edges with the same label. (a)  $T'_n$ ,  $n \geq 4$ ,  $n$  is even; (b)  $T''_n$ ,  $n \geq 2$ ,  $n$  is even; (c)  $\bar{T}_6$ , where  $T'_n$  and  $\bar{T}_6$  have no chord,  $T''_n$  has exactly one chord  $a$ .

An edge of a tubule  $T$  is a *chord* if its two ends are on the outer-perimeters (the top and bottom perimeters)  $c_1$  and/or  $c_2$  of  $T$  but  $e \notin c_1 \cup c_2$ . A chord  $e$  of a tubule  $T$  is of *type II* if one end is on  $c_1$  and the other is on  $c_2$ . A chord  $e$  of a tubule  $T$  is of *type I* if its both ends of  $e$  are on the same perimeter  $c_1$  or  $c_2$ .

Given a chord  $e$  of type I,  $T$  is separated by  $e$  into two parts. One is a tubule, say,  $T(e)$ . The other is a benzenoid system, say,  $B(e)$ . A chord  $e^*$  of type I is *maximal* if for any chord  $e \neq e^*$  of type I,  $B(e^*)$  is not the subgraph of  $B(e)$ .

From the result in ref. [29], it can see that for a  $k(k \geq 3)$ -resonant coronoid system there are at least two chords. But in the present case, there are 3-resonant tubules having no chord ( $T_n'$  and  $\bar{T}_6$  in figure 5) and there are 3-resonant tubules having exactly one chord ( $T_n''$  in figure 5). This fact shows the difference between the coronoid systems and tubules again.

A tubule without a chord of type I is a *pure* tubule. The construction method of 3-resonant pure tubules was given by Zhang and Wang.

**Theorem 11** <sup>[31]</sup>. Let  $T$  be a 3-resonant pure tubule. Then

- (1) if  $T$  has no chord, then  $T$  is  $T_n'$ ,  $\bar{T}_6$  or  $\bar{T}_4$ ;
- (2) if  $T$  has exact one chord, then  $T$  is  $T_n''$  or  $\bar{T}_3$ ;
- (3) if  $T$  has more than one chord (of type II) arranged clockwise as  $e_1, e_2, \dots, e_n$ , then  $T$  can be splitted into sections:  $T(e_i, e_{i+1})$ ,  $i = 1, 2, \dots, n \pmod n$ , such that each section is either  $T_n$ , or a crown, or a hexagon, and the attachable edges  $e_i$  and  $e_{i+1}$  of which constitute an attachable combination.

**Theorem 12** <sup>[31]</sup>. A pure 3-resonant tubule must be  $k(k \geq 3)$ -resonant.

In general case, a 3-resonant tubule  $T$  may have chords of type I. Let  $T$  be a tubule with maximal chords of type I:  $e_1^*, e_2^*, \dots, e_n^*$ . It is clear that  $\hat{T} = T(e_1^*) \cap T(e_2^*) \cap \dots \cap T(e_n^*)$  is a pure tubule and  $B(e_i^*)$  is a 3-resonant benzenoid system. Thus, Zhang and Wang can give a construction method of 3-resonant tubules based on 3-resonant benzenoid systems and 3-resonant pure tubules.

**Theorem 13** <sup>[31]</sup>. Let  $T$  be a tubule with chord of type I,  $e_1', e_2', \dots, e_m'$  be maximal chords of type I. Then  $T$  is  $k(k \geq 3)$ -resonant, iff  $B(e_i')$ ,  $i = 1, 2, \dots, m$ , is a  $k(k \geq 3)$ -resonant benzenoid system and  $\hat{T} = T(e_1') \cap T(e_2') \cap \dots \cap T(e_m')$  is



a  $k(k \geq 3)$ -resonant pure tubule.

**Corollary 14** <sup>[31]</sup>. A 3-resonant tubule must be  $k(k \geq 3)$ -resonant.

#### 4. $k$ -Resonance in Toroidal Polyhexes

A *toroidal polyhex* is a 3-regular (cubic or trivalent) graph embedded on the torus such that each face is a hexagon, described by three parameters  $p$ ,  $q$  and  $t$ , denoted by  $H(p, q, t)$  <sup>[40,41]</sup>, and drawn in the plane (equipped with the regular hexagonal lattice  $L$ ) using the representation of the torus by a  $p \times q$ -parallelogram  $P$  with the usual boundary identification (see figure 6): each side of  $P$  connects the centers of two hexagons, and is perpendicular to an edge-direction of  $L$ , both top and bottom sides pass through  $p$  vertical edges of  $L$  while two lateral sides pass through  $q$  edges. First identify its two lateral sides, then rotate the top cycle  $t$  hexagons, finally identify the top and bottom at their corresponding points. From this one get a toroidal polyhex  $H(p, q, t)$  with the torsion  $t$  ( $0 \leq t \leq p-1$ ).

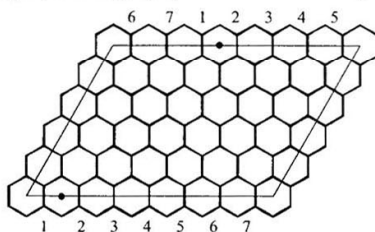


Figure 6. A toroidal polyhex  $H(p, q, t)$  for  $p = 7$ ,  $q = 5$ ,  $t = 2$ .

$k$ -resonance of benzenoid systems and open-ended carbon nanotubes were naturally extended to toroidal polyhexes by Shiu, Lam, and Zhang <sup>[30\*\*]</sup>.

The vertex-transitivity of toroidal polyhexes were respectively given by Thomassen <sup>[40]</sup>, Marusic and Pisanski <sup>[41]</sup>.

**Lemma 15** <sup>[40,41]</sup>.  $H(p, q, t)$  is vertex-transitive.

In ref. [33], the authors defined some hexagon-preserving automorphisms of  $H(p, q, t)$ , and showed the hexagon-transitivity of toroidal polyhexes.

**Lemma 16** <sup>[33]</sup>.  $H(p, q, t)$  is hexagon-transitive.

Some sufficient and necessary conditions or sufficient conditions for  $H(p, q, t)$  to be  $k(\leq 3)$ -resonant were also given in ref. [33].

**Theorem 17** <sup>[33]</sup>. A toroidal polyhex  $H(p, q, t)$  ( $p, q \geq 2$ ) is 1-resonant if and only if  $(p, q, t) \neq (2, 2, 0)$ .

**Lemma 18** <sup>[33]</sup>.  $H(p, q, t)$  is 2-resonant for  $p \geq 3$  and  $q \geq 3$ .

**Lemma 19** <sup>[33]</sup>. For  $p \geq 4$ ,  $H(p, 2, t)$  is 2-resonant if and only if  $t$  is neither 0 nor  $p \geq 2$ .

**Lemma 20** <sup>[33]</sup>. For  $q \geq 1$ ,  $H(2, q, t)$  is not 2-resonant.

**Theorem 21** <sup>[33]</sup>. For  $p \geq 2$  and  $q \geq 2$ , a toroidal polyhex  $H(p, q, t)$  is 2-resonant if and only if one of the following cases appears:

- (1)  $\min(p, q) \geq 3$ ,
- (2)  $p \geq 4$ ,  $q = 2$  and  $t \notin \{0, p - 2\}$ ,
- (3)  $(p, q) = (3, 2)$  or  $(2, 3)$ ,
- (4)  $(p, q, t) = (2, 2, 1)$ .

**Lemma 22** <sup>[33]</sup>. For  $p, q \geq 4$ ,  $H(p, q, t)$  is not 3-resonant.

**Lemma 23** <sup>[33]</sup>. For  $q \geq 2$ ,  $H(3, q, t)$  is 3-resonant.

**Lemma 24** <sup>[33]</sup>. For  $p \geq 4$ ,  $H(p, 3, t)$  is 3-resonant if and only if  $t = 0, p - 3, p - 2$  or  $p - 1$ .

**Lemma 25** <sup>[33]</sup>. For  $p \geq 3$ ,  $H(p, 2, t)$  is 3-resonant if and only if  $t = 1, p - 3, p - 1$ .

**Theorem 26** <sup>[33]</sup>. For  $p \geq 2$  and  $q \geq 2$ , a toroidal polyhex  $H(p, q, t)$  is 3-resonant if and only if one of the following cases appears

- (1)  $(p, q, t) = (2, 2, 1)$ ,
- (2)  $p \geq 2$  and  $q = 3$ ,
- (3)  $p = 3$  and  $q \geq 2$ ,
- (4)  $p \geq 4$ ,  $q = 2$  and  $t \in \{1, p - 3, p - 1\}$ ,
5.  $p \geq 4$ ,  $q = 3$  and  $t \in \{0, p - 3, p - 2, p - 1\}$ .

## 5. $k$ -Cycle Resonant Graphs.

X. Guo and F. Zhang <sup>[34]</sup> generalized the concept of  $k$ -resonant graphs to general cases to introduce the concept of  $k$ -cycle resonant graphs.

The following theorems were given in ref. [34].

**Theorem 27** <sup>[34]</sup>. Let  $G$  be a  $k$ -cycle resonant graph. Then,

- (1)  $G$  is bipartite;
- (2) for  $1 \leq t \leq k$  and any  $t$  disjoint cycles  $C_1, C_2, \dots, C_t$  in  $G$ ,  $G - \bigcup_{i=1}^t C_i$  contains no odd component;
- (3) any two 2-connected components in  $G$  have no common vertex.

**Theorem 28** <sup>[34]</sup>. Let  $G$  be a  $k$ -cycle resonant graph. Then  $G$  is elementary or 1-extendable if and only if  $G$  is 2-connected.

Theorem 27 (1) and (2) give some necessary conditions for a graph to be  $k$ -cycle resonant. Theorem 3.1 in ref. [34] asserts that the necessary conditions are also sufficient. However the theorem has a negligence. In fact, the sufficient and necessary conditions are valid if  $G$  is 2-connected or  $G$  has a perfect matching.

The correct sufficient and necessary conditions were given in ref. [35].

**Theorem 29** <sup>[35]</sup>. A 2-connected graph  $G$  with at least  $k$  disjoint cycles is  $k$ -cycle resonant if and only if  $G$  is bipartite and, for  $1 \leq t \leq k$  and any  $t$  disjoint cycles  $C_1, C_2, \dots, C_t$  in  $G$ ,  $G - \bigcup_{i=1}^t C_i$  contains no odd component.

For general cases, we have the following.

**Theorem 30** <sup>[35]</sup>. A connected graph  $G$  with at least  $k$  disjoint cycles is  $k$ -cycle resonant if and only if  $G$  is a bipartite graph with perfect matchings and, for  $1 \leq t \leq k$  and any  $t$  disjoint cycles  $C_1, C_2, \dots, C_t$  in  $G$ ,  $G - \bigcup_{i=1}^t C_i$  contains no odd component.

From Theorems 27(3), 28, 30, it is not difficult to see that the following theorem 31 holds.

**Theorem 31** <sup>[35]</sup>. Let  $G$  be a  $k$ -cycle resonant graph. Then,

- (1) for a 2-connected component  $G'$  of  $G$  with the maximum number  $k^*$  of disjoint cycles, if  $k^* \leq k$ ,  $G'$  is  $k^*$ -cycle resonant, otherwise  $G'$  is  $k$ -cycle resonant;
- (2) the forest induced by all the vertices of  $G$  not in any 2-connected component of  $G$  has a perfect matching.

The above theorems imply that a non-2-connected  $k$ -cycle resonant graph with  $k \geq 3$  can be constructed from some disjoint 2-connected  $k^*$  (or  $k$ )-cycle resonant graphs and a forest with perfect matching by adding some edges between the 2-connected graphs and the forest so that the resultant graph is connected and the added edges are cut edges. Hence we

need only to consider 2-connected  $k$ -cycle resonant graphs. However, in general cases, the construction of 2-connected  $k$ -cycle resonant graphs is still an open problem.

The necessary and sufficient conditions in Theorem 30 is simple and formally graceful. However, when it is used to determine whether or not a graph to be  $k$ -cycle resonant, one need to check any  $t$  disjoint cycles. It is obviously tedious. This is why we need to find new simpler necessary and sufficient conditions for planar graphs to be  $k$ -cycle resonant.

For a class of planar graphs,  $k$ -cycle resonant hexagonal systems, we obtained the following theorems.

A path  $P$  in a graph  $G$  is said to be a *chain* if all internal vertex of  $P$  are of degree 2 in  $G$  and the degree of any end vertex of  $P$  is not equal to two in  $G$ . A hexagonal system is said to a catacondensed hexagonal system if any vertex of it lies on the boundary.

**Theorem 32**<sup>[34]</sup>. A hexagonal system  $H$  is 1-cycle resonant if and only if  $H$  is a catacondensed hexagonal system.

**Theorem 33**<sup>[34]</sup>. A hexagonal system  $H$  is 2-cycle resonant if and only if (1)  $H$  contains at least two disjoint cycles, and

(2)  $H$  is a catacondensed hexagonal system with no chain of even length.

**Theorem 34**<sup>[34]</sup>. Let  $H$  be a 2-cycle resonant hexagonal system, and let  $k^*$  be the maximum number of disjoint cycles in  $H$ . Then  $H$  is  $k^*$ -cycle resonant.

**Theorem 35**<sup>[34]</sup>. A hexagonal system  $H$  with  $k^* \geq 2$  is  $k^*$ -cycle resonant if and only if  $H$  is a catacondensed hexagonal system with no chain of even length, where  $k^*$  is the maximum number of disjoint cycles in  $H$ .

It was pointed out in ref. [34] that in the hexagonal systems with  $h$  hexagons obtained from a same parent hexagonal system with  $h-1$  hexagons,  $k^*$ -cycle resonant hexagonal systems have greater resonance energies than 1-cycle resonant hexagonal systems, also 1-cycle resonant hexagonal systems have greater resonance energies than hexagonal systems not being 1-cycle resonant, where  $k^*$  is the maximum number of disjoint hexagons of a hexagonal system.

For general planar  $k$ -cycle resonant graphs, their characterization is more difficult. However for the cases of  $k=1,2$ , we had given some new necessary and sufficient conditions for a graph to be planar 1-cycle resonant graphs or planar 2-cycle resonant graphs<sup>[35]</sup>.

Before stating these results, we need to give some terminology and notations

Let  $G$  be a connected graph, and  $H$  a subgraph of  $G$ . A vertex in  $H$  is said to be an *attachment vertex* of  $H$  if it is incident with an edge in  $G - E(H)$ . The set of all attachment vertices of  $H$  is denoted by  $V_A(H)$ . A *bridge*  $B$  of  $H$  in  $G$  is either an edge in  $G - E(H)$  with two end vertices being in  $H$ , or a subgraph of  $G$  induced by all the edges in a connected component  $B'$  of  $G - V(H)$  together with all the edges with an end vertex in  $B'$  and the other in  $H$ . The vertices in  $V(B) \cap V(H)$  are also attachment vertices of  $B$  to  $H$ . A bridge with  $k$  attachment vertices is called a  $k$ -bridge.

The attachment vertices of a  $k$ -bridge  $B$  of a cycle  $C$  in  $G$  divide  $C$  into  $k$  edge-disjoint paths, called the segments of  $B$ . Two bridges of  $C$  avoid one another if all the attachment vertices of one bridge lie in a single segment of the other bridge, otherwise they overlap. Two bridges  $B$  and  $B^*$  of  $C$  are skew if there are four distinct vertices on  $C$ , in the cyclic order  $u, u^*, v, v^*$ , such that  $u$  and  $v$  are attachment vertices of  $B$ ,  $u^*$  and  $v^*$  are attachment vertices of  $B^*$ .

For a bipartite graph  $G$ , we always colour vertices of  $G$  white and black so that any two adjacent vertices have different colours.

We first gave several equivalent propositions.

**Theorem 36** <sup>[35]</sup>. Let  $G$  be a 2-connected bipartite planar graph. Then the following statements are equivalent:

- (1)  $G$  is 1-cycle resonant.
  - (2) For any cycle  $C$  in  $G$ ,  $G - V(C)$  has no odd component.
  - (3) For any cycle  $C$  in  $G$ , any bridge of  $C$  has exactly two attachment vertices which have different colours.
  - (4) For any cycle  $C$  in  $G$ , any two bridges of  $C$  avoid one another.
- Moreover, for any 2-connected subgraph  $B$  of  $G$  with exactly two attachment vertices, the attachment vertices of  $B$  have different colours.

From the above theorem, we can give the following necessary and sufficient conditions for a graph to be planar 1-cycle resonant.

**Theorem 37** <sup>[35]</sup>. A 2-connected graph  $G$  is planar 1-cycle resonant if and only if  $G$  is bipartite and, for any cycle  $C$  in  $G$ , any bridge of  $C$  has exactly two attachment vertices which have different colours.

**Theorem 38** <sup>[35]</sup>. A 2-connected graph  $G$  is planar 1-cycle resonant if and only if  $G$  is bipartite and, for any cycle  $C$  in  $G$ , any two bridges of  $C$  avoid

one another and, for any 2-connected subgraph  $B$  of  $G$  with exactly two attachment vertices, the attachment vertices of  $B$  have different colours.

A vertex  $u$  of a graph  $G$  is said to be *cycle-related* to another vertex  $v$  of  $G$  if  $u$  is contained in a 2-connected block of  $G$  and any cycle containing  $u$  must also contain  $v$ . If  $v$  is also cycle-related to  $u$ , then  $u$  and  $v$  are *mutually cycle-related*.

**Property 1** <sup>[35]</sup>. If a vertex  $u$  of a connected graph  $G$  is cycle-related to another vertex  $v$  of  $G$ , then  $u$  and  $v$  belong to a same 2-connected block  $B$  in  $G$  and all the edges in  $B-v$  incident with  $u$  are cut edges of  $G-v$ .

For a chain  $P$  in a graph  $G$ , let  $V_I(P)$  denote the set of internal vertices of  $P$ . For a subgraph  $B$  of  $G$ , let  $\bar{B}$  denote the subgraph of  $G$  induced by  $E(G) \setminus E(B)$ . The necessary and sufficient conditions for a planar graph to be 2-cycle resonant were also given in ref. [30].

**Theorem 39** <sup>[35]</sup>. A 2-connected graph  $G$  is planar 2-cycle resonant if and only if,

- (1)  $G$  is planar 1-cycle resonant,
- (2) for a chain  $P$  with even length and end vertices  $v_1$  and  $v_2$ ,  $G-V_I(P)$  has exactly two blocks each of which is 2-connected and  $v_1$  and  $v_2$  are cycle-related to the common vertex of the two blocks,
- (3) for a chain  $P$  with odd length and end vertices  $v_1$  and  $v_2$  such that  $G-V_I(P)$  is not 2-connected, either (a)  $G-V_I(P)$  has exactly three blocks, each of which is a 2-connected, and each of  $v_1$  and  $v_2$  is cycle-related to the other attachment vertex of the block containing it, and the attachment vertices of the third block are mutually cycle-related in the third block, or (b) any two 2-connected blocks of  $G-V_I(P)$  are disjoint,
- (4) for a 2-connected subgraph  $B_1$  of  $G$  with exactly two attachment vertices, if  $\bar{B}_1$  is not 2-connected and every block of  $\bar{B}_1$  is 2-connected, then  $\bar{B}_1$  has exactly three blocks, say  $B_2, B_3, B_4$ , and the attachment vertices of each of  $B_1, B_2, B_3, B_4$  are mutually cycle-related in the block.

Based on the above necessary and sufficient conditions, the constructions and decompositions of planar 1-cycle resonant and 2-cycle resonant graphs were respectively investigated by Xu and Guo <sup>[36]</sup>, Zhao and Guo <sup>[37,38]</sup>, Guo and Zhang <sup>[39]</sup>. Some efficient algorithms for recognizing whether or not a 2-connected graph to be planar 1-cycle resonant or 2-cycle resonant were developed.

Particularly, in ref. [39], Guo and Zhang investigated 1-cycle resonant reducible (simply 1-CR reducible) chains and ear decompositions of

1-cycle resonant graph  $G$ , where a 1-CR reducible chain of  $G$  is a maximal chain  $P$  in  $G$  such that  $G - V(P)$  (simply,  $G - P$ ) is still 1-cycle resonant.

**Theorem 39** <sup>[39]</sup>. Let  $G$  be a 2-connected planar 1-cycle resonant graph with cyclomatic number  $\nu(G) \geq 2$ . Then  $G$  has at least  $\nu(G) + 1$  1-CR-reducible chains.

**Theorem 40** <sup>[39]</sup>. Let  $G$  be a 2-connected 1-cycle resonant graph. Then  $G$  has at most  $3\nu(G) + 1$  1-CR-reducible chains.

**Theorem 41** <sup>[39]</sup>. Let  $G$  be a 2-connected planar 1-cycle resonant graph with cyclomatic number  $\nu(G) \geq 2$ . Then  $G$  has an ear decomposition  $G = C_0 + P_1 + P_2 + \dots + P_{\nu-1}$  such that  $C_0$  is a cycle and, for  $i = 1, 2, \dots, \nu - 1$ ,  $G_i = C_0 + P_1 + P_2 + \dots + P_i$  is a 2-connected planar 1-cycle resonant graph.

**Theorem 42** <sup>[39]</sup>. Let  $G$  be a 2-connected planar 1-cycle resonant graph, and  $P$  a path disjoint from  $G$ . Then  $(G + P)_{(x,y)}$  is planar 1-cycle resonant if and only if (i)  $P$  is of odd length, (ii)  $x$  and  $y$  have different colours in  $G$ , (iii) either  $x$  and  $y$  are adjacent in  $G$  or  $\{x, y\}$  is a vertex cut of  $G$ .

Let  $G$  be a planar 1-cycle resonant graph,  $P$  a path disjoint from  $G$ , and  $G^* = (G + P)_{(x,y)}$ . If  $(G + P)_{(x,y)}$  satisfies the conditions in Theorem 42, we say that  $G^*$  is obtained from  $G$  by a 1-CR-operation.

**Theorem 43** <sup>[39]</sup>. Let  $G$  be a planar 1-cycle resonant graph with cyclomatic number  $\nu(G) \geq 2$ . Then  $G$  can be constructed from a cycle by using 1-CR-operations successively.

$k$ -cycle resonant hexagonal systems are a special class of planar  $k$ -cycle resonant graphs, the construction of which was completely characterized in ref. [34]. For general planar  $k$ -cycle resonant graphs, their construction is more complex. Further investigations are needed.

## 5. Conclusion.

Investigations of  $k$ -resonant graphs (such as  $k$ -resonant benzenoid systems,  $k$ -resonant tubules,  $k$ -resonant toroidal polyhexes) and  $k$ -cycle resonant graphs have obtained great advance. The above many results are very interesting. The classes of graphs not only have strong chemistry background, but are also natural topics in matching theory. In the investigation of matching theory, Lovasz et. al <sup>[43-53]</sup> introduced and investigated elementary graphs, 1-extendable graphs, and  $n$ -extendable

graphs etc. A graph  $G$  is said to be  $n$ -extendable if any  $n$  independent edges of  $G$  is contained in a perfect matching of  $G$ . We can similarly call  $k$ -cycle resonant graphs as  $k$ -cycle extendable graphs, and call  $k$ -resonant graphs as  $k$ -hexagon extendable graphs. The above investigations are also a new advance of matching theory research. There are still some open problems for further investigations.

**Problem 1.** The construction and recognition of 2-resonant (generalized) benzenoid systems, 2-resonant tubules.

**Problem 2.** The characterization of  $k(>3)$ -resonant toroidal polyhexes.

**Problem 3.** The construction and recognition of  $k$ -cycle resonant graphs.

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