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An upper bound for the Clar number of fullerene graphs

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A fullerene graph is a three-regular and three-connected plane graph exactly 12 faces of which are pentagons and the remaining faces are hexagons. Let F_n be a fullerene graph with n vertices. The Clar number $c(F_n)$ of F_n is the maximum size of sextet patterns, the sets of disjoint hexagons which are all M-alternating for a perfect matching (or Kekulé structure) M of F_n. A sharp upper bound of Clar number for any fullerene graphs is obtained in this article: $c(F_n) \leqslant \lfloor \frac{n-12}{6} \rfloor$. Two famous members of fullerenes C_{60} (Buckministerfullerene) and C_{70} achieve this upper bound. There exist infinitely many fullerene graphs achieving this upper bound among zigzag and armchair carbon nanotubes.

KEY WORDS: fullerene graph, carbon nanotube, Clar number, sextet pattern, Clar formula, perfect matching, Kekulé structure

1. Introduction

Fullerenes are carbon-cage molecules exclusively consisting of carbon atoms arranged on a sphere with 12 five-membered faces and other six-membered faces. The icosahedral C_{60} molecule, Buckministerfullerene, proposed firstly by Kroto et al. [1] and confirmed by later experiments [2,3], is the archetype of fullerenes. A *fullerene graph* as a molecular graph of a fullerene is a three-regular and three-connected plane graph where exactly 12 faces are pentagons and remaining faces are hexagons. It is well known that fullerene graphs F_n with n vertices exist for all $n \geqslant 20$, expect for $n = 22$ [4]. For construction and enumeration of fullerene isomers, readers may refer to [4,5].

Let G be a plane graph. A *perfect matching* (or Kekulé structure) M of G is a set of pairwise disjoint edges of G such that every vertex of G is incident with an edge in M. A cycle of G is M-*alternating* if its edges appear alternately in and off M. A set $\mathcal{H}$ of disjoint face-boundaries of G that are even cycles is called

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a *resonant pattern* if G has a perfect matching M such that all cycles in $\mathcal{H}$ are M-alternating. Equivalently, G–$\mathcal{H}$ has a perfect matching, where G–$\mathcal{H}$ denotes the subgraph obtained from G by deleting the vertices in $\mathcal{H}$ together with their incident edges. A *sextet pattern* is a special types of resonant pattern that only consists of hexagons. In Clar's modes [6], a sextet pattern is denoted by those cycles depicted within such hexagons and the remainder is placed a perfect matching designated by the double bonds; for example, a sextet pattern of F_{24} is illustrated in figure 3 (right). For benzenoid systems or fullerene graphs G, the *Clar number* of G, denote by $c(G)$, is the maximum size of all sextet patterns of G; *Clar formula* always means a sextet pattern with the maximum number of hexagons.

The concept of resonant pattern originates from Clar's aromatic theory [6]: within benzenoid hydrocarbon isomers, one with larger Clar number is more stable. Some upper bounds for the Clar number of benzenoid hydrocarbons, were given by Hansen and Zheng [7]. An integer linear programming was proposed by the same authors [8] to compute the Clar number of benzenoid hydrocarbons. Abeledo and Atkinson [9] showed that relaxing the integer-restrictions in such a programme always yields an integral solution, accordingly settled a corresponding conjecture in [8]. For other researches on the Clar number of benzenoid hydrocarbons, see [10–15].

Recently, Zhang and Wang [16] investigated sextet patterns of open-end carbon nanotubes or tubule. For Buckministerfullerene (C_{60}), El-Basil [17] found that $c(C_{60}) = 8$ and C_{60} has exactly 5 Clar formulas; Further, Shiu et al. [18] obtained Clar and sextet polynomials. For any fullerene graphs Zhang and He [19] obtained that the sextet pattern count is no larger than the Kekulé structure count.

In this paper, we obtain an upper bound for the Clar number of fullerene graphs F_n, which is described in the following main theorem.

Theorem 1. $c(F_n) \leqslant \lfloor \frac{n-12}{6} \rfloor$.

In the next section we will give a rigorous proof to this theorem. In the last section we show that there are infinitely many fullerene graphs which can achieve this upper bound, including C_{60} and C_{70}, and zigzag and armchair carbon nanotubes as well. By the way, theorem 1 shows that none of fullerene graphs is "fully benzenoid" [20].

2. Proof of theorem 1

To prove the theorem, we now introduce some useful notions. Let G be any graph with the vertex-set $V(G)$ and edge-set $E(G)$. For a subgraph or a set of vertices S of G, we say S *meets* a subgraph G' of G if $S \cap G' \neq \emptyset$, and let

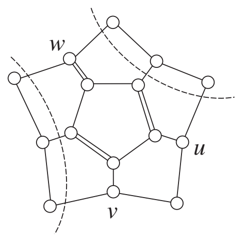

Figure 1. A half part B of dodecahedron and illustration for the proof of lemma 1.

G–S denote the subgraph obtained from G by deleting the vertices in S together with their incident edges. For a 2-connected plane graph G, each face of G is bounded by a cycle. For convenience, a face is often represented by its boundary if unconfused. For example, an edge uv meeting a face f always means $\{u, v\} \cap f \neq \emptyset$; and a face f of G *adjoins* a subgraph G' of G if f is not a face of G' and f has an edge in common with G'. Further, the boundary of G always means the boundary of its infinite face.

For any fullerene graph F, any *pentagon*, a cycle with length 5, of F must bound a face since F is three-connected; any *hexagon*, a cycle with length 6, of F also bounds a face since F is cyclically 5-edge connected [21].

In what follows we always denote by F any given fullerene graph and by $\mathcal{H}$ any given Clar formula of F. Let $U_{\mathcal{H}} := V(F) - V(\mathcal{H})$ be the set of vertices of F that are not included in hexagons of $\mathcal{H}$.

Let B be the half part of dodecahedron as shown in figure 1. Then B is a plane graph with 15 vertices and 6 pentagons, where the 5 pentagons adjoin the central pentagon. Our proof to theorem 1 entirely relys on the following two crucial lemmas.

Lemma 1. If a fullerene graph F contains B as its subgraph, then $|V(B) \cap U_{\mathcal{H}}| \geqslant 12$.

Proof. If a hexagon h in $\mathcal{H}$ adjoins B, the intersection $h \cap B$ is a path of length 2 along the boundary of B and its end-vertices are of degree 2 in B. So, among all faces of F adjoining B at most two belong to $\mathcal{H}$ since the faces in $\mathcal{H}$ are pairwise disjoint hexagons. If there are precisely two faces of them in $\mathcal{H}$, let u, v and w be the three 3-degree vertices of B which lie on the boundary of B and which are not included in $\mathcal{H}$ such that both u and v are adjacent to a vertex of degree 2 in B (see figure 1). Then w is a vertex of degree one in B–$\mathcal{H}$. From this we can show that one of u and v would not be matched by any perfect matching of F–$\mathcal{H}$, which contradicts that $\mathcal{H}$ is a sextet pattern of F. So at most 3 vertices of B are included in $\mathcal{H}$, and $|V(B) \cap U_{\mathcal{H}}| \geqslant 15 - 3 = 12$. □

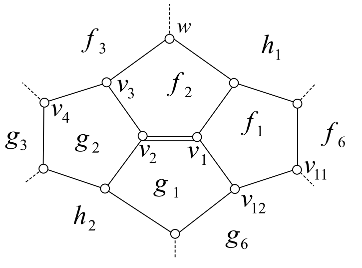

Figure 2. The subgraph G_1.

Lemma 2. If a subgraph G of a fullerene graph F has at least k pentagons, then $|V(G) \cap U_{\mathcal{H}}| \geqslant k$.

Proof. Let G be a subgraph of F with at least k pentagons. Since F has exactly 12 pentagons, $k \leqslant 12$. If G contains B, lemma 1 implies the assertion. So, from now on we suppose that G contains no B. We prove this lemma by induction on k. If $k = 1$, we have $|V(G) \cap U_{\mathcal{H}}| \geqslant 1$ since a pentagon has at least one vertex that cannot be included in any sextet pattern of F. So suppose $k \geqslant 2$ and the lemma holds for smaller k.

If $U_{\mathcal{H}}$ has a non-empty subset S that is contained in $V(G)$ such that S meets at most $|S|$ pentagons of G, then $G - S$ will have at least $k - |S|$ pentagons. By induction hypothesis we have that $|V(G - S) \cap U_{\mathcal{H}}| \geqslant k - |S|$. Since $S \subseteq V(G) \cap U_{\mathcal{H}}$, $|V(G) \cap U_{\mathcal{H}}| \geqslant k$ and the lemma holds. So it is sufficient to show the existence of such an S.

($*$) *Suppose, on the contrary, that there is no* $\emptyset \neq S \subseteq V(G) \cap U_{\mathcal{H}}$ *such that* S *meets at most* $|S|$ *pentagons of* G.

Let M be a perfect matching of F–$\mathcal{H}$. Then $M \neq \emptyset$ covers precisely all vertices in $U_{\mathcal{H}}$. There exists an edge $e = v_1 v_2 \in M$ meeting G since G has $k \geqslant 2$ pentagons and any pentagon contains at least one vertex in $U_{\mathcal{H}}$; let ψ_e denote the number of pentagons of G met by e. We claim that $3 \leqslant \psi_e \leqslant 4$ for any such edge e: If $\psi_e \leqslant 2$, $S := \{v_1, v_2\} \cap V(G)$ meets ψ_e pentagons of G, a contradiction follows; $\psi_e \leqslant 4$ holds since F is three-regular. Further, every edge in M meeting G must belong to G. In the following there are two cases to be considered.

Case 1. There exists an edge $e = v_1 v_2 \in M \cap E(G)$ with $\psi_e = 4$. Then G contains a subgraph G_1 consisting of 4 pentagons g_1, g_2, f_1 and f_2, meeting the same edge $v_1 v_2$ (see figure 2). The faces adjoining G_1 in F are denoted by h_1, f_6, g_6, h_2, g_3 and f_3, which are illustrated in figure 2. Clearly, $\{h_1, f_3\} \nsubseteq \mathcal{H}$, and $\{h_2, g_6\} \nsubseteq \mathcal{H}$. If $\{h_1, f_3\} \cap \mathcal{H} = \emptyset$, $S := V(f_2) \subseteq U_{\mathcal{H}}$ meets at most 5 pentagons of G since G contains no B as its subgraph. This contradicts the above supposition ($*$). Hence $\mathcal{H}$ contains exactly one of h_1 and f_3, and exactly one of h_2 and g_6 in a similar manner.

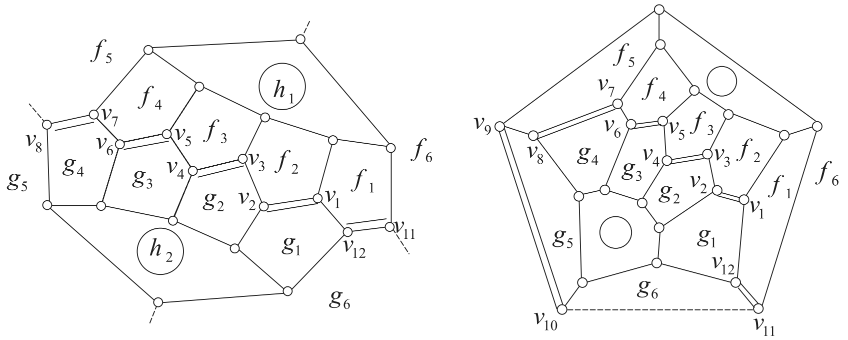

Figure 3. Illustration for case 1.

If $\{f_3, h_2\} \subseteq \mathcal{H}$, then $\{h_1, g_6\} \cap \mathcal{H} = \emptyset$. Since $B \nsubseteq G$, f_1 adjoins at most 4 pentagons of G. Then $S := V(f_1) \subseteq U_{\mathcal{H}}$ meets at most 5 pentagons of G. This also contradicts supposition ($*$). For the case that $\{h_1, g_6\} \subseteq \mathcal{H}$, a similar contradiction happens.

So the remaining case is either $\{h_1, h_2\} \subseteq \mathcal{H}$ or $\{f_3, g_6\} \subseteq \mathcal{H}$. Without loss of generality, we suppose that $h_1, h_2 \in \mathcal{H}$, considering their symmetry. The faces adjoining h_1 in F are enumerated clockwise as $f_1, f_2, \ldots, f_6$, and the faces adjoining h_2 in F are enumerated counterclockwise as $g_1, g_2, \ldots, g_6$ (see figure 3). As denoted in figures 2 and 3, $v_{11}v_{12}$ is the common edge of f_1 and g_6, and v_3v_4 the common edge of f_3 and g_2. Then $v_{11}v_{12} \in M$ and $v_3v_4 \in M$. Further, $f_3 \cap g_3 = v_4v_5$.

Let $P_{2i} := v_{11}v_{12}v_1v_2v_3v_4 \cdots v_{2i-1}v_{2i}$ be a path with $2i + 2$ vertices. Obviously P_4 is an M-alternating path in G_1 and $V(P_4) \subseteq U_{\mathcal{H}}$. Then at least three of f_3, g_3, f_6 and g_6 are pentagons of G: otherwise $S := V(P_4)$ meets at most 6 pentagons of G, a contradiction. By the symmetry, without loss of generality we suppose that both f_3 and g_3 are pentagons of G. So f_4 and g_3 have an edge v_5v_6 in common, and $v_5v_6 \in M$. Further, $f_4 \cap g_4 = v_6v_7$. Hence P_6 is an M-alternating path in G and $V(P_6) \subseteq U_{\mathcal{H}}$. By the same reason we have that at least 3 faces in f_4, g_4, f_6 and g_6 are pentagons of G. By the symmetry we may suppose that f_4 and g_4 are pentagons of G (see figure 3 (left)). Then $v_7v_8 := f_5 \cap g_4$ is an edge in M. Let v_8v_9 be an edge of f_5 and g_5 in common. Similarly we may suppose that both f_5 and g_5 are pentagons of G (see figure 3 (right)). Then f_6 and g_5 have an edge v_9v_{10} in common and $v_9v_{10} \in M$. Then P_{10} is an M-alternating path in G both end-edges of which belong to M and $V(P_{10}) \subseteq \mathcal{H}$. Obviously $S := V(P_{10})$ meets at most 12 pentagons since F contains precisely 12 pentagons. This contradicts supposition ($*$).

Case 2. $\psi_e = 3$ for any $e = v_1v_2 \in M \cap E(G)$. Then the 3 pentagons, g_1, g_2 and g_3, met by v_1v_2 may form two distinct subgraphs G_2 and G_3 of G such that for G_2, only g_2 contains v_1v_2, but for G_3 both g_1 and g_2 contain v_1v_2 (see figure 4).

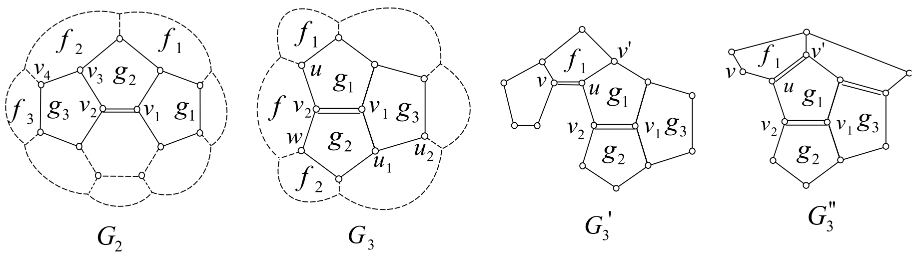

Figure 4. Illustration for case 2.

Subcase 2.1. $G_2 \subseteq G$. Let f_1, f_2 denote the faces outside G_2 that adjoin g_2 in F (see G_2 in figure 4). Then f_1 and f_2 have an edge in common and $\{f_1, f_2\} \nsubseteq \mathcal{H}$. It follows that precisely one of f_1 and f_2 belongs to $\mathcal{H}$; Otherwise $S := V(g_2) \subseteq U_{\mathcal{H}}$ meets at most 5 pentagons of G (possible g_1, g_2, g_3, f_1, f_2), which contradicts supposition $(*)$. Without loss of generality, let $f_1 \in \mathcal{H}$. Then $v_3v_4 := f_2 \cap g_3$ is an edge. Further, $v_3v_4 \in M$ and $\psi_{v_3v_4} = 3$ (Case 2). Hence $S := \{v_1, v_2, v_3, v_4\} \subseteq U_{\mathcal{H}}$ meets precisely 4 pentagons of G, a contradiction to supposition $(*)$.

Subcase 2.2. $G_3 \subseteq G$, but $G_2 \nsubseteq G$. The faces adjoining g_1, g_2 but not g_3 are denoted by f_1, f and f_2 (see G_3 in figure 4). If both of f_1 and f_2 are in $\mathcal{H}$, then $V(g_3) \subseteq U_{\mathcal{H}}$. Since $B \nsubseteq G$, $S := V(g_3)$ meets at most 5 pentagons of G, a contradiction. So, without loss of generality let $f_1 \notin \mathcal{H}$. Let u be the vertex meeting g_1, f_1 and f. Then $u \in U_{\mathcal{H}}$. Let $uv := f_1 \cap f$ and $uv' := f_1 \cap g_1$. Then $uv' \in M$; otherwise, $uv \in M$. Since $\psi_{uv} = 3$ and f is not a pentagon of G, G_2 appears in G, contradicting this subcase (see G_3' in figure 4). So suppose $uv' \in M$. Further, let $S := V(g_1) \subseteq U_{\mathcal{H}}$. Since f is not a pentagon of G, S meets at most five pentagons of G. This contradicts supposition $(*)$ and completes the entire proof of the lemma. □

Proof of theorem 1. Let $G := F_n$. Since F_n has exactly 12 pentagons, by lemma 2 we have $|U_{\mathcal{H}}| \geqslant 12$. By $U_{\mathcal{H}} = V(F_n) - V(\mathcal{H})$, we have $|V(\mathcal{H})| = |V(F_n)| - |U_{\mathcal{H}}| \leqslant n - 12$. On the other hand, $|V(\mathcal{H})| = 6c(F_n)$ and $c(F_n)$ is an integer. So we have $c(F_n) \leqslant \lfloor \frac{n-12}{6} \rfloor$ and the main theorem is proved. □

3. Sharpness for the upper bound

In this section we will show there exist infinitely many fullerenes whose Clar numbers attain the upper bound in Theorem 1. Two famous members of fullerenes C_{60} and C_{70} synthesized in experiments [4] are such fullerenes: Sextet patterns of C_{60} and C_{70} in figure 5 are their Clar formulas by theorem 1. Hence $c(C_{60}) = 8$ and $c(C_{70}) = 9$. Further, infinitely many examples of such fullerenes

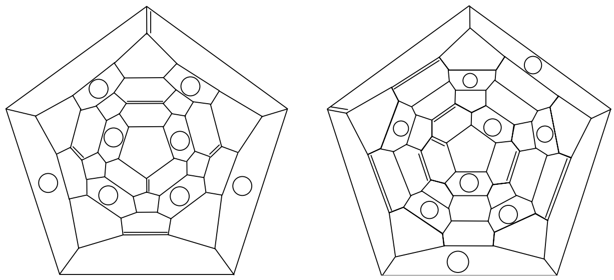

Figure 5. Clar formulas of C_{60} (left) and C_{70} (right).

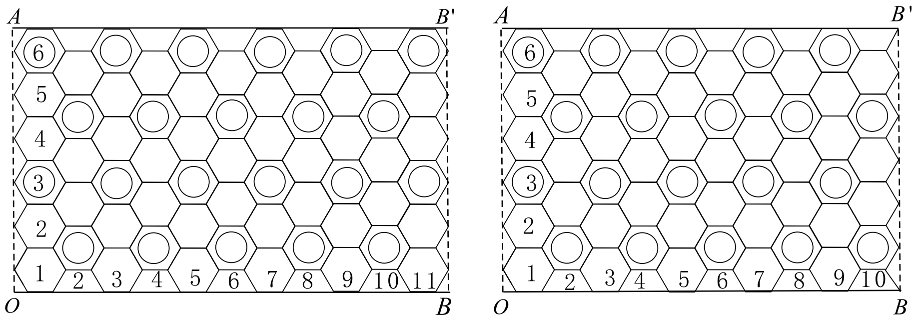

Figure 6. The unrolled honeycomb lattices of zigzag open-end nanotubes.

can be found in zigzag and armchair carbon nanotubes, where the chiral angles are equal to 30° and 0° respectively [22].

3.1. Zigzag-carbon nanotubes

We cut a rectangular section $OAB'B$ from the hexagonal lattice in the plane. The *zigzag* open-end nanotube $T_Z(p, q)$ is obtained by rolling the rectangular section $OAB'B$ shown in figure 6 so that segments OB and AB' are glued, where p denotes the number of layers parallel to OA and q the number of hexagons on each layer. For example, the rectangular sections in figure 6 (left) and (right) are rolled into zigzag open-end nanotubes $T_Z(11, 6)$ and $T_Z(10, 6)$ according to odd and even number p of layers.

Let B_1 be a half of a F_{36} illustrated in figure 7 (left). Then B_1 as a cap is added to each end of $T_Z(p, 6)$ to obtain a zigzag nanotube $N_Z(p, 6)$ for any non-negative integers p: along their boundaries identify the 3 (resp. 2)-degree vertices of B_1 with the 2 (resp. 3)-degree vertices on an end of a tubule $T_Z(p, 6)$. Figure 7 illustrates such a generation procedure of a zigzag nanotube $N_Z(3, 6)$: for convenience, a tube $T_Z(3, 6)$ is deformed to the plane, two copies of B_1 are added to faces f_1 and f_2 of $T_Z(3, 6)$ along their boundaries.

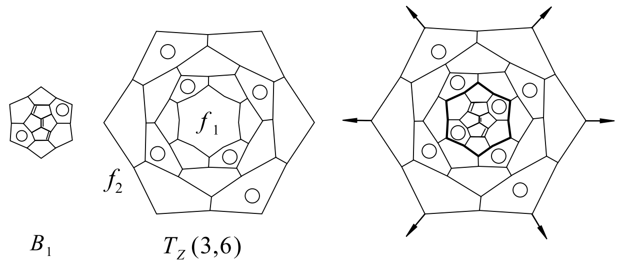

Figure 7. A generation of zigzag carbon nanotubes with sextet patterns.

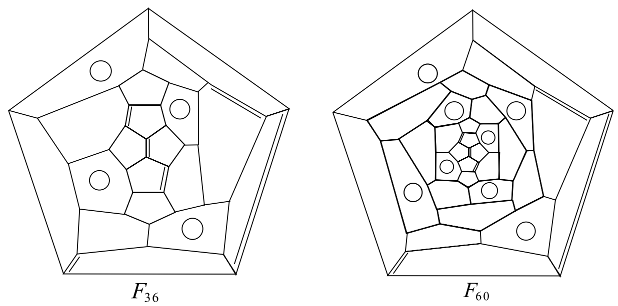

Figure 8. Zigzag nanotubes $N_Z(0,6)$ and $N_Z(2,6)$ with Clar formulas.

Any zigzag nanotube $N_Z(p,6)$ is a fullerene graph F_n and $n = 36 + 12p$ by a routine computation. We now calculate their Clar numbers. We can see that the zigzag tubule $T_Z(p,6)$ with cycles within some hexagons in figure 6 and both caps B_1 with cycles and double bonds in figure 7 are combined into a zigzag nanotube $N_Z(p,6)$ with a sextet pattern, which has $2p+4$ aromatic sextets. On the other hand, this number is just the upper bound of the Clar number in theorem 1. Hence for any non-negative integer p the $N_Z(p,6)$ achieve the upper bound. Further, the sextet pattern constructed as above is a Clar formula of $N_Z(p,6)$ and $c(N_Z(p,6)) = 2p+4$. In particular, zigzag nanotubes $N_Z(0,6)$ and $N_Z(2,6)$ are F_{36} and F_{60} respectively, which together with Clar formulas are illustrated in figure 8.

3.2. *Armchair carbon nanotubes*

The *armchair* open-end nanotube $T_A(p,q)$ (resp. $T'_A(p,q)$) is obtained by rolling the rectangular section $OAB'B$ shown in figure 9 (left) (resp. (right)) so that segments OB and AB' are glued, where q denotes the number of layers parallel to the axis direction or to OB. For $T_A(p,q)$, p is the number of hexagons on each layer; For $T'_A(p,q)$, p is the number of hexagons on each short layer, whereas all longer layers have $p+1$ hexagons. For example, the rectangular section in figure 9 (left) and (right) are rolled into armchair open-end nanotube

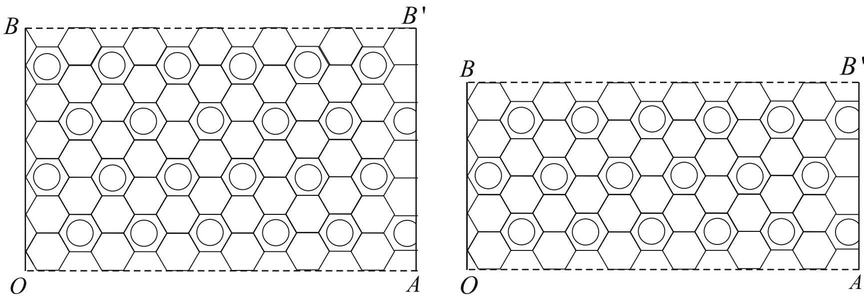

Figure 9. The unrolled honeycomb lattice of armchair open-end nanotubes.

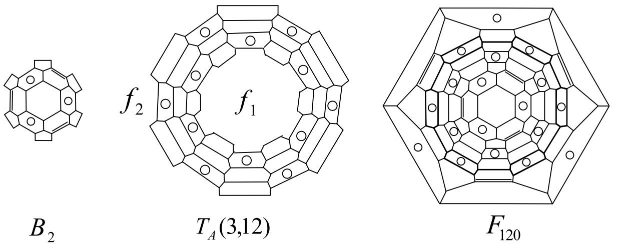

Figure 10. A generation of armchair nanotubes $N_A(3k, 12)$ with Clar formulas.

$T_A(6, 12)$ and $T'_A(4, 12)$; other examples are $T_A(3, 12)$ in figure 10 (middle) and $T'_A(1, 12)$ in figure 11 (middle).

As in the above subsection to each end of a tubule $T_A(p, 12)$ a cap B_2 (see figure 10 (left)) is added to obtain an armchair nanotube $N_A(p, 12)$ for any non-negative integers p: along their boundaries identify the 3 (resp. 2)-degree vertices of B_2 with the 2 (resp. 3)-degree vertices on an end of $T_A(p, 12)$. Figure 10 illustrates such a generation procedure of an armchair nanotube $N_A(3, 12)$, which is a fullerene F_{120}.

Any armchair nanotube $N_A(p, 12)(p \geqslant 1)$ is a fullerene graph F_n with $n = 48 + 24p$ vertices. If $p = 3k, k$ is any positive integer, the set of hexagons with cycles from a tubule $T_A(3k, 12)$ in figure 9 (left) and both caps B_2 in figure 10 forms a sextet pattern of $N_A(3k, 12)$, which is a Clar formula by theorem 1 since it misses exactly 12 vertices. Hence any armchair nanotube $N_A(3k, 12)$ achieve the upper bound in theorem 1 and $c(N_A(3k, 12)) = 12k + 6$. For example, $N_A(3, 12)$ is a fullerene graph F_{120}, which together with a Clar formula is illustrated in figure 10 (right).

In an analogous manner an armchair tubule $T'_A(p, 12)$ is added double caps B_2 to get an armchair nanotube $N'_A(p, 12)$ (see figure 11), which is a fullerene graph F_n with $n = 60 + 24p$. For any non-negative integer k, a Clar formula of $N'_A(3k+1, 12)$ missing exactly 12 vertices can be constructed. Hence all armchair nanotubes $N'_A(3k + 1, 12)$ achieve the upper bound in theorem 1 and

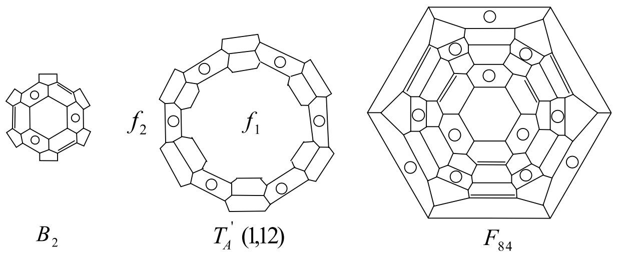

Figure 11. Generation of armchair nanotubes $N'_A(3k+1, 12)$ with Clar formulas.

$c(N'_A(3k + 1, 12)) = 12 + 12k$. For example, the construction of an armchair nanotube $N'_A(1, 12)$ (F_{84}) with a Clar formula is illustrated in figure 11.

Acknowledgment

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