J Math Chem (2010) 48:676–686
DOI 10.1007/s10910-010-9700-8

ORIGNAL PAPER

Maximal resonance of cubic bipartite polyhedral graphs

Wai Chee Shiu · Heping Zhang · Saihua Liu

Received: 16 December 2009 / Accepted: 24 May 2010 / Published online: 12 June 2010

Abstract Let $\mathcal{H}$ be a set of disjoint faces of a cubic bipartite polyhedral graph G. If G has a perfect matching M such that the boundary of each face of $\mathcal{H}$ is an M-alternating cycle (or in other words, $G - \mathcal{H}$ has a perfect matching), then $\mathcal{H}$ is called a resonant pattern of G. Furthermore, G is k-resonant if every i $(1 \leqslant i \leqslant k)$ disjoint faces of G form a resonant pattern. In particular, G is called maximally resonant if G is k-resonant for all integers $k \geqslant 1$. In this paper, all the cubic bipartite polyhedral graphs, which are maximally resonant, are characterized. As a corollary, it is shown that if a cubic bipartite polyhedral graph is 3-resonant then it must be maximally resonant. However, 2-resonant ones need not to be maximally resonant.

Keywords Polyhedral graph · k-resonant · Cyclical edge-connectivity

This work is supported by NSFC (grant no. 10831001) and FRG, Hong Kong Baptist University.

W. C. Shiu (✉)
Department of Mathematics, Hong Kong Baptist University, Kowloon Tong, Hong Kong, People's Republic of China
e-mail: wcshiu@hkbu.edu.hk

H. Zhang · S. Liu
School of Mathematics and Statistics, Lanzhou University, Lanzhou, Gansu 730000, People's Republic of China

H. Zhang
e-mail: zhanghp@lzu.edu.cn

S. Liu
e-mail: liush2005@lzu.cn

1 Introduction

The concept of resonance was proposed according to Clar's aromatic sextet theory [2] and Randić's conjugated circuit model [9–13]. The k-resonance of many molecular graphs, including fullerene graphs and boron-nitrogen fullerene graphs, were investigated [1,7,14,15,17–20,22,23]. Every fullerene graph is shown to be 1-resonant but not all fullerene graphs are 2-resonant [17]. 3-resonant ones were also characterized. Especially, it was shown that 3-resonant fullerene graphs are also k-resonant ($k > 3$). However, every boron-nitrogen fullerene graph is 2-resonant [19]. Likely, 3-resonant boron-nitrogen fullerene graphs are k-resonant ($k > 3$). Both fullerene graphs and boron-nitrogen fullerene graphs are cubic polyhedral graphs. Here a *polyhedral graph* is the graph formed from the vertices and edges of a convex polyhedron. By Steinitz's Theorem [16], a graph is a polyhedral graph if and only if it is a 3-connected simple planar graph. In this paper, we consider the k-resonance of general cubic (i.e., 3-regular) bipartite polyhedral graphs.

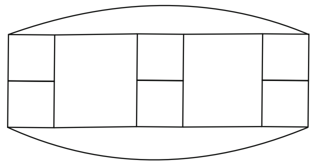
Let G be a polyhedral graph in the plane. Its every face corresponds to a face of the corresponding convex polyhedron of G. By Euler's formula, there are at least six square faces in every cubic bipartite polyhedral graph. When a cubic bipartite polyhedral graph has exactly six squares, it is a boron-nitrogen fullerene graph (i.e., 3-connected cubic plane bipartite graphs with six square faces and others hexagonal). A set of disjoint even faces $\mathcal{H}$ of a polyhedral graph G is a *resonant pattern* if $G - \mathcal{H}$ has a perfect matching. For a positive integer k, if every set of no more than k disjoint faces (the outer face may be included) of G (if it has) forms a resonant pattern, then G is called *k-resonant*. Especially, if G is k-resonant for every integer $k \geqslant 1$, then it is called *maximal resonant*.

It was shown in [21] that each face of a plane bipartite graph is a resonant pattern if and only if this graph is *elementary* (i.e., its every edge lies in some perfect matching of the graph). Since the edges of an r-regular bipartite graph G can be decomposed into r disjoint perfect matchings [8], G is elementary. Hence every cubic bipartite polyhedral graph is 1-resonant.

For boron-nitrogen fullerene graphs [19] as well as benzenoid systems [22,23], coronoid systems [1], open-end nanotubes [18], toroidal polyhexes [14,20], Klein-bottle polyhexes [7,15] and fullerene graphs [17], it was shown that if they are 3-resonant, then they are maximally resonant; that is to say, to decide whether they are maximally resonant, it suffices to decide whether they are 3-resonant. For detail information on resonant theory and the corresponding results, we may refer to [2,4–6,9–13,21]. In this paper, our aim is to characterize the maximally resonant cubic bipartite polyhedral graphs and find the smallest positive integer k such that any k-resonant cubic bipartite polyhedral graph must be maximal resonant.

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. Since a cubic bipartite polyhedral graph has at least six squares and is 3-connected, its cyclical edge-connectivity is either 3 or 4. The following result was already shown in [19].

Fig. 1 The graph G_0



Theorem 1.1 *All boron-nitrogen fullerene graphs with cyclical edge-connectivity 3 are k-resonant for any* $k \geqslant 1$ *(i.e., maximally resonant).*

Surprisingly, we show that if a cubic bipartite polyhedral graph with cyclical edge-connectivity 3 is k-resonant ($k \geqslant 3$), then it is necessarily a boron-nitrogen fullerene graph. But if a cubic bipartite polyhedral graph has cyclical edge-connectivity 4, then it is k-resonant ($k \geqslant 3$) if and only if all its vertices can be covered by a set of disjoint squares with only one exception G_0 (the graph described in Fig. 1) which is also a boron-nitrogen fullerene graph. The maximally resonant cubic bipartite polyhedral graphs are then characterized. The main results we obtain in this paper contain the special case of boron-nitrogen fullerene graphs [19].

Moreover, it implies that if a cubic bipartite polyhedral graph is 3-resonant, then it is necessarily maximally resonant. However, Fig. 10. provides an example to show that 3 is the smallest positive integer k such that any k-resonant cubic bipartite polyhedral graph must be maximally resonant.

2 Maximal resonance of cubic bipartite polyhedral graphs with cyclical edge-connectivity 3

In a graph G, let $V(G)$ and $E(G)$ be the vertex set and edge set of G, respectively. $|V(G)|$ and $|E(G)|$ denote their sizes. The vertices of degree 2 of a path P are called the *internal vertices* of P. Note that if G has n vertices and more than $n-1$ edges, then G must contain a cycle. Moreover, in a 3-connected cubic plane graph, each vertex is incident to exactly three faces and two adjacent faces share at least one edge.

Let T_n ($n \geqslant 1$) [3] be the graph consisting of n concentric layers of hexagons, capped on each end by a cap formed by three pairwise adjacent squares (see Fig. 2). Then T_n is a boron-nitrogen fullerene graph with cyclical edge-connectivity 3. In fact [3,19], T_n ($n \geqslant 1$) are the only boron-nitrogen fullerene graphs with cyclical edge-connectivity 3. Although boron-nitrogen fullerene graphs form a small class of cubic bipartite polyhedral graphs, we find that T_n ($n \geqslant 1$) are the only maximally resonant cubic bipartite polyhedral graphs with cyclical edge-connectivity 3.

Theorem 2.1 *A cubic bipartite polyhedral graph G with* $c\lambda(G) = 3$ *is k-resonant* ($k \geqslant 3$) *if and only if* $G \cong T_n$ *for some* $n \geqslant 1$.

Proof It is known in [19] that T_n is k-resonant for every integer $n \geqslant 1$. It suffices to prove the only if part.

Let G be a cubic bipartite polyhedral graph with $c\lambda(G) = 3$ and $L = \{e_1, e_2, e_3\}$ a cyclical 3-edge cut set of G. Suppose that H_1 and H_2 are the two components of

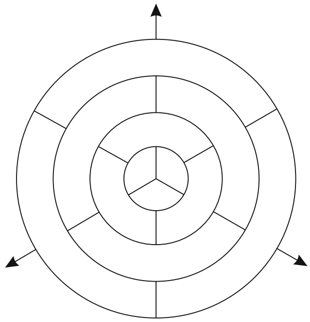


Fig. 2 The graph T_3

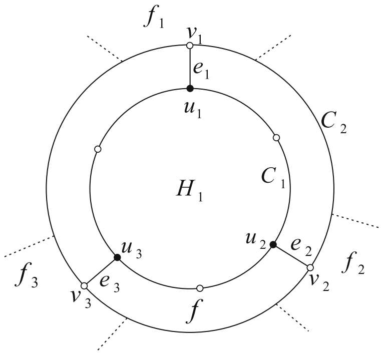


Fig. 3 The illustration for the proof of Theorem 2.1

$G - L$. Since G is cubic and 3-connected, e_1, e_2 and e_3 are disjoint and H_1, H_2 are 2-connected. Let F_i $(i = 1, 2)$ be the face of H_i that contains H_j $(i \neq j \in \{1, 2\})$ and C_i the boundary of F_i. Then C_1 and C_2 are cycles. And then each of e_1, e_2 and e_3 has one end on C_1 and the other one on C_2. Let $e_i = u_i v_i$, where $u_i \in V(C_1)$ and $v_i \in V(C_2)$ for $i = 1, 2, 3$. Since H_i $(i = 1, 2)$ contains three 2-degree vertices and the others of degree 3, $|V(H_i)|$ is odd. Since G is bipartite, we color the vertices of G properly by black and white.

To obtain the structure of G, by symmetry it suffices to discuss the structure of one of H_1 and H_2. Without loss of generality, we take H_1 into consideration. The cycle C_1 is divided into three edge disjoint segments (paths) by u_1, u_2 and u_3. Namely, they are $u_1 - u_2, u_2 - u_3$ and $u_3 - u_1$ (see Fig. 3). Let f_i $(i = 1, 2, 3)$ be the face of H_2 containing v_i which is different from F_2. Firstly, we have the following assertion.

Claim 1 Each of $u_1 - u_2, u_2 - u_3$ and $u_3 - u_1$ contains odd number of internal vertices.

Proof We only need to show that u_1, u_2 and u_3 receive the same color. Suppose to the contrary that u_1 receives the color different from the other two. Without loss of generality, suppose that u_1 is black and u_2, u_3 are white. Let f be the faces of G whose boundary contains e_2 and e_3. Since G is 1-resonant, $G - f$ has a perfect matching M. If $e_1 \in M$, then $|V(H_1 - f - u_1)|$ is even. Since u_2 and u_3 are white, $|V(f \cap H_1)|$ is odd. Then $|V(H_1)|$ is even. It is a contradiction. If $e_1 \notin M$, then $H_1 - f$ contains the same number, say n_1, of black vertices and white vertices, among them only u_1 is of

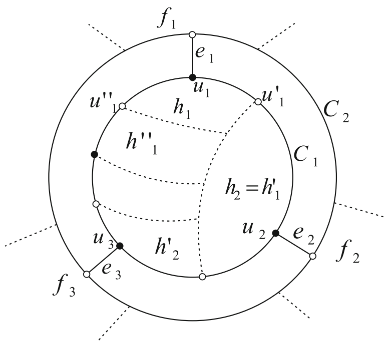


Fig. 4 The illustration for the proof of Case 1 of Theorem 2.1

degree 2. $f \cap H_1$ is a path with the two end vertices u_2 and u_3 colored white. Suppose that $f \cap H_1$ has n_2 white vertices. Then $f \cap H_1$ has $n_2 - 1$ black vertices. The degree sum of black vertices of H_1 is $3n_1 - 1 + 3(n_2 - 1) = 3(n_1 + n_2) - 4$ while the degree sum of white vertices of H_1 is $3n_1 + 3n_2 - 2 = 3(n_1 + n_2) - 2$. This is impossible, since in the bipartite graph H_1, the degree sums of black vertices and white vertices are equal. Hence u_1, u_2 and u_3 receive the same color. □

Claim 2 Each of $u_1 - u_2$, $u_2 - u_3$ and $u_3 - u_1$ contains exactly one internal vertex.

Proof Suppose to the contrary that at least one of the three segments, say $u_3 - u_1$, contains more than one internal vertex. Let u''_1 be an internal vertex of $u_3 - u_1$ adjacent to u_1. Note that u_1, u_2 and u_3 are all 2-degree vertices in H_1. Let h_i $(i = 1, 2, 3)$ be the face of H_1 different from F_1, whose boundary contains u_i. We consider two cases:

Case 1 There exists a segment, say $u_1 - u_2$, containing only one internal vertex, say u'_1 (see Fig. 4).

There are two faces of H_1 different from F_1 and h_1 containing u'_1 and u''_1, respectively. Denote these two faces by h'_1 and h''_1, respectively. Then $h'_1 = h_2$. There is also a face of H_1 different from F_1 and h_2, named h'_2, whose boundary contains the neighbor, say u'_2, of u_2 on $u_2 - u_3$.

If $h'_1 (= h_2)$ and h''_1 are disjoint, then u_1 is an isolated vertex of $G - h_2 - h''_1 - f_1$. This contradicts the 3-resonance of G. But if h_2 is adjacent to h''_1, then h_1 and h'_2 are disjoint. Then u_2 is an isolated vertex of $G - h_1 - h'_2 - f_2$. This is also a contradiction.

Case 2 Each of the three segments has at least three vertices.

Let u'_i and u''_i $(i = 1, 2, 3)$ be the two neighbors of u_i on C_1. Let h'_i and h''_i be the two faces of H_1 different from F_1 and h_i that contain u'_i and u''_i, respectively (see Fig. 5). If h'_i and h''_i are disjoint for some i $(1 \leqslant i \leqslant 3)$, then $G - h'_i - h''_i - f_i$ leaves the isolated vertex u_i. This is a contradiction. Hence, h'_i and h''_i are adjacent or the same face for $i = 1, 2, 3$. Then h_1, h_2, h_3 are pairwise disjoint. Since $|V(H_1)|$ is odd, $H_1 - h_1 - h_2 - h_3$ has at least one odd component which is also a component of $G - h_1 - h_2 - h_3$. This contradicts the 3-resonance of G. □

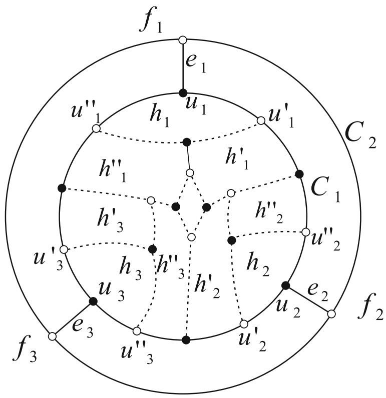


Fig. 5 The illustration for the proof of Case 2 of Theorem 2.1

Hence, there is exactly one internal vertex on each segment and these three internal vertices have the same color. Moreover, $|V(H_1 - C_1)|$ is odd. If $|V(H_1 - C_1)| = 1$, then H_1 is a cap consists of three pairwise adjacent squares. Otherwise $|V(H_1 - C_1)| = n \geqslant 3$. Then the number of edges of $H_1 - C_1$ is $\frac{3n-3}{2} = n - 1 + \frac{n-1}{2} > n - 1$, which means that $H_1 - C_1$ contains a cycle. Let e'_1, e'_2 and e'_3 be the three edges between C_1 and $H_1 - C_1$. Then $\{e'_1, e'_2, e'_3\}$ is another cyclical 3-edge cut set and each of them has one end on C_1 and the other end on a cycle, named C_3, of $H_1 - C_1$. Then the whole situation is repeated for C_3 until we get the cap consisting of three pairwise adjacent squares.

For H_2, the discussion is similar. Hence $G \cong T_n$ for some $n \geqslant 1$. □

3 Maximal resonance of cubic bipartite polyhedral graphs with cyclical edge-connectivity 4

Throuhout this section, we use G to denote a cubic bipartite polyhedral graph with $c\lambda(G) = 4$. Then G has the following structural property.

Lemma 3.1 *G has no edge cuts consisting of at most three edges, where two of them are disjoint.*

Proof Suppose to the contrary that C is an edge cut of three edges and two edges of C are disjoint. Let H_1 and H_2 be the two components of $G - C$. Let n_i $(i = 1, 2)$ be the number of vertices of H_i. Since two edges of C are disjoint, $n_i \geqslant 2$ for $i = 1, 2$. Then the degree sum of H_i $(i = 1, 2)$ is $3n_i - 3$. Thus the number of edges of H_i is $\frac{3n_i-3}{2} = n_i - 1 + \frac{n_i-1}{2} > n_i - 1$. Hence each of H_1 and H_2 contains a cycle and C is thus a cyclical edge cut set with size less than 4. This contradicts the fact that $c\lambda(G) = 4$. □

The following property has been proved for the special case of boron-nitrogen fullerene graphs [19]. It holds also in the general case.

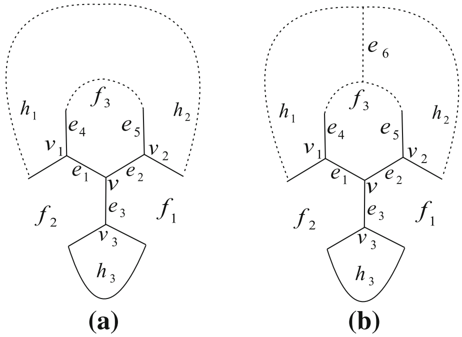


Fig. 6 The illustration for the proof of Lemma 3.2

Lemma 3.2 *If G is 3-resonant, then each vertex of G is covered by a square.*

Proof Suppose to the contrary that there is a vertex v of G that does not lie on any square.

Let v_1, v_2 and v_3 be the three neighbors of v and $e_i = vv_i$ for $i = 1, 2, 3$. f_i $(i = 1, 2, 3)$ denotes the face of G whose boundary contains $\{e_1, e_2, e_3\}\backslash\{e_i\}$. By the hypothesis, the sizes of f_1, f_2 and f_3 are greater than 4. Let h_i $(i = 1, 2, 3)$ be the face of G, whose boundary contains v_i but different from f_1, f_2 and f_3 (see Fig. 6).

First we claim that h_1, h_2 and h_3 are distinct. If not, suppose that $h_1 = h_2$ without loss of generality. Let e_4 and e_5 be the two edges of $h_1 \cap f_3$ which take v_1 and v_2 as one of their ends, respectively (see Fig. 6a). Since f_3 is neither a triangular nor a square, e_4 and e_5 are disjoint. Then the $v_1 - v_2$ segment of h_1 through e_4 and e_5 has internal vertices. Hence, $\{e_4, e_5\}$ is an edge cut of G. This is a contradiction, since G is 3-connected.

Then we claim that h_1, h_2 and h_3 are pairwise disjoint. If not, suppose that h_1 and h_2 are adjacent. Let e_4 and e_5 be the two edges of $h_1 \cap f_3$ and $h_2 \cap f_3$ which take v_1 and v_2 as one of their ends, respectively (see Fig. 6b). As before, e_4 and e_5 are disjoint. Let e_6 be an edge of $h_1 \cap h_2$. Then $\{e_4, e_5, e_6\}$ forms an edge cut with size three in which e_4 and e_5 are disjoint. By Lemma 3.1, this is impossible.

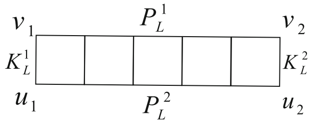
Hence, h_1, h_2 and h_3 are three pairwise disjoint distinct faces of G. Then v is an isolated vertex of $G - (h_1 \cup h_2 \cup h_3)$. This contradicts the 3-resonance of G. □

Lemma 3.3 *If there are three squares of G sharing a common vertex, then* $G \cong C_4 \times K_2$.

Proof Suppose that G contains a subgraph H consisting of three pairwise adjacent squares f_1, f_2 and f_3. Let e_1, e_2 and e_3 be the three edges incident to f_1, f_2 and f_3, respectively, but not in H. Suppose that e_1, e_2 and e_3 are not incident to the same vertex. Then $|V(G-H)| = n > 1$ and $|E(G-H)| = \frac{3n-3}{2} = n-1+\frac{n-1}{2} > n-1$. Thus there are cycles in $G-H$. Then $\{e_1, e_2, e_3\}$ is a cyclical 3-edge cut set, which is impossible. Therefore, e_1, e_2 and e_3 are incident to the same vertex. Hence $G \cong C_4 \times K_2$. □

We call the graph $P_n \times K_2$ $(n \geqslant 2)$ a *square chain*. Let $L = P_n \times K_2$ for $n \geqslant 2$. We use $\|L\|$ to denote the number of squares (4-faces) of L. Then $\|L\| = n - 1$. Especially, if $\|L\|$ is odd (resp. even), we call L an *odd* (resp. *even*) square chain.

Fig. 7 A square chain $P_6 \times K_2$



Let v_1, v_2, u_1, u_2 be the four 2-degree vertices of a square chain $L = P_n \times K_2$. Suppose that the shortest $v_1 - v_2$ path and $u_1 - u_2$ path are the two P_n layers and the shortest $v_1 - u_1$ path and $v_2 - u_2$ path are two layers of K_2 (see Fig. 7). Denote the shortest $v_1 - v_2$ path, $u_1 - u_2$ path, $v_1 - u_1$ path and $v_2 - u_2$ path by P_L^1, P_L^2, K_L^1 and K_L^2, respectively. Then $P_L^1 \cup P_L^2 \cup K_L^1 \cup K_L^2$ forms a cycle bounding L. Let F be a face of G. Denote the boundary of F by $\partial(F)$. Since G is 3-connected with $c\lambda(G) = 4$, at most one of $\{P_L^1, P_L^2, K_L^1, K_L^2\}$ is a subgraph of $\partial(F)$.

Theorem 3.4 *If G is k-resonant ($k \geqslant 3$), then $G \cong G_0$ or $G \cong C_{2n} \times K_2 (n \geqslant 2)$ or $V(G)$ is covered by a set of disjoint odd square chains.*

Proof If G has three squares sharing a common vertex, then by Lemma 3.3 $G \cong C_4 \times K_2$. If G contains a subgraph isomorphic to $C_{2n} \times K_2$, then $G \cong C_{2n} \times K_2$. Then we only need to consider the case that vertices of G are covered by all the maximal square chains $\mathcal{L} = \{L_0, L_1, \ldots, L_t\}$ $(t \geqslant 1)$. If there is an edge connecting two vertices of two maximal square chains L_i and L_j $(i \neq j)$, respectively, then it is denoted as $L_i \leftrightarrow L_j$.

Suppose that there is an even maximal square chain L_0 consists of squares $h_1, h_2, \ldots, h_{2n}$ $(n \geqslant 1)$ consecutively. Let v_1, v_2 be the two end vertices of $P_{L_0}^1$ and u_1, u_2 the two end vertices of $P_{L_0}^2$. Then u_1, u_2, v_1, v_2 are the four 2-degree vertices of L_0. Since G does not have odd cycles, $u_1u_2, v_1v_2 \notin E(G)$. Let F_1 and F_2 be two faces of G such that $P_{L_0}^1 \subset \partial(F_1)$ and $P_{L_0}^2 \subset \partial(F_2)$. Let e_1, e_2 be the common edges of h_1 and F_1, F_2, respectively. We assert that $F_1 \cap F_2 = \varnothing$. Suppose not, let e_3 be a common edge of F_1 and F_2. Then $\{e_1, e_2, e_3\}$ is an edge cut of G with two disjoint edges e_1 and e_2. This is a contradiction by Lemma 3.1. Hence $F_1 \cap F_2 = \varnothing$.

Claim 1 Each of F_1 and F_2 is incident to at most two chains in $\mathcal{L}$.

Proof Suppose to the contrary that one of F_1 and F_2, say F_1, is adjacent to at least two other square chains in $\mathcal{L}$ except L_0. Let L_1 and L_2 be the two closest square chains from L_0 which are incident to F_1. Then $L_0 \leftrightarrow L_1$ and $L_0 \leftrightarrow L_2$. Let w_1 be the neighbor of u_1 on L_1 and f_1 the square of L_1 containing w_1. Label the other three vertices of f_1 by w_2, w_3, w_4 (see Fig. 8). Let f_2 be the square of L_2 containing the neighbor of u_2 on L_2.

Since $L_1, L_2, \ldots, L_t$ are pairwise disjoint, f_1 and f_2 are disjoint. On the other hand, we assert that f_1 and F_2 are disjoint. Since $F_1 \cap F_2 = \varnothing$, $w_1w_4 \notin \partial(F_2)$ and $w_2w_3 \notin \partial(F_2)$. If $w_3w_4 \in \partial(F_2)$, then since G is planar, $\partial(F_2) - P_{L_0}^2 - w_3w_4$ consists of a $v_1 - w_4$ path and a $v_2 - w_3$ path. If the $v_1 - w_4$ path contains internal vertices, then the two end edges of the $v_1 - w_4$ path form a 2-edge cut set. This is impossible. But if the $v_1 - w_4$ path does not contain internal vertices, then the union

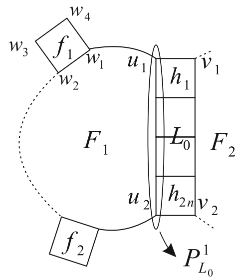


Fig. 8 The illustration for the proof of Claim 1 of Theorem 3.4

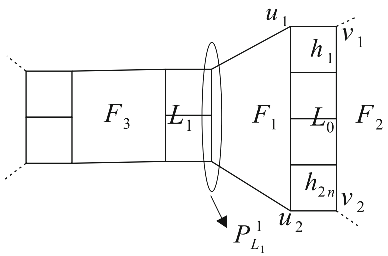


Fig. 9 The illustration for the proof of Claim 2 of Theorem 3.4

of v_1u_1, u_1w_1, w_1w_4, w_4v_1 form a square adjacent to L_0 and L_1. This is a contradiction to the fact that L_0 is a maximal square chain. Hence $F_2 \cap f_1 = \varnothing$. Similarly, $F_2 \cap f_2 = \varnothing$.

Then $G - f_1 - f_2 - F_2$ has an odd component $P^1_{L_0}$. That is a contradiction to the 3-resonance of G. The claim is proved. □

By Claim 1, F_1 is incident to exactly one other square chain in $\mathcal{L}$, say L_1. If $K^s_{L_1} \subset \partial(F_1)$ for some $s \in \{1, 2\}$, then $\partial(F)$ is an odd cycle, a contradiction to the bipartiteness of G. Hence, we may assume $P^1_{L_1} \subset \partial(F_1)$. Since $\|L_0\|$ is even and G is bipartite, $\|L_1\|$ must be even. If F_2 is also incident to L_1, then $P^2_{L_1} \subset \partial(F_2)$ similarly. Hence the face whose boundary contains v_1u_1 but different from h_1 is a square not in L_0. Thus L_0 is not a maximal square chain. This is a contradiction.

Hence, F_2 is not incident to L_1. Let F_3 be the face of G such that $P^2_{L_1} \subset \partial(F_3)$. Also, by the bipartiteness of G, $K^1_{L_0}, K^2_{L_0} \not\subseteq \partial(F_3)$. Hence, F_3 and L_0 are disjoint.

If $\|L_0\| \geqslant 4$, then h_1 and h_{2n} are disjoint. Hence $G - h_1 - h_{2n} - F_3$ leaves $P^1_{L_1}$ as an odd component (see Fig. 9). This is a contradiction. Thus we have $\|L_0\| = 2$.

Since G is a cubic polyhedral graph, G is the graph as shown in Fig. 10.

Claim 2 $t = 2$.

Proof If $t = 1$, then $G \cong C_6 \times K_2$ and L_1, L_2 are not maximal. If $t \geqslant 3$, then $G - f_1 - f_2 - f_3$ contains an odd component with the five vertices in black, where f_1, f_2 and f_3 are chosen as shown in Fig. 10. Hence $t = 2$. □

By the above claims, if G has an even maximal square chain, then $G \cong G_0$. Otherwise, $V(G)$ is covered by a set of disjoint odd square chains. □

On the other hand, there is a sufficient condition for cubic bipartite polyhedral graphs to be k-resonant, which was proved in [19].

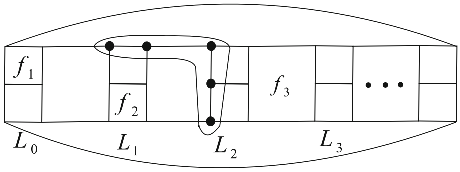


Fig. 10 The illustration for the proof of Claim 3 of Theorem 3.4

Lemma 3.5 (**[19]**) *Let G be a 2-connected cubic plane bipartite graph. If all the vertices of G are covered by a set of disjoint faces of size* 4, *then every set of disjoint faces of G forms a resonant pattern.*

Hence, if G is a cubic bipartite polyhedral graph with a set of disjoint squares covering all its vertices, then G is maximally resonant. Consequently we have the following result.

Theorem 3.6 *A cubic bipartite polyhedral graph G with $c\lambda(G) = 4$ is maximally resonant if and only if $G \cong G_0$ or $V(G)$ is covered by a set of disjoint squares.*

Proof It is easy to verify that G_0 is k-resonant ($k \geqslant 1$). If $V(G)$ is covered by a set of disjoint squares, then by Lemma 3.5, it is k-resonant ($k \geqslant 1$).

Conversely, suppose G is a cubic bipartite polyhedral graph G with $c\lambda(G) = 4$ and it is maximally resonant. Then by Theorem 3.4, $G \cong G_0$ or $G \cong C_{2n} \times K_2$ or $V(G)$ is covered by a set of disjoint odd square chains. In the latter two cases, it is easy to see that G contains a set of disjoint squares covering $V(G)$. □

The graphs in Fig. 11 are cubic bipartite polyhedral graphs with cyclical edge connectivity 4. Moreover their vertices can be covered by sets of disjoint squares (squares inserted within black points). Hence, by Theorem 3.6, they are k-resonant for any $k \geqslant 1$. In fact, for a cubic bipartite polyhedral graph G with $c\lambda(G) = 4$, if it is not isomorphic to T_n ($n \geqslant 1$), G_0 or $C_{2n} \times P_2$ ($n \geqslant 2$), then to decide its maximal

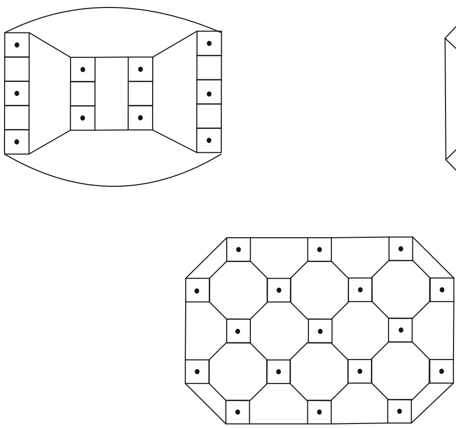


Fig. 11 Cubic bipartite polyhedral graphs with cyclical edge connectivity 4, whose vertices are covered by sets of disjoint squares (inserted within black points)

resonance we only need to find out all its maximal square chains and decide whether the maximal square chains are all odd.

The relation of 3-resonance and maximal resonance holds not only for boron-nitrogen fullerene graphs but also for the general cubic bipartite polyhedral graphs by Theorems 2.1, 3.4 and 3.6. So we have the following corollary.

Corollary 3.7 *Let G be a cubic bipartite polyhedral graph. Then G is maximally resonant if and only if G is 3-resonant.*

Remarks 3 is the smallest positive integer k such that a k-resonant cubic bipartite polyhedral graph must be maximally resonant , since there are 2-resonant ones which are not maximally resonant. Figure 10 provides an example (one can easily check that the graph is 2-resonant).

References

1. R. Chen, X. Guo, k-coverable coronoid systems. J. Math. Chem. **12**, 147–162 (1993)
2. E. Clar, *The Aromatic Sextet* (Wiley, London, 1972)
3. T. Došlić, Cyclical edge-connectivity of fullerene graphs and (k, 6)-cages. J. Math. Chem. **33**(2), 103–112 (2003)
4. X. Guo, k-Resonace in benzenoid systems, open-ended carbon nanotubes, toroidal polyhexes; and k-cycle resonant graphs. MATCH Commun. Math. Comput. Chem. **56**, 439–456 (2006)
5. D.J. Klein, Elemental benzenoids. J. Chem. Inf. Comput. Sci. **34**, 453–459 (1994)
6. D.J. Klein, H. Zhu, Resonance in elemental benzenoids. Discret. Appl. Math. **67**, 157–173 (1996)
7. Q. Li, S. Liu, H. Zhang, 2-extendability and k-resonance of non-bipartite Klein-bottle polyhexes, preprint, (2009)
8. L. Lovasz, M.D. Plummer, *Matching Theory, Annals of Discrete Math*, vol. 29 (North-Holland, Amsterdam, 1986)
9. M. Randić, On the characterization of local aromatic properties in benzenoid hydrocarbons. Tetrahedron **30**(14), 2067–2074 (1974)
10. M. Randić, Graph theoretical approach to local and overall aromaticity of benzenoid hydrocarbons. Tetrahedron **31**(11–12), 1477–1481 (1975)
11. M. Randić, Aromaticity and conjugation. J. Amer. Chem. Soc. **99**, 444–450 (1977)
12. M. Randić, Conjugated circuits and resonance energies of benzenoid hydrocarbons. Chem. Phys. Lett. **38**, 68–70 (1976)
13. M. Randić, Aromaticity of polycyclic conjugated hydrocarbons. Chem. Rev. **103**(9), 3449–3605 (2003)
14. W.C. Shiu, P.C.B. Lam, H. Zhang, k-resonance in toroidal polyhexes. J. Math. Chem. **38**(4), 451–466 (2005)
15. W.C. Shiu, H. Zhang, A complete characterization for k-resonant Klein-bottle polyhexes. J. Math. Chem. **43**, 45–59 (2008)
16. E. Steinitz, Polyeder und Raumeinteilungen, Encyclopädie der Mathematischen Wissenschaften, Band 3 (Geometrie) Teil 3AB12 (1922), pp. 1–139
17. D. Ye, Z. Qi, H. Zhang, On k-resonant fullerene graphs, SIAM J. Discret. Math. **23**(2), 1023–1044 (2009)
18. F. Zhang, L. Wang, k-Resonance of open-ended carbon nanotubes. J. Math. Chem. **35**(2), 87–103 (2004)
19. H. Zhang, S. Liu, 2-resonance of plane bipartite graphs and its applications to boron-nitrogen fullerenes, preprint (2009)
20. H. Zhang, D. Ye, k-resonant totoidal polyhexes. J. Math. Chem. **44**(1), 270–285 (2008)
21. H. Zhang, F. Zhang, Plane elementary bipartite graphs. Discret. Appl. Math. **105**, 291–311 (2000)
22. M. Zheng, k-Resonant benzenoid systems. J. Mol. Struct. (Theochem) **231**, 321–334 (1991)
23. M. Zheng, Construction of 3-resonant benzenoid systems. J. Mol. Struct. (Theochem) **277**, 1–14 (1992)