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Anti-Kekulé number of the {(3, 4), 4}-fullerene*

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A *{(3,4),4}-fullerene graph* G is a 4-regular plane graph with exactly eight triangular faces and other quadrangular faces. An edge subset S of G is called an *anti-Kekulé set*, if $G - S$ is a connected subgraph without perfect matchings. The *anti-Kekulé number* of G is the smallest cardinality of anti-Kekulé sets and is denoted by $ak(G)$. In this paper, we show that $4 \le ak(G) \le 5$; at the same time, we determine that the {(3, 4), 4}-fullerene graph with anti-Kekulé number 4 consists of two kinds of graphs: one of which is the graph $\mathcal{H}_1$ consisting of the tubular graph Q_n $(n \ge 0)$, where Q_n is composed of n $(n \ge 0)$ concentric layers of quadrangles, capped on each end by a cap formed by four triangles which share a common vertex (see Figure 2 for the graph Q_n); and the other is the graph $\mathcal{H}_2$, which contains four diamonds D_1, D_2, D_3, and D_4, where each diamond D_i $(1 \le i \le 4)$ consists of two adjacent triangles with a common edge e_i $(1 \le i \le 4)$ such that four edges e_1, e_2, e_3, and e_4 form a matching (see Figure 7D for the four diamonds $D_1 - D_4$). As a consequence, we prove that if $G \in \mathcal{H}_1$, then $ak(G) = 4$; moreover, if $G \in \mathcal{H}_2$, we give the condition to judge that the anti-Kekulé number of graph G is 4 or 5.

KEYWORDS

anti-Kekulé set, anti-Kekulé number, {(3,4),4}-fullerene, perfect matching, matching

1 Introduction

A *{(3,4),4}-fullerene graph* G is a 4-regular plane graph with exactly eight triangular faces and other quadrangular faces. This concept of the {(3, 4), 4}-fullerene comes from Deza's *{(R,k)}-fullerene* (Deza and Sikirić, 2012). Fixing $R \subset N$, a $\{(R, k)\}$-fullerene graph is a k-regular $(k \ge 3)$, and it is mapped on a sphere whose faces are i-gons $(i \in R)$. A *{(a,b),k}-fullerene* is $\{(R, k)\}$-fullerene with $R = \{a, b\}$ $(1 \le a \le b)$. The $\{(a, b), k\}$-fullerene draws attention because it includes the mostly widely researched graphs, such as fullerenes (i.e.,{(5, 6), 3}-fullerenes), boron–nitrogen fullerenes (i.e.,{(4, 6), 3}-fullerenes), and (3,6)-fullerenes (i.e.,{(3, 6), 3}-fullerenes) (Yang and Zhang, 2012).

The anti-Kekulé number of a graph was introduced by Vukičević and Trinajstić (2007). They introduced the anti-Kekulé number as the smallest number of edges that have to be removed from a benzenoid to remain connected but without a Kekulé structure. Here, a Kekulé structure corresponds to a perfect matching in mathematics; it is known that benzenoid hydrocarbon has better stability if it has a lower anti-Kekulé number. Veljan and Vukičević (2008) found that the anti-Kekulé numbers of the infinite triangular, rectangular, and hexagonal grids are 9, 6 and 4, respectively. Zhang et al. (2011) proved that the anti-Kekulé number of cata-condensed phenylenes is 3. For fullerenes, Vukičević (2007) proved that C_{60} has anti-Kekulé number 4, and Kutnar et al. (2009) showed that the leapfrog fullerenes have the anti-Kekulé number 3 or 4 and that for each leapfrog fullerene, the anti-Kekulé number can be established by observing the finite number of cases independent of the size of the fullerene. Furthermore, this result was improved by Yang et al. (2012) by proving that all fullerenes have anti-Kekulé number 4.

In general, Li et al. (2019) showed that the anti-Kekulé number of a 2-connected cubic graph is either 3 or 4; moreover, all (4,6)-fullerenes have the anti-Kekulé number 4, and all the (3,6)-fullerenes have anti-Kekulé number 3. Zhao and Zhang (2020) confirmed all (4,5,6)-fullerenes have anti-Kekulé number 3, which consist of four sporadic (4,5,6)-fullerenes (F_{12}, F_{14}, F_{18}, and F_{20}) and three classes of (4,5,6)-fullerenes with at least two and at most six pentagons.

Here, we consider the {(3, 4), 4}-fullerene graphs. In the next section, we recall some concepts and results needed for our discussion. In Section 3, by using Tutte's Theorem on perfect matching of graphs, we determine the scope of the anti-Kekulé number of the {(3, 4), 4}-fullerene. Finally, we show that the {(3, 4), 4}-fullerene with anti-Kekulé number 4 consists of two kinds of graphs $\mathcal{H}_1, \mathcal{H}_2$. As a consequence, we prove that if $G \in \mathcal{H}_1$, then $ak(G) = 4$. Moreover, if $G \in \mathcal{H}_2$, we give the condition to judge that the anti-Kekulé number of graph G is 4 or 5.

2 Definitions and preliminary results

Let $G = (V, E)$ be a simple and connected plane graph with vertex set $V(G)$ and edge set $E(G)$. For $V' \subseteq V(G)$, $G - V'$ denotes the subgraph obtained from G by deleting the vertices in V' together with their incident edges. If $V' = v$, we write $G - v$. Similarly, for $E' \subseteq E(G)$, $G - E'$ denotes the graph with vertex set $V(G)$ and edge set $E(G) - E'$. If $E' = e$, we write $G - e$. Let V' be a non-empty set; $G[V']$ denotes the induced subgraph of G induced by the vertices of V'; similarly, if $E' \subseteq E(G)$, $G[E']$ denotes the induced subgraph of G induced by the edges of E'.

For a subgraph H of G, the induced subgraph of G induced by vertices of $V(G) - V(H)$ is denoted by $\bar{H}$. A plane graph G partitions the rest of the plane into a number of arcwise-connected open sets. These sets are called the *faces* of G. A face is said to be *incident* with the vertices and edges in its boundary, and two faces are *adjacent* if their boundaries have an edge in common. Let $F(G)$ be the set of the faces of G.

An *edge-cut* of a connected plane graph G is a subset of edges $C \subseteq E(G)$ such that $G - C$ is disconnected. A *k-edge-cut* is an edge-cut with k edges. A graph G is *k-edge-connected* if G cannot be separated into at least two components by removing less than k edges. An edge-cut C of a graph G is *cyclic* if its removal separates two cycles. A graph G is *cyclically k-edge-connected* if G cannot be separated into at least two components, each containing a cycle, by removing less than k edges. A cycle is called a facial cycle if it is the boundary of a face.

For subgraphs H_1 and H_2 of a plane graph G, $E(H_1, H_2) = E(V(H_1), V(H_2))$ represents the set of edges whose two end vertices are in $V(H_1)$ and $V(H_2)$ separately. If $V(H_1)$ and $V(H_2)$ are two non-empty disjoint vertex subsets such that $V(H_1) \cup V(H_2) = V(G)$, then $E(H_1, H_2)$ is an edge-cut of G, and we simply write $\nabla(H_1) = \nabla(V(H_1))$ or $\nabla(H_2) = \nabla(V(H_2))$. We use $\partial(G)$ to denote the *boundary* of G, that is, the boundary of the infinite face of G.

A *matching* M of a graph G is a set of edges of G such that no two edges from M have a vertex in common. A matching M is *perfect* if it covers every vertex of G. A *perfect matching* is also called a Kekulé structure in chemistry.

Let G be a connected graph with at least one perfect matching. For $S \subseteq E(G)$, we call S an *anti-Kekulé* set if $G - S$ is connected but has no perfect matchings. The smallest cardinality of anti-Kekulé sets of G is called the *anti-Kekulé number* and denoted by $ak(G)$.

For the edge connectivity of the {(3, 4), 4}-fullerene, we have the following results.

Lemma 2.1. ((Yang et al., 2023) *Lemma 2.3*) *Every* {(3, 4), 4}-*fullerene is cyclically 4-edge-connected.*

Lemma 2.2. ((Yang et al., 2023) *Corollary 2.4*) *Every* {(3, 4), 4}-*fullerene is 4-edge-connected.*

Q_n is the graph consisting of n concentric layers of quadrangles, capped on each end by a cap formed by four triangles which share a common vertex as shown in Figure 2. In particular, Q_0 is what we call an octahedron (see Figure 5F).

Lemma 2.3. ((Yang et al., 2023) *Lemma 2.5*) *If G has a cyclical 4-edge-cut* $E = \{e_1, e_2, e_3, e_4\}$, *then* $G \cong Q_n$ $(n \geq 1)$, *where the four edges* e_1, e_2, e_3, *and* e_4 *form a matching, and each* e_i *belongs to the intersection of two quadrilateral faces for* $i = 1, 2, 3, 4$.

Tutte's theorem plays an important role in the process of proof.

Theorem 2.4. (Lovász and Plummer, 2009) *(Tutte's theorem) A graph G has a perfect matching if and only if for any* $X \subseteq V(G)$, $o(G - X) \leq |X|$, *where* $o(G - X)$ *denotes the number of odd components of* $G - X$.

Here, an odd component of $G - X$ is *trivial* if it is just a single vertex and *non-trivial* otherwise.

All graph-theoretical terms and concepts used but unexplained in this article are standard and can be found in many textbooks, such as Lovász and Plummer (2009).

3 Main results

From now on, let G always be a {(3, 4), 4}-fullerene; we called a 4-edge-cut E in G *trivial* if $E = \nabla(v)$, that is, E consists of the four edges incident to v. By Lemma 2.3, if E is a cyclical 4-edge-cut, then the four edges in E form a matching. Moreover, if E is not a cyclical 4-edge-cut, then E is trivial. So, we have the following lemma.

Lemma 3.1. *Let G be a* {(3, 4), 4}-*fullerene,* $E = \{e_1, e_2, e_3, e_4\}$ *be an 4-edge-cut, but it is not cyclical, then E is trivial.*

Proof. Since $E = \{e_1, e_2, e_3, e_4\}$ is an 4-edge-cut, $G - E$ is not connected. Then, $G - E$ has at least two components. Moreover, as G is 4-edge-connected by Lemma 2.2, $G - E$ has at most two components. So, $G - E$ has exactly two components.

Let G_1, G_2 be two components of $G - E$. Since E is not cyclical, without loss of generality, we suppose that G_1 is a forest; then, we have

$$n - e = l, \tag{1}$$

where n, e, l is the number of vertices, edges, and trees in G_1, respectively. Furthermore, since each vertex of G is of degree 4, we have

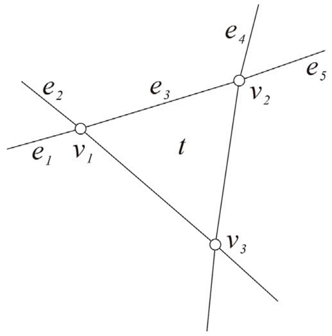

FIGURE 1
Edges e_1e_2, e_3, e_4, and e_5.

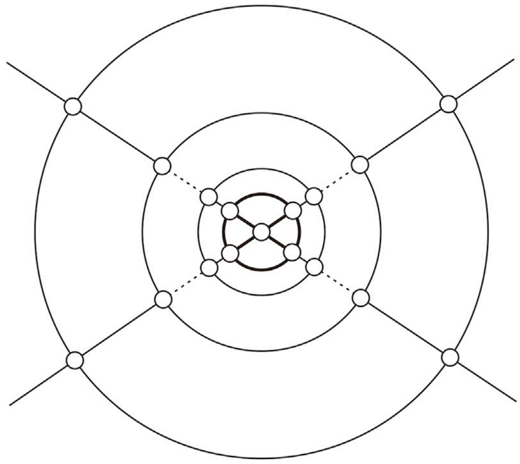

FIGURE 2
{(3,4),4}-Fullerene Q_n, where the bold segments indicate the cap of Q_n ($n \geq 0$).

$$4n - 4 = 2e. \tag{2}$$

Combing with equalities 1) and 2), we know $n = l = 1$ and $e = 0$, which means G_1 only consists of a single vertex. So, E is trivial. □

Lemma 3.1 plays an important role in the proof of the following theorem. Next, we explore the scope of the anti-Kekulé number of {(3, 4), 4}-fullerene.

Theorem 3.2. *Let G be a* {(3, 4), 4}*-fullerene, then* $4 \leq ak(G) \leq 5$.

Proof. First, we show $ak(G) \leq 5$. Let t be any triangle in G and the boundary of t was labeled $v_1v_2v_3$ along the clockwise direction. Denote the other two edges incident to v_1 (v_2) by e_1, e_2 (e_4, e_5), set $e_3 = v_1v_2$, then e_1, e_2, e_3, e_4, and e_5 are pairwise different, set $E' = \{e_1, e_2, e_3, e_4, e_5\}$ (see Figure 1) and $G' = G - E'$.

In order to show $ak(G) \leq 5$, we only need to prove that G' is connected and has no perfect matchings. Then, G' has no perfect matchings since the two edges v_1v_3, v_2v_3 cannot be covered by a perfect matching at the same time in G'.

In the following, we show that G' is connected. We proved this using reduction to absurdity, suppose G' is not connected, then G' has a component (say G_1) containing vertices v_1, v_2, and v_3, as v_1, v_2, and v_3 are connected by the path $v_1v_3v_2$ in G_1. On the other hand, since $e_3 = v_1v_2$ connects two vertices v_1, v_2 in G and $E' = \{e_1, e_2, e_3, e_4, e_5\}$ is an edge cut of G, even if we remove five edges, e_1, e_2, e_3, e_4, and e_5, to disconnect G, it is actually the same as removing four edges, e_1, e_2, e_4, and e_5 (see Figure 1); that is, $E_1 = \{e_1, e_2, e_4, e_5\}$ is an 4-edge-cut. Moreover, due to Lemma 2.3, E_1 cannot be a cyclical 4-edge-cut as e_1, e_2, e_4, and e_5 is not a matching. Then, according to Lemma 3.1, E_1 is a trivial 4-edge-cut. Thus, G_1 or $\overline{G_1}$ is a single vertex, both of which are impossible by the definition of G. So G' is connected. Thus,

$$ak(G) \leq 5. \tag{3}$$

Finally, we show $ak(G) \geq 4$. By the definition of an anti-Kekulé set, suppose $E_1' = \{e_1', e_2', e_3', \ldots, e_k'\}$ was the smallest anti-Kekulé set of G, that is, $ak(G) = k$. Then, $G_1' = G - E_1'$ was connected and has no perfect matching. Hence, according to Theorem 2.4, there exists a non-empty subset $X_0 \subseteq V(G_1')$ such that $o(G_1' - X_0) > |X_0|$, since $|V(G_1')| = |V(G)|$ and $|V(G)|$ is even, $o(G_1' - X_0)$ and $|X_0|$ have the same parity. Consequently,

$$o(G_1' - X_0) \geq |X_0| + 2 \tag{4}$$

For the sake of convenience, we let $\alpha = o(G_1' - X_0)$. If we chose an X_0 with the maximum size, then $G_1' - X_0$ has no even components. On the contrary, we suppose there exists an even component (say F) of $G_1' - X_0$. For any vertex $v \in V(F)$, $o(F - v) \geq 1$. Let $X' = X_0 \cup \{v\}$, thus $o(G_1' - X') = o(G_1' - X_0)$ $+o(F - v) \geq |X_0| + 2 + 1 = |X'| + 2$, which is a contradiction to the choice of X_0.

In addition, E_1' is the smallest anti-Kekulé set of G, then $G_1' + e_i'$ has perfect matchings for any edge $e_i' \in E_1'$ for $1 \leq i \leq k$. On the other hand, the number of odd components of $G_1' - X_0$ was not decreased or decreased by at most one or two if we add one edge e_i' to G_1', that is,

$$|X_0| \geq o(G_1' + e_i' - X_0) \geq \alpha\text{-}2. \tag{5}$$

By inequality (4), we have

$$|X_0| \leq \alpha\text{-}2. \tag{6}$$

Combined with inequalities (5) and (6), we have $\alpha = |X_0| + 2$ and each edge $e_i' \in E_1'$ connects two odd components of $G_1' - X_0$. Let $H_1, H_2, H_3, \ldots, H_\alpha$ be the odd components of $G_1' - X_0$. Then, due to Lemma 2.2, $|\nabla(H_i)| \geq 4$ $(1 \leq i \leq \alpha)$; therefore,

$$4\alpha - 2k \leq \sum_{i=1}^{\alpha} |\nabla(H_i)| - 2|E_1'| \leq 4|X_0| = 4(\alpha - 2). \tag{7}$$

Thus, $k \geq 4$, that is, $ak(G) \geq 4$. We know that $4 \leq ak(G) \leq 5$.

By Theorem 3.2, we know that $4 \leq ak(G) \leq 5$. Next, we give the characterization of {(3, 4), 4}-fullerenes with anti-Kekulé number 4. Before, we define $\mathcal{H}_1 = \{Q_n \mid n \geq 0\}$, where Q_n is shown in Figure 2. The structure of two adjacent triangles is called a *diamond*. In a diamond, the common edge of the two triangles is called the *diagonal edge*. The subgraph consisting of four diamonds such that the four diagonal edges form a matching is denoted by D, that is, $D = \bigcup_{i=1}^{4} D_i$ (see Figure 7D for the four diamonds $D_1 - D_4$). Let $\mathcal{H}_2 = \{G | D \subseteq G\}$. So, we have the following theorem.

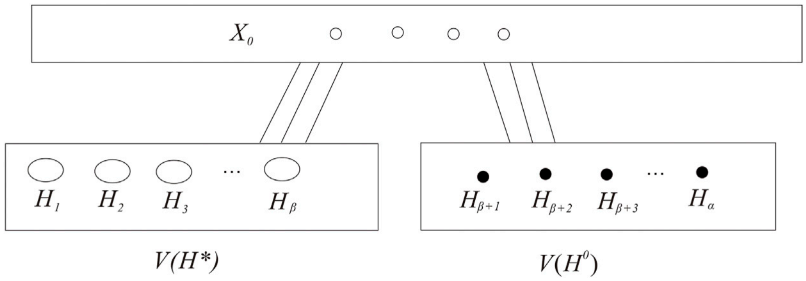

FIGURE 3
$V(G)$ is divided into X_0, $V(H^*)$, and $V(H^0)$.

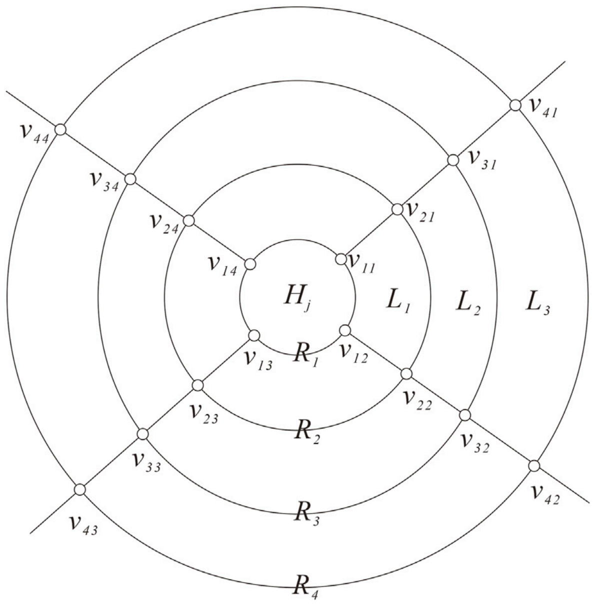

FIGURE 4
Labeling of $G[V(\overline{H_j} \cup \partial(H_j))]$.

Theorem 3.3. *Let G be a* {(3, 4), 4}*-fullerene, if* $ak(G) = 4$*, then* $G \in \mathcal{H}_1$ *or* $G \in \mathcal{H}_2$.

Proof. Let E_0 be the anti-Kekulé set of G such that $|E_0| = 4$, set $G_0 = G - E_0$. Then, G_0 is connected without perfecting matchings. Thus, by Theorem 2.4, there exists a non-empty subset $X_0 \subseteq V(G_0)$ such that $o(G_0 - X_0) > |X_0|$. For convenience, let $\alpha = o(G_0 - X_0)$, since α and $|X_0|$ have the same parity, that is,

$$\alpha \geq |X_0| + 2. \tag{8}$$

We choose an X_0 satisfying Ineq. (8) with the maximum size. Then, a proof similar to the proof of Theorem 3.2 is used to prove $ak(G) \geq 4$. We can know $G_0 - X_0$ has no even components. Let $H_1, H_2, H_3, \ldots, H_\alpha$ be all the odd components of $G_0 - X_0$, set $H = \cup_{i=1}^{\alpha} H_i$.

Let H_1, H_2, H_3, …, H_β be the non-trivial odd components of $G_0 - X_0$, set $H^* = \cup_{i=1}^{\beta} H_i$. Let $H_{\beta+1}, H_{\beta+2}, H_{\beta+3}, \ldots, H_\alpha$ be the trivial odd components of $G_0 - X_0$, set $H^0 = \cup_{i=\beta+1}^{\alpha} H_i$. Then, $V(G)$ is divided into X_0, $V(H^*)$, $V(H^0)$(see Figure 3 the partition of $V(G)$).

Since $ak(G) = 4$, all equalities in Ineq. (7) of Theorem 3.2 hold. The first equality in Ineq. (7) holds if and only if $|\nabla(H_i)| = 4\,(1 \leq i \leq \alpha)$, and the second equality in Ineq. 7) holds if and only if there is no edge in the subgraph $G_0[X_0]$; that is, X_0 is an independent set of G_0. Moreover, each edge of E_0 connects two components in H and $|X_0| = \alpha - 2$. Since $|\nabla(H_j)| = 4$ $(1 \leq j \leq \alpha)$, $\nabla(H_j)$ is a cyclical 4-edge-cut of G or not.

Next, we distinguish the following two cases to complete the proof of Theorem 3.3.

Case 1: There exists one H_j such that $\nabla(H_j)$ is a cyclical 4-edge-cut.

By Lemma 2.3, $G \cong Q_n$ $(n \geq 1)$, which means the four edges of $\nabla(H_j)$ form a matching. Without loss of generality, we supposed H_j consists of s layers of quadrangular faces and the cap of H_j is entirely in the interior of the boundary cycle $\partial(H_j)$. Then, $G[V(\overline{H_j} \cup \partial(H_j))]$ induced by the vertices of $\overline{H_j}$ and the boundary of $\partial(H_j)$ consists of $n - s$ layers of quadrangular faces and a cap, for convenience, set $m = n - s$, let $L_1, L_2, L_3, \ldots, L_m$ be all the layers and C be the cap of $G[V(\overline{H_j} \cup \partial(H_j))]$, where quadrangular layer L_i is adjacent to L_{i-1} and L_{i+1} for $2 \leq i \leq m - 1$, L_1 is adjacent to H_j, and L_m is adjacent to C. Set $R_1 = H_j \cap L_1$ and $R_{m+1} = C \cap L_m$. For $2 \leq i \leq m$, let $R_i = L_{i-1} \cap L_i$. The vertices on R_i $(i = 1, 2, 3, \ldots, m+1)$ are recorded as v_{i1}, v_{i2}, v_{i3}, and v_{i4} $(i = 1, 2, 3, \ldots, m+1)$ in a clockwise direction and v_{i1}, v_{i3}, and v_{i2}, v_{i4}, are on the same line, respectively (see Figure 4). Since $\nabla(H_j)$ is a cyclical 4-edge-cut, set $\nabla(H_j) = \{e_1', e_2', e_3', e_4'\}$. Without loss of generality, set $e_i' = v_{1i}v_{2i}$ $(1 \leq i \leq 4)$. The vertices shared by the four triangles on the two caps are represented by v', v'', respectively, such that v' is in H_j and v'' is in $\overline{H_j}$.

Next, we analyze whether the edges of $\nabla(H_j)$ belongs to E_0 or not, which is divided into the following five subcases.

Subcase 1.1: All the edges of $\nabla(H_j)$ belong E_0.

That is, $e_i' \in E_0$ for all $i = 1, 2, 3, 4$. Since each edge of E_0 connects two components of H and there are four edges e_1', e_2', e_3', e_4' belonging to E_0. All the vertices of $\overline{H_j}$ belong to $V(H^*)$, which means $X_0 = \varnothing$, a contradiction.

Subcase 1.2: Exactly three edges of $\nabla(H_j)$ belong to E_0.

Without loss of generality, suppose $e_1', e_2', e_3' \in E_0$, then $v_{24} \in X_0$ and $v_{21}, v_{22}, v_{23} \in V(H)$, that is, v_{21}, v_{22}, v_{23} belong to $V(H^*)$ or $V(H^0)$.

If all of v_{21}, v_{22}, and v_{23} belong to $V(H^0)$, then $v_{21}v_{22}, v_{22}v_{23} \in E_0$, immediately $|E_0| > 4$, which contradicts $|E_0| = 4$. This contradiction means at least one of v_{21}, v_{22}, and v_{23} belongs to $V(H^*)$ (say $V(H_1)$),

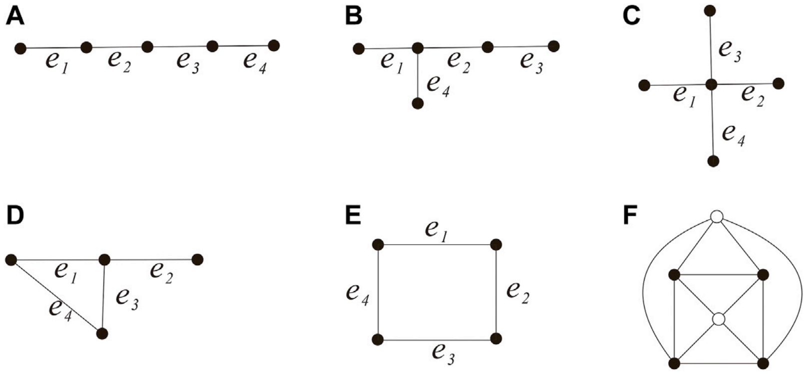

FIGURE 5
$G[E_0]$ has one component and the {(3,4),4}-fullerene Q_0 **(A–F)**.

then by Lemma 2.3 and Lemma 3.1, either $\nabla(H_1)$ is a cyclical 4-edge-cut and the four edges in $\nabla(H_1)$ form a matching or $\nabla(H_1)$ is trivial. However, since H_1 is a non-trivial odd component of $G_0 - X_0$, $|V(H_1)| \geq 3$. Thus, $\nabla(H_1)$ is not a trivial 4-edge-cut. That is, $\nabla(H_1)$ is a cyclical 4-edge-cut, and the four edges in $\nabla(H_1)$ form a matching. Now, if v_{21} (or v_{23}) belong to $V(H_1)$, then $v_{21}v_{24}$, $v_{21}v_{11}$ (or $v_{23}v_{24}$, $v_{23}v_{13}$) belong to $\nabla(H_1)$, but they do not form a matching, a contradiction. Thus, both $v_{21}, v_{23} \in V(H^0)$ and $v_{22} \in V(H_1)$. Immediately, we have $v_{21}v_{22}$, $v_{22}v_{23} \in E_0$ and $|E_0| > 4$, which contradicts $|E_0| = 4$. This contradiction means there cannot be three edges of $\nabla(H_j)$ belonging to E_0.

Subcase 1.3: Exactly two edges of $\nabla(H_j)$ belong to E_0.

Then, by symmetry, $e_1', e_2' \in E_0$ or $e_1', e_3' \in E_0$.

First, if $e_1', e_2' \in E_0$, then $v_{23}, v_{24} \in X_0$ and $v_{23}v_{24} \in E(X_0)$, which contradicts that $E(X_0) = \varnothing$.

Claim 1: For a quadrangular face q with $\partial(q) = abcda$ with clock direction such that $a \in X_0, b \in V(H^0)$, then $c, d \in V(H^0)$ or $c, d \in V(H^*)$ or $c \in X_0, d \in V(H^0)$.

Proof. Since $E(X_0) = \varnothing$, $d \in V(H^0) \cup V(H^*)$. If $d \in V(H^0)$, then $c \notin V(H^*)$ by Lemma 2.3 and Lemma 3.1, thus $c \in X_0$ or $c \in V(H^0)$.

If $d \in V(H^*)$, then also by Lemma 2.3 and Lemma 3.1, we can know $c \in V(H^*)$ and the claim holds.

By Claim 1, next, if $e_1', e_3' \in E_0$, then $v_{22}, v_{24} \in V(X_0)$, $v_{21}, v_{23} \in V(H)$. If all the vertices of v_{21}, v_{22}, v_{23}, and v_{24} belong to the cap of $\overline{H_j}$, that is, all of v_{21}, v_{22}, v_{23}, and v_{24} are adjacent to v'', then as $|E_0| = 4$ and $e_1', e_3' \in E_0$, we can know $v'' \in H^0$ and $v_{21}v''$, $v_{23}v'' \in E_0$, and we have the {(3, 4), 4}-fullerenes Q_{s+1}, that is, $m = 1$.

If all the vertices of v_{21}, v_{22}, v_{23}, and v_{24} do not belong to the cap of $\overline{H_j}$, that is, the layer L_2 consists of four quadrangular faces, then, for the quadrangular face $q \in F(L_2)$, the vertices on $\partial(q)$ belong to X_0, H^0, H^0, H^0 or X_0, H^0, H^*, H^* or X_0, H^0, X_0, H^0 by Claim 1.

If the former case holds, that is, there exists one face $q \in F(L_2)$ such that the boundary of q is of the form X_0, H^0, H^0, and H^0, then immediately we can have $|E_0| > 4$, a contradiction.

If the second case holds, that is, there exists one face $q \in F(L_2)$ such that the boundary of q is of the form X_0, H^0, H^*, and H^*, then by Claim 1 and since $|E_0| = 4$, we can know all the faces of L_2 are of the form X_0, H^0, H^*, and H^*, that is, all the vertices of $\overline{H_j \cup L_1}$ belong to $V(H^*)$. In this case, we also have $G \in \mathcal{H}_1$.

By the aforementioned discussion and Claim 1, next, we suppose all the quadrangular faces of L_2 are of the form X_0, H^0, X_0, and H^0. Then, we can use the aforementioned same analysis to the layer L_3 as L_2, since $G \cong Q_n$ and H_j consists of s layers of quadrangular faces; after finite steps (say t steps), we obtain t layers $L_2, L_3, \ldots, L_{t+1}$ such that all the faces of L_i $(2 \leq i \leq t+1)$ are of form X_0, H^0, X_0, and H^0 and either the four vertices on $\partial(R_{t+2})$ are adjacent to v'' $(v'' \in V(H^0))$ or all the vertices of $\overline{H_j \cup L_1 \cup L_2 \cup \cdots \cup L_{t+1}}$ belong to $V(H^*)$.

If the four vertices on $\partial(R_{t+2})$ are adjacent to v'' $(v'' \in V(H^0))$, then $m = t + 1$, $n = s + t + 1$ and $G \in \mathcal{H}_1$. If all the vertices of $\overline{H_j \cup L_1 \cup L_2 \cup \cdots \cup L_{t+1}}$ belong to $V(H^*)$ (say $V(H_1)$), suppose H_1 consists of p layers of quadrangular faces, then $m = t + p + 2$, $n = s + t + p + 2$, and also $G \in \mathcal{H}_1$.

To sum up, if exactly two edges of $\nabla(H_j)$ belong to E_0, then $G \in \mathcal{H}_1$.

Subcase 1.4: Exactly one edge of $\nabla(H_j)$ belong to E_0.

Without loss of generality, suppose $e_1' \in E_0$, then v_{22}, v_{23}, $v_{24} \in X_0$, $v_{22}v_{23}, v_{23}v_{24} \in E(X_0)$, which contradicts that X_0 is an independent set of G_0.

Subcase 1.5: No edge of $\nabla(H_j)$ belongs to E_0.

Thus, $\bigcup_{i=1}^{4} v_{2i} \subseteq X_0$, so $v_{21}v_{22}, v_{22}v_{23}, v_{23}v_{24}, v_{24}v_{21} \in E(X_0)$, which contradicts $E(X_0) = \phi$.

Case 2: $\nabla(H_j)$ is not a cyclical 4-edge-cut of G for all $1 \leq j \leq \alpha$.

For convenience, set $E_0 = \{e_1, e_2, e_3, e_4\}$. Here, first, we give the idea of proof, then we will show that $G_0 = G - E_0$ is bipartite by proving $|V(H_i)| = 1$ $(1 \leq i \leq \alpha)$. Since G has exactly eight triangular faces and $|E_0| = 4$, which implies that each edge e_i of E_0 is the common edge of two triangles, by discussing all possible subgraphs formed by facial cycles containing an edge of E_0, we show that $G \in \mathcal{H}_1$ or $G \in \mathcal{H}_2$.

Since $\nabla(H_j)$ is not a cyclical 4-edge-cut of G for all $1 \leq j \leq \alpha$, H_j or $\overline{H_j}$ is a singleton by Lemma 3.1. Since X_0 is non-empty and $\alpha = |X_0| + 2$, which means H_j is a singleton vertex, that is, $|V(H_j)| = 1$ $(1 \leq j \leq \alpha)$.

Let Y_0 denote the set of all singletons y_i from each H_i $(1 \leq i \leq \alpha)$, and denote the vertices of X_0 by x_i $(1 \leq i \leq |X_0|)$, so $G_0 = (X_0, Y_0)$ is bipartite. For convenience, we color the vertices white in X_0 and black in Y_0.

Next, we consider possible subgraphs of G containing all edges of E_0. By the Euler theorem, G has exactly eight triangular faces

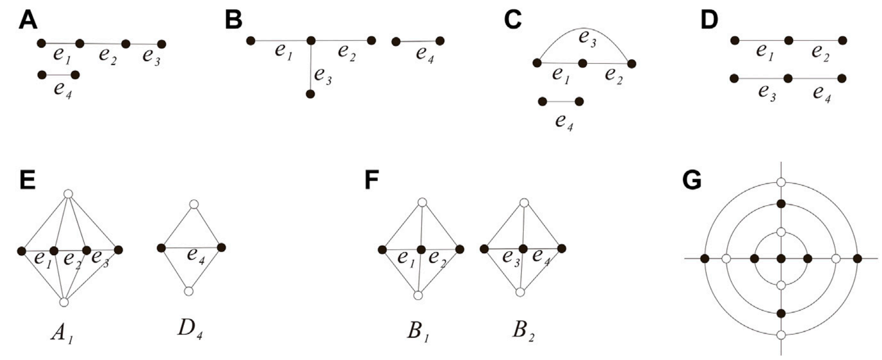

FIGURE 6
$G[E_0]$ has two components and the {(3,4),4}-fullerenes Q_l $(l \geq 1)$ **(A–G)**.

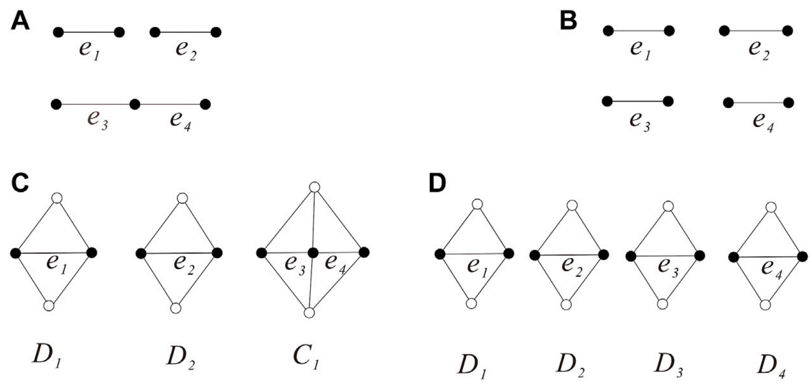

FIGURE 7
$G[E_0]$ has three components **(A,C)** or four components **(B,D)**.

because $G_0 = (X_0, Y_0)$ is bipartite; each edge e_i of E_0 is the common edge of two triangles and connects two vertices in Y_0, that is, every edge $e_i \in E_0$ belongs to a diamond, say D_i, i = 1, 2, 3, 4 and $F(D_i) \cap F(D_j) = \varnothing$ $(i \neq j, i, \quad j = 1, 2, 3, 4)$.

Claim 2: If $G[E_0]$ has one component, then $G \cong Q_0$, where Q_0 is the octahedron.

Proof. If $G[E_0]$ has one component, then we have the subgraphs shown in Figures 5A, B, C) if $G[E_0]$ is a tree and Figures 5D, E if $G[E_0]$ has cycles. If $G[E_0]$ is isomorphism to the graph shown in Figure 5A, then the two diamonds D_1, D_2 are adjacent and they form one cap of Q_n. Set $D_{12} = D_1 \cup D_2$, then $\nabla(D_{12})$ forms an 4-edge-cut. On the other hand, by Lemma 2.3 and Lemma 3.1, $\nabla(D_{12})$ is a cyclical 4-edge-cut and $G \cong Q_p$ or $\nabla(D_{12})$ is trivial. If $\nabla(D_{12})$ is a cyclical 4-edge-cut, then $G \cong Q_p\,(p \geq 1)$ and e_3 belongs to a quadrangular face, which contradicts that the two faces containing e_3 are triangles. If $\nabla(D_{12})$ is a trivial 4-edge-cut, that is, $\overline{D_{12}}$ is a singleton, which is impossible as the two vertices of e_4 belong to $V(\overline{D_{12}})$. Thus, $G[E_0]$ cannot be isomorphism to the subgraph shown in Figure 5A. All the situations of Figures 5B–D contradicts $F(D_i) \cap F(D_j) = \varnothing$ $(i \neq j, i, \quad j = 1, 2, 3, 4)$.

If $G[E_0]$ is isomorphic to the graph shown in Figure 5E, then in order to guarantee $F(D_i) \cap F(D_j) = \varnothing$ $(i \neq j, i, \quad j = 1, 2, 3, 4)$, the four diamonds D_1, D_2, D_3, and D_4 forms two caps of Q_n such that the cycle induced by E_0 is exactly the intersecting of the two caps. Immediately, we have the graph Q_0 (see Figure 5F the octahedron Q_0), that is, $G \cong Q_0$ if $G[E_0]$ has one component, so $G \in \mathcal{H}_1$.

In accordance with Claim 2, next, we assume that $G[E_0]$ is not connected, so $G[E_0]$ has at least two and at most four components. Then, we have the following three cases.

Subcase 2.1: $G[E_0]$ has exactly two components.

By symmetry, the subgraph induced by E_0 has four cases as shown in Figures 6A–D. Then, the graph G which contains the subgraphs shown in Figure 6B contradicts $F(D_i) \cap F(D_j) = \varnothing$ $(i \neq j, i, \quad j = 1, 2, 3, 4)$. If G contains the subgraph shown in Figure 6C, then the three edges e_1, e_2, and e_3 belong to the same triangular face as every 3-length cycle of a {(3, 4), 4}-fullerene must be the boundary of a triangular face by Lemma 2.2, which contradicts that $F(D_i) \cap F(D_j) = \varnothing$ $(i \neq j, i, \quad j = 1, 2, 3, 4)$.

If $G[E_0]$ is isomorphic to the graph as shown in Figure 6A, then the three edges e_1, e_2, and e_3 belong to three diamonds D_1, D_2, and D_3, respectively, and we have the subgraph A_1 consisting of D_1, D_2, and D_3 (see Figure 6E) such that $|\nabla(A_1)| = 2$ and A_1, D_4 are disjoint. By the definition of G, we can know the two 3-degree vertices on

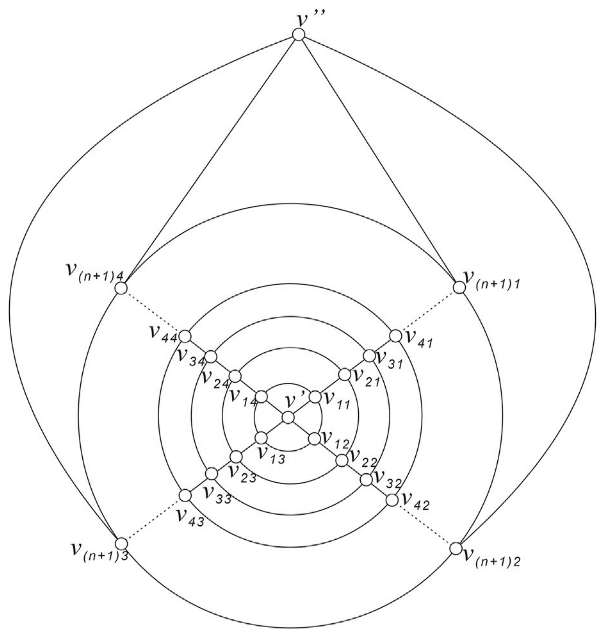

FIGURE 8
{(3,4),4}-Fullerenes Q_n.

$\partial(A_1)$ must be adjacent and we obtain $G \cong Q_0$, which contradicts that A_1, D_4 are disjoint.

If $G[E_0]$ is isomorphic to the graph as shown in Figure 6D, then D_1, D_2 are adjacent, and D_3, D_4 are adjacent. Set $B_1 = D_1 \cup D_2$, $B_2 = D_3 \cup D_4$. Since the two edges e_1, e_2 are disjoint, the edges e_3, e_4, B_1, B_2 are disjoint. Then, $\nabla(B_i)$ $(i = 1, 2)$ forms a cyclical 4-edge-cut (see Figure 6F), by Lemma 2.3, $G \cong Q_l\,(l \geq 1)$.

Since $G_0 = (X_0, Y_0)$ is bipartite, it should be noted that each edge e_i of E_0 is in these eight triangles and connects two vertices in Y_0; thus, the edges of $E(G) - E(B_1) - E(B_2)$ are X_0Y_0 − edges and $G - B_1 - B_2$ has only quadrangles (see Figure 6G). Moreover, by Lemma 2.3, we can know $G - B_1 - B_2$ consists of $l - 2$ $(l \geq 2)$ layers of quadrangles (each layer is made up of four quadrangles). Thus, we have $G \in \mathcal{H}_1$.

Subcase 2.2: $G[E_0]$ has exactly three components.

Then, both of the two components of $G[E_0]$ are K_2, and one component is $K_{1,2}$ (see Figure 7A). Without loss of generality, we suppose the component $K_{1,2}$ is induced by the edges e_3, e_4. Then, the two diamonds D_3, D_4 are adjacent, and D_1, D_2 are disjoint. Set $C_1 = D_3 \cup D_4$ (see Figure 7C).

Then, due to Lemma 2.3 and Lemma 3.1, $\nabla(C_1)$ forms a cyclical 4-edge-cut, thus, $G \cong Q_s$, where Q_s is the tubular $\{(3,4),4\}$-fullerene as shown in Figure 2, which means each of the two caps of Q_s must contain two adjacent diamonds, contradicts that D_1, D_2 are disjoint.

Subcase 2.3: $G[E_0]$ has four components.

Then, the four diagonal edges e_1, e_2, e_3, and e_4 are disjoint (see Figure 7B), that is, the four diamonds D_1, D_2, D_3, and D_4 cannot intersect at the diagonal edges. We have the four diamonds D_1, D_2, D_3, and D_4 as shown in Figure 7D. Then, $G \in \mathcal{H}_2$.

So far, we have completed the proof of Theorem 3.3.

Inspired by Theorem 3.3, we immediately get the following theorems.

Theorem 3.4. *Let G be a {(3, 4), 4}-fullerene, if* $G \in \mathcal{H}_1$, *then* $ak(G) = 4$.

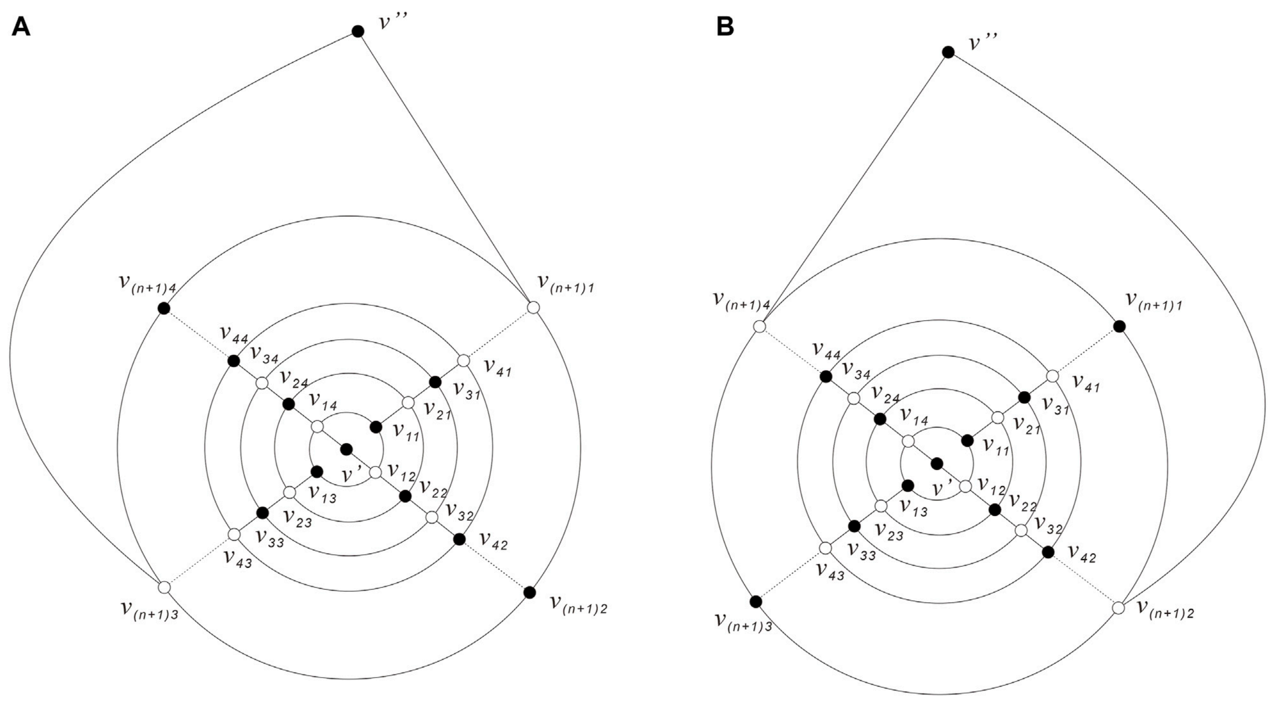

FIGURE 9
Graph $G - E_0$; n is an odd number **(A)**, and n is an even number **(B)**.

Proof. Let $G \in \mathcal{H}_1$, that is, $G \cong Q_n$ $(n \geq 0)$. By Theorem 3.2 and the definition of the anti-Kekulé number, we only need to find an anti-Kekulé set E_0 of G such that $|E_0| = 4$.

For convenience, let the plane embedding graph of Q_n as shown in Figure 8. Q_n consist of $n+1$ concentric rings with four vertices on each ring and two vertices on two caps; these $n+1$ concentric rings are recorded as $R_1, R_2, R_3, \ldots, R_{n+1}$ from the inside to the outside. Next, the vertices of Q_n are labeled as follows: the vertices shared by the four triangles on the two caps are represented by v', v'', respectively, and the vertices on R_i $(i = 1, 2, 3, \ldots, n+1)$ are recorded as v_{i1}, v_{i2}, v_{i3}, and v_{i4} $(i = 1, 2, 3, \ldots, n+1)$ in a clockwise direction such that v_{i1}, v_{i3} (v_{i2}, and v_{i4}) are on the same line (see Figure 8 the labeling of Q_n).

Next, we will prove Theorem 3.4 in two cases.

Case 1: n is an odd number.

Let $E_0 = \{v'v_{11}, v'v_{13}, v''v_{n+1,2}, v''v_{n+1,4}\}$ (see Figure 9A), and set $G_1 = G - E_0$. Then, E_0 is not a cyclically 4-edge-cut of G by Lemma 2.3. Moreover, E_0 is not a trivial 4-edge-cut as the four edges in E_0 are not incident with a common vertex. That is, G_1 is connected.

Then, we prove that $G_1 = G - E_0$ has no perfect matching, and there are only quadrangular faces in G_1, so, G_1 is bipartite. We color the vertices of G_1 with black and white such that adjacent vertices in G_1 are assigned two distinct colors (see Figure 9A). Let M_0 denote the set of white vertices and N_0 denote the set of black vertices, then $G_1 = G_1(M_0, N_0)$, $|M_0| = 2n+2$, $|N_0| = 2n+4$. In accordance with Theorem 2.4, there exist $M_0 \subseteq V(G_1)$ such that $o(G_1 - M_0) = |N_0| = 2n+4 > |M_0| = 2n+2$, so G_1 has no perfect matching.

Case 2: n is an even number.

Let $E_0 = \{v'v_{11}, v'v_{13}, v''v_{n+1,1}, v''v_{n+1,3}\}$ (see Figure 9B), and set $G_2 = G - E_0$. Also, G_2 is connected.

There are only quadrangular faces in G_2; so, G_2 is also bipartite with one bipartition $2n+2$ vertices and the other bipartition $2n+4$ vertices, which means G_2 has no perfect matching.

Therefore, we find the anti-Kekulé set E_0 of G with $|E_0| = 4$, which means $ak(G) = 4$, if $G \in \mathcal{H}_1$.

Due to Theorem 3.4, if $G \in \mathcal{H}_1$, then $ak(G) = 4$. However, the anti-Kekulé number of G can be 4 or 5 if $G \in \mathcal{H}_2$. Next, we use a method to judge whether the anti-Kekulé number of G can be 4 or 5 when $G \in \mathcal{H}_2$. Before we give some definitions of G if $G \in \mathcal{H}_2$. Let $G \in \mathcal{H}_2$, the four diamonds of G be D_1, D_2, D_3, and D_4 and the four diagonal edges be e_1, e_2, e_3, and e_4 such that $e_i \in E(D_i)$, $i = 1, 2, 3, 4$. Set $E_0 = \{e_1, e_2, e_3, e_4\}$ and $e_1 = v_1v_2$, $e_2 = v_3v_4$, $e_3 = v_5v_6$, and $e_4 = v_7v_8$. The eight vertices of the four diagonal edges are called eight *stars*, and their union is denoted by $V_0 = \bigcup_{i=1}^{8} v_i$.

Set $G_0 = G - E_0$. Then, G_0 is bipartite, without loss of generality, we supposed the bipartitions of G_0 were V_1, V_2. Then, by the proof of Theorem 3.3, we can know if $ak(G) = 4$, then $V_0 \subset V_1$ or $V_0 \subset V_2$, which means $ak(G) = 5$ when $V_0 \not\subset V_1$ and $V_0 \not\subset V_2$. Thus, we have the following theorem.

Theorem 3.5. *Let G be a $\{(3, 4), 4\}$-fullerene, $G \in \mathcal{H}_2$, if $V_0 \subset V_1$ or $V_0 \subset V_2$, then $ak(G) = 4$, otherwise, $ak(G) = 5$.*

Proof. By Theorem 3.2, we only need to show if $V_0 \subset V_1$ or $V_0 \subset V_2$, then $ak(G) = 4$. Without loss of generality, suppose $V_0 \subset V_1$. Then, $G[V_1]$ consists of the four edges e_1, e_2, e_3, and e_4 and some singleton vertices. Since the four edges e_1, e_2, e_3, and e_4 cannot be incident with a common vertex, E_0 is not a trivial 4-edge-cut. However, E_0 also cannot be a cyclical 4-edge-cut by Lemma 2.3, as e_i belongs to the intersection of two triangular faces for $i = 1, 2, 3, 4$. Thus, $G_0 = G - E_0$ is connected.

On the other hand, by the degree-sum formula $4|V_2| = 4|V_1| - 8$, which means $|V_1| \neq |V_2|$. Thus, G_0 cannot have perfect matchings by Theorem 2.4. So, we find the anti-Kekulé set E_0 with $|E_0| = 4$. Immediately, we have $ak(G) = 4$. Otherwise, by Theorem 3.2, $ak(G) = 5$.

By Theorem 3.5, for a $\{(3, 4), 4\}$-fullerene G with $G \in \mathcal{H}_2$, we can give the method to judge the anti-Kekulé number of graph G is 4 or 5 as follows:

Step 1: Delete the four diagonal edges e_1, e_2, e_3, and e_4.
Step 2: Color the vertices of $G_0 = G - \{e_1, e_2, e_3, e_4\}$ with black and white.
Step 3: If we find the eight stars are in the same color, then $ak(G) = 4$, otherwise, $ak(G) = 5$.

4 Conclusion

In this paper, we have obtained the scope of the anti-Kekulé number of $\{(3, 4), 4\}$-fullerenes in Theorem 3.2; at the same time, we characterized $\{(3, 4), 4\}$-fullerenes with anti-Kekulé number 4 in Theorem 3.3, which includes two kinds of graphs $\mathcal{H}_1, \mathcal{H}_2$.

As a consequence, we proved that if $G \in \mathcal{H}_1$, then $ak(G) = 4$. Interestingly, by the proof of Theorem 3.3, we found the $\{(3, 4), 4\}$-fullerene G belongs to $\mathcal{H}_2$, but the anti-Kekulé number of G is not always 4; therefore, at the end of this paper, we gave a condition for judging whether the anti-Kekulé number of graph G is 4 or 5.

Data availability statement

The original contributions presented in the study are included in the article/Supplementary Material, further inquiries can be directed to the corresponding author.

Author contributions

RY performed the ideas and the formulation of overarching research goals and aims. HJ wrote the first manuscript draft and performed the review and revision of the first draft.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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