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The Clar Number of Fullerenes on Surfaces*

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Abstract

There are only four surfaces in which a fullerene can be embedded: the sphere, projective plane, torus and Klein bottle. Let F be a fullerene on surface Σ. A resonant pattern of a fullerene F is a set $\mathcal{H}$ of pairwise disjoint hexagons such that $F-\mathcal{H}$ has a perfect matching. The Clar number $c(F)$ of F is the maximum cardinality of all resonant patterns of F. In this paper, as a generalization of spherical fullerenes we obtain a sharp upper bound for the Clar number of any fullerene F with n vertices on surface Σ, that is, $c(F) \leq \lfloor \frac{n}{6} \rfloor - \chi(\Sigma)$, where $\chi(\Sigma)$ stands for the Euler characteristic of Σ. Moreover, we present five families of projective fullerenes which can attain the upper bound $\frac{n}{6} - 1$, and characterize all fully-benzenoid toroidal and Klein-bottle fullerenes.

1 Introduction

The discovery of buckminsterfullerene C_{60} has generated an epidemic of new research into fullerene science. Fullerenes are closed carbon-cage molecules made up entirely of pentagons and hexagons. Their molecular graphs are finite trivalent graphs on the sphere with only hexagonal and pentagonal faces. Such structures also exist on other surfaces [7]. The Euler characteristic χ of a surface Σ is given by $\chi(\Sigma) = 2 - 2g$ if $\Sigma = S_g$, while $\chi(\Sigma) = 2 - \overline{g}$ if $\Sigma = N_{\overline{g}}$, where S_g and $N_{\overline{g}}$ are obtained from the sphere by adding

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g handles and $\overline{g}$ crosscaps respectively. From Euler's formula, one can obtain that the number of pentagons f_5 of a fullerene F on surface Σ is equal to $6\chi(\Sigma)$. So there are only four possible surfaces on which fullerenes exist, namely, the sphere S_0, projective plane N_1, torus S_1 and Klein bottle N_2 since their Euler characteristics are respectively 2, 1, 0 and 0, and the other surfaces have negative Euler characteristics. The fullerenes on these surfaces are called spherical, projective, toroidal and Klein-bottle fullerenes, respectively. Hence there are exactly 12, 6, 0 and 0 pentagons in a spherical, projective, toroidal and Klein-bottle fullerene, respectively.

Let F be a fullerene on surface Σ. A *perfect matching* (or *Kekulé structure*) M of F is a set of edges such that each vertex is incident with exactly one edge in M. A cycle of F is *M-alternating* if its edges appear alternately in and off M. A set $\mathcal{H}$ of pairwise disjoint faces of F is called a *resonant pattern* if F has a perfect matching M such that the boundary of each face in $\mathcal{H}$ is an M-alternating cycle. A *Clar set* of F is a resonant pattern with the maximum number of faces. The number of faces of a Clar set is called the *Clar number* of F, denoted by $c(F)$. A *fully-benzenoid fullerene* F is a fullerene admitting a Clar set that includes all vertices of F.

The Clar number is an important chemical index which was introduced by Clar [4] for predicting the stability of the benzenoid hydrocarbon isomers. Given two isomeric benzenoid hydrocarbons, the one with larger Clar number is both chemically and thermodynamically more stable. Hansen and Zheng [15] computed the Clar number of benzenoid hydrocarbons using integer linear programming and conjectured that the linear programming relaxation was sufficient for benzenoid hydrocarbons. Abeledo and Atkinson [1] confirmed this conjecture for general 2-connected plane bipartite graphs. This result implies that the Clar number can be computed in polynomial time for 2-connected plane bipartite graphs. Salem [24, 25] also attempted to give a combinatorial algorithm to solve the Clar problem of benzenoid hydrocarbons. However Bernáth and Kovács [3] proved that the Clar number problem is NP-complete for planar non-bipartite graphs. For other relevant researches on the Clar number, we refer to [14, 19, 26, 31].

Zhang and Ye [32] presented an upper bound of Clar number of spherical Fullerenes. A new proof was given by Hartuny [16].

Theorem 1.1. [32] *Let F be a spherical fullerene with n vertices. Then $c(F) \le \lfloor \frac{n}{6} \rfloor - 2$.*

The experimental spherical fullerenes C_{60}:1, C_{70}:1, C_{76}:1, C_{78}:1, C_{82}:3, C_{84}:22 and

C_{84}:23 attain the upper bound in Theorem 1.1, where C_n:m [9] occurs at position m in a list of lexicographically ordered spirals that describe isolated-pentagon isomers with n atoms. For buckminsterfullerene C_{60}, El-Basil [8] found that it has exactly 5 Clar sets, each of which consists of 8 hexagons. Ye and Zhang [30] gave a characterization of spherical fullerenes whose Clar numbers attain the bound $\frac{n}{6} - 2$ and constructed all 18 spherical fullerenes whose Clar numbers attain the maximum value 8 among all fullerene isomers of C_{60}. Further Zhang et al. [33] proposed a combination of Clar number and Kekulé count of spherical fullerenes, as a stability predictor of spherical fullerenes, which distinguishes uniquely the icosahedral C_{60} from its all 1812 fullerene isomers. Recently, Hartuny [16] gave another characterization of spherical fullerenes whose Clar numbers attain the bound $\frac{n}{6} - 2$.

Altshuler [2] showed that any toroidal fullerene can be determined by a unique string of three integers. For convenience, we adopt the notation $H(p, q, t)$ ($p \geq 1$, $q \geq 1$, $0 \leq t \leq p - 1$), which was introduced by Marušič and Pisanski [21], to represent a toroidal fullerene. Kirby and Pollak [18] described a simple algorithm for enumerating all isomers of a toroidal fullerene. Thomassen [29] classified Klein-bottle fullerenes with girth 6 into five classes. Li et al. [20] reclassified the five classes of Klein-bottle fullerenes into two new classes $K(p, q, t)$ and $N(p, q, t)$.

In this paper, Theorem 1.1 is extended to any fullerenes on surface Σ as follows.

Theorem 1.2. *Let F_n be a fullerene graph with n vertices on surface Σ. Then $c(F_n) \leq \lfloor \frac{n}{6} \rfloor - \chi(\Sigma)$.*

In Section 2 of this paper, we will present the proof of Theorem 1.2. We say a fullerene with n vertices on a surface Σ *extremal* if the Clar number of the fullerene attains the bound $\frac{n}{6} - \chi(\Sigma)$. In addition to the experimental extremal spherical fullerenes pointed out previously, Zhang and Ye [32] constructed infinitely many examples of extremal fullerenes in zigzag and armchair carbon nanotubes. In Section 3, we give five families of extremal projective fullerenes, whose Clar numbers attain the upper bound $\frac{n}{6} - 1$. Since there is a one to one correspondence from projective fullerenes to centrosymmetric spherical fullerenes [7], we also obtain five families of the corresponding extremal spherical fullerenes. Since the Euler characteristics of torus and Klein-bottle are zero, a toroidal or Klein-bottle fullerene is fully-benzenoid if and only if it is extremal. In Section 4, we characterize all extremal toroidal and Klein-bottle fullerenes.

2 Proof of Theorem 1.2

The projective plane is the simplest compact nonorientable surface which can be obtained from the sphere by adding one crosscap. Alternately, the projective plane can be obtained by identifying antipodal points of the sphere. Similarly, a graph on projective plane is the antipodal quotient of a centrosymmetric spherical graph on the sphere which has vertices, edges and faces obtained by identifying antipodal vertices, edges and faces of the centrosymmetric spherical graph. Graphs on projective plane are usually drawn inside a circular frame where antipodal boundary points are to be identified.

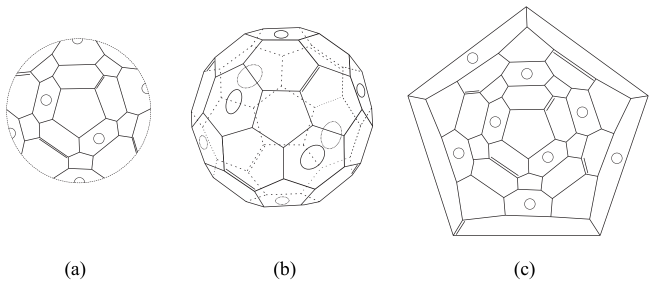


Figure 1. (a) A resonant pattern of a projective fullerene; (b) A resonant pattern of the corresponding centrosymmetric spherical fullerene of projective fullerene in (a); (c) A resonant pattern of the Schlegel diagram of spherical fullerene in (b).

In Clar's modes [4], a resonant pattern is denoted by those cycles depicted within such hexagons and the remainder is placed a perfect matching designated by the double bonds. If some hexagon in the resonant pattern of a projective fullerene is located in the boundary region in the circular representation and is divided into two parts by the boundary of the circular, we assign each part a halfcycle. If some edge of the remainder perfect matching is divided into two parts by the boundary of the circular, we place each part a half double bonds. For example, a resonant pattern of a projective fullerene with 30 vertices is illustrated in Figure 1(a). If we draw a projective graph G inside a circular frame, we can always obtain the corresponding centrosymmetric spherical graph G_1 as follows: take a copy G, each boundary point is being identified to the copy of its antipodal point, then stretch it to the corresponding centrosymmetric spherical graph G_1. A resonant pattern of the corresponding centrosymmetric spherical fullerene of projective fullerene in Figure 1(a) is illustrated in Figure 1(b). Graphs on sphere are usually drawn on plane as Schlegel diagrams. Figure 1(c) illustrate a resonant pattern of the Schlegel diagram of the spherical fullerene in 1(b).

Proof of Theorem 1.2. The theorem holds for a toroidal or Klein-bottle fullerene since it has the Euler characteristic 0 and consists entirely of hexagons. By Theorem 1.1, it holds for any spherical fullerenes. So we only need to prove that $c(F) \leq \lfloor \frac{n}{6} \rfloor - 1$ for any projective fullerene F with n vertices. To this end, let $\mathcal{H}$ be a Clar set of F. Then there exists a perfect matching M of F such that the boundary of each face in $\mathcal{H}$ are M-alternating. Since each edges of M is obtained by identifying two antipodal edges of the corresponding centrosymmetric spherical fullerene F_1, the set of edges in F_1 corresponding to M form a perfect matching M_1 of F_1. Since each face of $\mathcal{H}$ is obtained by identifying two antipodal faces of the corresponding centrosymmetric spherical fullerene F_1, the set of faces $\mathcal{H}_1$ in F_1 corresponding to $\mathcal{H}$ is a set of pairwise disjoint faces of F_1 and the boundary of each face in $\mathcal{H}_1$ is M_1-alternating. So we have $|\mathcal{H}_1|$=2$|\mathcal{H}|$, and $\mathcal{H}_1$ is a resonant pattern of F_1. By Theorem 1.1, we have $c(F) = |\mathcal{H}| = \frac{|\mathcal{H}_1|}{2} \leq \frac{c(F_1)}{2} \leq \frac{\lfloor \frac{2n}{6} \rfloor - 2}{2} = \lfloor \frac{n}{6} \rfloor - 1$. □

3 Extremal projective fullerenes

In this section we will present five families of extremal projective fullerenes, which implies five families of extremal spherical centrosymmetric fullerenes. From now on, we always omit the boundary of the circular frame when we draw a projective fullerene.

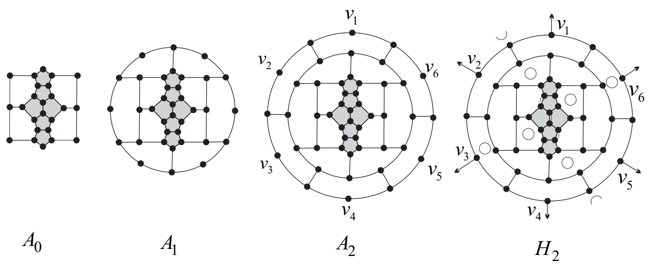


Figure 2. The construction of the first family of projective fullerenes H_k.

(1) Extremal projective fullerenes H_k

From A_0, add k layers of hexagons to obtain A_k for a natural number k (see Figure 2). We label the 2-degree vertices of A_k along the boundary of A_k counterclockwise with $v_1, v_2, v_3, v_4, v_5, v_6$, and connect v_1 with v_4, v_2 with v_5, v_3 with v_6. Now we get a projective fullerene H_k. Figure 2 illustrates the construction of H_2. The graph H_k $(k = 0, 1, 2, \dots)$ has $12k + 24$ vertices, $18k + 36$ edges, $6k + 7$ hexagons and $c(H_k) = 2k + 3$.

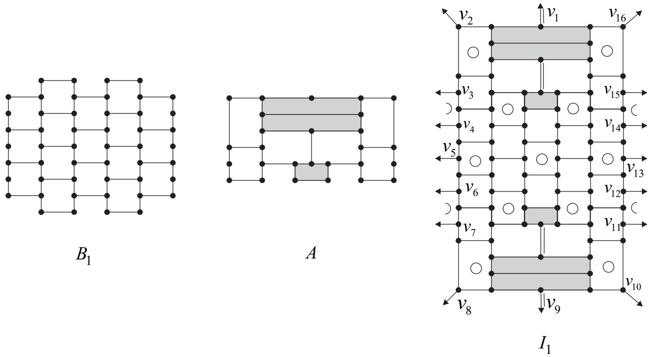


Figure 3. The construction of the second family of projective fullerenes I_k.

(2) Extremal projective fullerenes I_k

Extremal projective fullerenes I_k can be constructed as follows: first display a linear hexagonal chain with $3k$ hexagons along the vertical direction, then paste two linear hexagonal chains with $3k + 1$ and $3k$ hexagons to the each lateral side gradually, and denote the resulting graph by B_k, where k is a natural number. Now we paste a copy of A to the top side of B_k and rotate another copy of A 180 degrees, then paste it to the bottom side of B_k. Note that the resulting graph has $6k + 10$ 2-degree vertices. We label these 2-degree vertices along the boundary of B_k counterclockwise with $v_i, i = 1, 2, \dots, 6k+10$, and connect v_i with v_{i+3k+5}, where $i = 1, 2, \dots, 3k + 5$. Now we get projective fullerenes I_k. Figure 3 illustrates the construction of I_1. The graph I_k $(k = 0, 1, \dots)$ has $36k + 48$ vertices, $54k + 72$ edges, $18k + 19$ hexagons and $c(I_k) = 6k + 7$.

(3) Extremal projective fullerenes J_k

Start from B, then paste k linear hexagonal chains with 3, 6,…, $3k$, $3k + 1$ hexagons to each lateral side gradually, and denote the resulting graph by D_k, where k is a positive integer. For simplicity of our notation, we denote C_2 by rotating C_1 180 degrees and D by rotating C 180 degrees. Now we paste $k - 1$ copies of C_1 to the top side of D_k gradually,

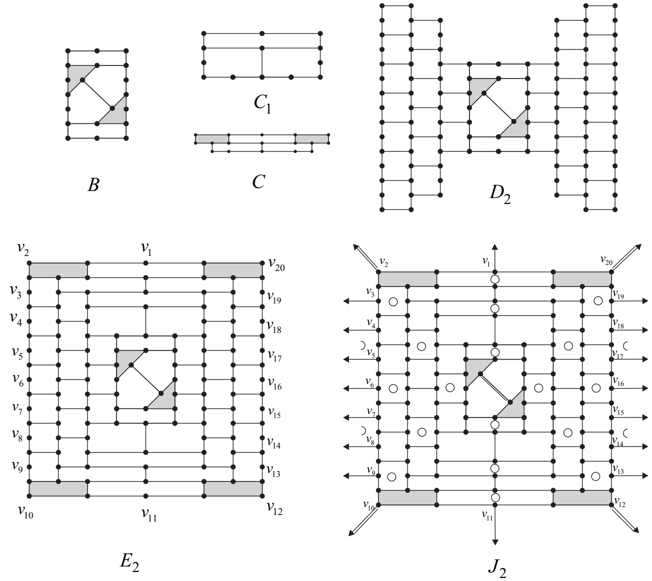


Figure 4. The construction of the third family of projective fullerenes J_k.

and paste $k-1$ copies of C_2 to the bottom side of D_k gradually, then paste a copy of C to the top side of resulting graph, and a copy of D to the bottom side of the resulting graph. Now we get a graph E_k. Clearly, E_k has $6k+8$ 2-degree vertices. We label these 2-degree vertices along the boundary of E_k counterclockwise with $v_i, i = 1, 2, \ldots, 6k+8$, and connect v_i with v_{i+3k+4}, where $i = 1, 2, \ldots, 3k+4$. Now we get a projective fullerene J_k. Figure 4 illustrates the construction of J_2. The graph J_k $(k = 1, 2, \ldots)$ has $6k^2+36k+30$ vertices, $9k^2+54k+45$ edges, $3k^2+18k+10$ hexagons and $c(J_k) = k^2+6k+4$.

(4) Extremal projective fullerenes L_k

From F_0, add k layers of hexagons to obtain F_k, where k is a natural number. We label vertices along the boundary of F_k counterclockwise with $v_0, v_1, \ldots, v_{17}$, identify pairs of vertices v_i and v_{i+9} to u_i, identify pairs of edges v_iv_{i+1} and $v_{i+9}v_{i+10}$ to u_iu_{i+1}, $i = 0, 1, \ldots, 8$, where subscript addition operation is modulo 18. Now we get a projective fullerene L_k. Figure 5 illustrates the construction of L_1. The graph L_k $(k = 0, 1, \ldots)$ has $18k+30$ vertices, $27k+45$ edges, $9k+10$ hexagons and $c(J_k) = 3k+4$.

(5)Extremal projective fullerenes N_k

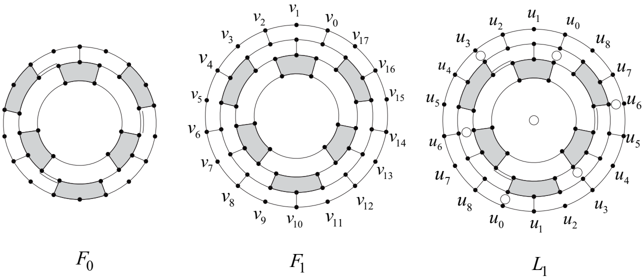


Figure 5. The construction of the fourth family of projective fullerenes L_k.

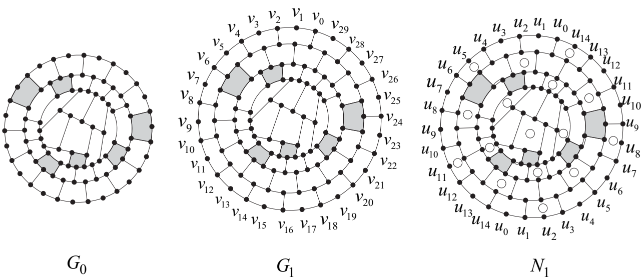


Figure 6. The construction of the fifth family of projective fullerenes N_k.

From G_0, then add k layers of hexagons to obtain G_k, where k is a natural number. We label vertices along the boundary of G_k counterclockwise with $v_0, v_1, \ldots, v_{29}$, identify pairs of vertices v_i and $v_i + 15$ to u_i, identify pairs of edges $v_i v_{i+1}$ and $v_{i+15} v_{i+16}$ to $u_i u_{i+1}$, $i = 0, 1, \ldots, 14$, where subscript addition operation is modulo 30. Now we get a projective fullerene N_k. Figure 6 illustrates the construction of N_1. The graph N_k $(k = 0, 1, \ldots)$ has $30k + 72$ vertices, $45k + 108$ edges, $15k + 31$ hexagons and $c(N_k) = 5k + 11$.

It is noticeable that by the same method mentioned in Section 2, we can also obtain zigzag nanotube $N_Z(2k + 1, 6)$ depicted in [32], which is the corresponding extremal centrosymmetric spherical fullerene of the projective fullerene H_k $(k = 0, 1, \ldots)$.

4 Extremal toroidal and Klein-bottle fullerenes

In this section, we obtain complete characterizations of the extremal toroidal and Klein-bottle fullerenes.

Now, we are going to illustrate the structures of toroidal and Klein-bottle fullerenes.

Let P be a $p \times q$-parallelogram in a hexagonal lattice, where p and q are positive integers. Every corner of P lies at the center of a hexagon. The top side and the bottom side intersect p vertical edges and each of the two parallel lateral sides passes through q edges perpendicular to them. A toroidal fullerene $H(p,q,t)$ (respectively, Klein-bottle fullerene $K(p,q,t)$) is obtained from P by the following boundary identification: first identify two lateral sides along the same direction and then identify the bottom side with the top side along the same (respectively, reverse) direction with a torsion t, where t is an integer and $0 \le t \le p-1$. For example, a toroidal fullerene $H(9,6,3)$ and a Klein-bottle fullerene $K(9,6,3)$ are illustrated in Figure 7(a) and (b) respectively.

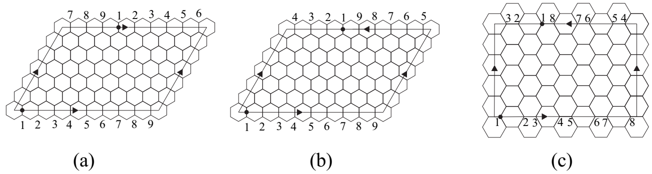


Figure 7. (a) A toroidal fullerene $H(9,6,3)$; (b) A Klein-bottle fullerene $K(9,6,3)$; (c) A Klein-bottle fullerene $N(8,9,2)$

Let R be a $p \times q$-rectangle in a hexagonal lattice, where p is a positive even integer and q is a positive integer. Every top corner of R lies at the center of a hexagon and every bottom corner of R lies at the center of a hexagon if q is even but at the center of a horizontal edge otherwise. The top side (respectively, the bottom side) covers $\frac{p}{2}$ horizontal edges and each of the two parallel lateral sides passes through $\lfloor \frac{q}{2} \rfloor$ edges perpendicular to them. A Klein-bottle fullerene $N(p,q,t)$ is obtained from R by the following boundary identification: first identify two lateral sides along the same direction and then identify the bottom side with the top side along the reverse direction with a torsion t, where t is an integer, t and q have the opposite parity, and $0 \le t \le q-1$. For example, a Klein-bottle fullerene $N(8,9,2)$ is illustrated in Figure 7(c).

It is easy to see that both $H(p,q,t)$ and $K(p,q,t)$ are bipartite graphs with pq faces,

$2pq$ vertices and $3pq$ edges, while $N(p,q,t)$ is non-bipartite with $\frac{pq}{2}$ faces, pq vertices and $\frac{3pq}{2}$ edges.

The following two lemmas will be useful.

Lemma 4.1. [27] *$H(p,q,t)$ is hexagon-transitive.*

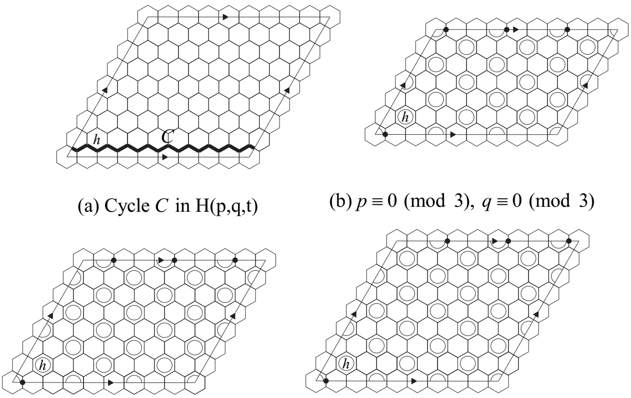
Lemma 4.2. [28] *All Klein-bottle fullerenes $K(p,q,t)$, $t = 0,1,\ldots,p-1$, are equivalent.*

Theorem 4.3. *$H(p,q,t)$ is extremal if and only if $p \equiv 0 \pmod 3$ and $q \equiv t \pmod 3$.*

Proof. Suppose $H(p,q,t)$ is extremal. Then there exists a Clar set of $H(p,q,t)$ covering all vertices of $H(p,q,t)$. Let C be the cycle induced by those vertices which are just upon the bottom horizontal line of parallelogram P (see Figure 8(a)). Then the length of C is $2p$. For a hexagon in a Clar set of $H(p,q,t)$, if C intersects it, then their intersection must be a path with 3 vertices. Hence $2p$ is divisible by 3. This implies that $p \equiv 0 \pmod 3$. So $p \geq 3$. Let h be the hexagon in the lower left corner of P without intersection with the boundary lines of P. Since $H(p,q,t)$ is hexagon-transitive and extremal, we can extend h to a unique Clar set $\mathcal{H}$ of $H(p,q,t)$ which covers all vertices of $H(p,q,t)$. The hexagons in $\mathcal{H}$ in the interior of the parallelogram P are first determined. Since $h \in \mathcal{H}$, the $(3i)$-th hexagon ($i = 0,1,\ldots,\frac{p}{3}-1$) from left to right along the bottom horizontal line of parallelogram P is in $\mathcal{H}$. If $q = 3s + r$, where s and $r < 3$ are non-negative integers, then the $(3j)$-th hexagon ($j = 0,1,\ldots,\ s$) from bottom to top along the left lateral line of P is in $\mathcal{H}$. Hence the r-th hexagon, and the $(3i+r)$-th hexagon ($i = 0,1,\ldots,\frac{p}{3}-1$) from left to right along the top horizontal line of P are in $\mathcal{H}$ (see Figure 8(b), (c) and (d)). The 0-th hexagon from left to right along the bottom horizontal line of P indeed is the same hexagon as one of the $(3i+r)$-th hexagons along the top horizontal line of P. So $0 \leq t = 3i + r \leq p - 1$, and we have $q \equiv t \pmod 3$.

Conversely, suppose $p \equiv 0 \pmod 3$ and $q \equiv t \pmod 3$. The 0-th hexagon h_0 from left to right along the bottom horizontal line of P is the same hexagon as t-th hexagon along the top horizontal line of P. Since $q \equiv t \pmod 3$, let $q = 3s + r$ and $t = (3i + r)$ where s, i and $r < 3$ are non-negative integers. Further, since $p \equiv 0 \pmod 3$, h_0 can be extended uniquely to a Clar set of $H(p,q,t)$ covering all vertices (see also Figure 8(b), (c) and (d)). So $H(p,q,t)$ is extremal. □

Theorem 4.4. *$K(p,q,t)$ is extremal if and only if $p \equiv 0 \pmod 3$.*

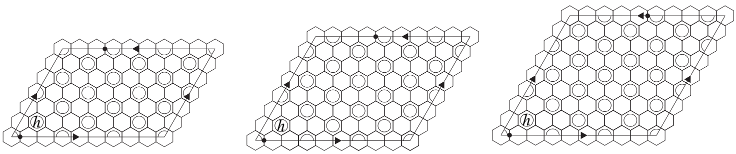


(a) Cycle C in H(p,q,t) (b) $p \equiv 0$ (mod 3), $q \equiv 0$ (mod 3)

(c) $p \equiv 0$ (mod 3), $q \equiv 1$ (mod 3) (d) $p \equiv 0$ (mod 3), $q \equiv 2$ (mod 3)

Figure 8. Illustration for the proof of Theorem 4.3: Toroidal fullerenes $H(p,q,t)$.

Proof. Suppose $K(p,q,t)$ is extremal. Using similar arguments as in Theorem 4.3, we can obtain that $p \equiv 0 \pmod 3$.



(a) $p \equiv 0$ (mod 3), $q \equiv 0$ (mod 3) (b) $p \equiv 0$ (mod 3), $q \equiv 1$ (mod 3) (c) $p \equiv 0$ (mod 3), $q \equiv 2$ (mod 3)

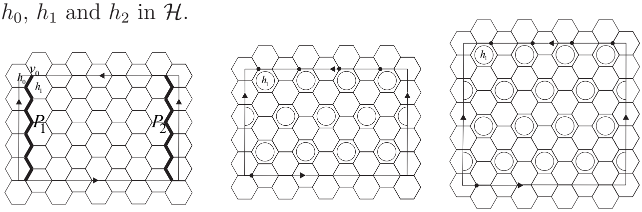
Figure 9. Illustration for the proof of Theorem 4.4: Klein-bottle fullerenes $K(p,q,t)$.

Conversely, suppose $p \equiv 0 \pmod 3$. The 0-th hexagon h_0 from left to right along the bottom horizontal line of P is the same hexagon as $(t+1)$-th hexagon along the top horizontal line of P. Let h be the hexagon in the lower left corner of P not intersecting the boundary of P. Suppose $q = 3s + r$, where s and $r < 3$ are non-negative integers. For $K(p,q,r+2)$, where $r+2$ is modulo p, since $p \equiv 0 \pmod 3$, by a similar argument as in Theorem 4.3, h can be extended uniquely to a Clar set of $K(p,q,r+2)$ covering all vertices (see Figure 9). So $K(p,q,r+2)$ is extremal. It follows immediately from Lemma 4.2 that all $K(p,q,t)$, $t = 0,1,\dots,p-1$, are extremal. $\square$

Theorem 4.5. *$N(p, q, t)$ is extremal if and only if $q \equiv 0 \pmod 3$.*

Proof. Suppose $N(p, q, t)$ is extremal. Then there exists a Clar set $\mathcal{H}$ of $N(p, q, t)$ covering all vertices of $N(p, q, t)$. Let P_1 be the subgraph induced by those vertices which are just at the right side of the left lateral line of rectangle R (see Figure 10(a)). Assume that $t = 0$. Then P_1 is a cycle and its length equals q. For any hexagon in $\mathcal{H}$, if P_1 intersects it, then their intersection must be a path with 3 vertices. Hence q is divisible by 3, i.e., $q \equiv 0 \pmod 3$.

So we may now assume that $t \neq 0$. Then P_1 is a path with $q + 1$ vertices. Let v_0 be the end vertex of P_1 on the top horizontal line of R. Let h_0 be the 0-th hexagon from top to bottom along the left lateral line of R, and h_1 be the hexagon in the upper left corner of R such that an edge of h_1 overlaps the top horizontal line of R. Suppose h_2 is the hexagon such that h_0, h_1 and h_2 have the common vertex v_0. By the structure of $N(p, q, t)$, h_2 is one of the hexagons just above the $\frac{p}{2}$ horizontal edges along the bottom horizontal line of R. Since $\mathcal{H}$ covers v_0 and $N(p, q, t)$ is 3-regular, there is exactly one hexagon of h_0, h_1 and h_2 in $\mathcal{H}$.



(a) Illustration for necessity (b) $q \equiv 1 \pmod 2$ (c) $q \equiv 0 \pmod 2$

Figure 10. Illustration for the proof of Theorem 4.5: Klein-bottle fullerenes $N(p, q, t)$.

If $h_0 \in \mathcal{H}$, then each hexagon intersecting the top and bottom horizontal lines of R at exactly two vertices of $N(p, q, t)$ is in $\mathcal{H}$. These hexagons cover exactly 4 vertices of P_1. For any other hexagon in $\mathcal{H}$, if P_1 intersects it, then their intersection must be a path with 3 vertices. Hence $q + 1 - 4$ is divisible by 3. This implies that $q \equiv 0 \pmod 3$.

If $h_1 \in \mathcal{H}$, then each hexagon just below the $\frac{p}{2}$ horizontal edges along the top horizontal line of R is in $\mathcal{H}$. By the structure of $N(p, q, t)$, one of these hexagons must cover the other end vertex of P_1. So these hexagons cover exactly 4 vertices of P_1. For any other hexagon in $\mathcal{H}$, if P_1 intersects it, then their intersection must be a path with 3 vertices. Hence $q + 1 - 4$ is divisible by 3. This implies that $q \equiv 0 \pmod 3$.

If $h_2 \in \mathcal{H}$, then each hexagon just above the $\frac{p}{2}$ horizontal edges along the bottom horizontal line of R is in $\mathcal{H}$. These hexagons cover exactly 4 vertices of P_1. For any other hexagon in $\mathcal{H}$, if P_1 intersects it, then their intersection must be a path with 3 vertices. Hence $q + 1 - 4$ is divisible by 3. This implies that $q \equiv 0 \pmod 3$.

Conversely, suppose $q \equiv 0 \pmod 3$. Then $q \geq 3$. Starting from h_1, we can always extend it to a Clar set of $N(p, q, t)$ (see Figure 10(b) and (c)). In fact, each hexagon just below the $\frac{p}{2}$ horizontal edges along the top horizontal line of R is in $\mathcal{H}$, and the hexagons in $\mathcal{H}$ without intersection with boundary lines of R are uniquely determined. Note that these hexagons, which are already determined, cover some vertices of P_1. Let P_2 be the subgraph induced by those vertices which are just at the left side of the right lateral line of rectangle R. The hexagons along the left lateral line of R covering the remaining vertices of P_1 also cover the remaining vertices of P_2. Hence h can be extended to a Clar set of $N(p, q, t)$ covering all vertices (see also Figure 10(b) and (c)). Furthermore, none of the hexagons which intersect the top and bottom horizontal lines of R at exactly two nonadjacent vertices is in $\mathcal{H}$, and none of hexagons just upper the $\frac{p}{2}$ horizontal edges along the bottom horizontal line of R is in $\mathcal{H}$. These facts guarantee that the Clar set $\mathcal{H}$ is irrelevant to the choice of t. Hence $N(p, q, t)$ is extremal for all possible t. □

5 Conclusions

Theorem 1.2 implies none of the spherical fullerenes and projective fullerenes is fully-benzenoid and all extremal toroidal and Klein-bottle fullerenes are fully-benzenoid. This paper also presents simple characterizations for fully-benzenoid toroidal and Klein-bottle fullerenes. The fully-benzenoid polycyclic aromatic hydrocarbons whose resonant patterns can be represented with only hexagons possess particularly high stability and lower reactivity [4, 5]. Gutman and Babić [12] early gave a characterization of fully-benzenoid hydrocarbons. Recently Gutman and Salem [11] showed that any fully-benzenoid hydrocarbon has a unique Clar set. We point out that fully-benzenoid $K(p, q, t)$ also has this property, but fully-benzenoid fullerene $H(p, q, t)$ and $N(p, q, t)$ each has exactly three Clar sets. For other researches on fully-benzenoid polycyclic aromatic hydrocarbons, we refer to [6, 10, 13, 22, 23].

Hartung [17] developed a method to calculate the Clar number directly for many infinitely families of spherical fullerenes. Such arguments also imply that, for any constant

c, there exists a spherical fullerene F with n vertices such that $c(F) < \frac{n}{6} - c$. The problem how to compute the Clar number of a given fullerene on the sphere or projective plane efficiently is still open.

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