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On the Clar Number of Benzenoid Graphs

Nino Bašić[a], István Estélyi[b], Riste Škrekovski[c,d], Niko Tratnik[e]

[a] *Faculty of Mathematics, Natural Sciences and Information Technologies, University of Primorska, Slovenia*
nino.basic@famnit.upr.si

[b] *NTIS, University of West Bohemia, Czech Republic*
estelyii@gmail.com

[c] *Faculty of Mathematics and Physics, University of Ljubljana, Slovenia*
riste.skrekovski@fmf.uni-lj.si

[d] *Faculty of information studies, Novo mesto, Slovenia*

[e] *Faculty of Natural Sciences and Mathematics, University of Maribor, Slovenia*
niko.tratnik@um.si

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Abstract

A Clar set of a benzenoid graph B is a maximum set of independent alternating hexagons over all perfect matchings of B. The Clar number of B, denoted by $\mathrm{Cl}(B)$, is the number of hexagons in a Clar set for B. In this paper, we first prove some results on the independence number of subcubic trees to study the Clar number of catacondensed benzenoid graphs. As the main result of the paper we prove an upper bound for the Clar number of catacondensed benzenoid graphs and characterize the graphs that attain this bound. More precisely, it is shown that for a catacondensed benzenoid graph B with n hexagons $\mathrm{Cl}(B) \leq [(2n+1)/3]$.

1 Introduction

The Clar number of a molecular graph G (for example benzenoid graph, fullerene or carbon nanotube) is the maximum number of independent alternating hexagons over all perfect matchings of G. This concept originates from Clar's aromatic sextet theory [4] and has been studied in many papers for benzenoid graphs [13,17] and fullerenes [2,15,22,25]. Also, the connections between the Clar number and the Fries number (i.e. the maximum number of alternating hexagons over all perfect matchings) were investigated in [10,14,23] and some relations to linear programming were considered in [1,12]. In [16] an algorithm for computing the Clar number of a catacondensed benzenoid graph was proposed.

Moreover, matchings and perfect matchings of a molecular graph play an important role in many fields of chemical graph theory. For example, they are essentially used in studying resonance graphs [7], saturation number [3], enumeration of matchings [20], Hosoya index [5,24], Zhang-Zhang polynomial [21], forcing and anti-forcing numbers [19], internal Kekulé structures [9], etc. Furthermore, there are connections between resonance graphs and Clar sets [18].

In the present paper, we prove an upper bound for the Clar number of catacondensed benzenoid graphs and characterize the graphs that attain the bound. We proceed as follows. In the following section we first formally define all the important concepts. Since the problem of studying the Clar number of a catacondensed benzenoid graph can be transformed into the problem of studying the independence number of its dualist tree, in Section 3 we prove some results on the independence number of subcubic trees. Finally, in Section 4 we prove the upper bound and characterize all extremal graphs with respect to this bound.

2 Preliminaries

In the existing (both mathematical and chemical) literature, there is inconsistency in the terminology pertaining to (what we call here) "benzenoid graph". In order to avoid any confusion, we first define our objects.

A *benzenoid graph* is a 2-connected graph in which all inner faces are hexagons (and all hexagons are faces), such that two hexagons are either disjoint or have exactly one common edge, and no three hexagons share a common edge.

Note that in some literature it is assumed that a benzenoid graph can be embedded into the regular hexagonal lattice [11]. Obviously, our definition is more general and includes graphs that cannot be embedded into the regular hexagonal lattice. For more details on these definitions see [6].

Let B be a benzenoid graph. A vertex shared by three hexagons of B is called an *internal* vertex of B. A benzenoid graph is said to be *catacondensed* if it does not possess internal vertices. Otherwise it is called *pericondensed*.

A *matching* M in a graph G is a set of edges of G such that no two edges from M share a vertex. If every vertex of G is incident with an edge of M, the matching M is called a *perfect matching* (in chemistry perfect matchings are known as *Kekulé structures*). Let B be a benzenoid graph and h a hexagon of B. If M is a matching that contains exactly 3 edges of h, then h is an *M-alternating* hexagon. In such cases we often draw a circle in h.

Let B be a benzenoid graph. We say that some set of hexagons of B is *independent* (or that the hexagons from this set are independent) if these hexagons are pairwise disjoint. A *Clar set* C is a maximum set of independent M-alternating hexagons over all perfect matchings M of B. If C is a Clar set and M a perfect matching such that every hexagon from C is M-alternating, then we say that the perfect matching M *gives* Clar set C. The *Clar number* of B, denoted by $\mathrm{Cl}(B)$, is the number of hexagons in a Clar set for B. It is easy to observe that a Clar set C is a maximum set of independent hexagons such that the graph obtained from B by removing hexagons from C (and all the edges incident to these hexagons) has a perfect matching.

An *independent set* is a set of vertices in a graph G, no two of which are adjacent. A *maximum independent set* is an independent set of largest possible cardinality for a given graph G. This cardinality is called the *independence number* of G, and denoted by $\alpha(G)$.

A *vertex cover* of a graph is a set of vertices such that each edge of the graph is incident to at least one vertex of the set. Moreover, a graph G is called *subcubic* if the degree of any vertex of G is at most 3.

3 Auxiliary results on trees

In this section some results about the independence number of subcubic trees are proved. These results will be used to establish the main result of the paper. First we prove the following lemma.

Lemma 3.1 *Every tree with more than one vertex has a maximum independent set which contains all the leaves.*

Proof. Let T be any tree and I be an independent set of maximum size that contains as many leaves as possible. Suppose that there exists a leaf u of T such that $u \notin I$. Denote by v the only neighbour of u. We consider the following two cases:

- if $v \in I$, then the set $(I \setminus \{v\}) \cup \{u\}$ is an independent set of the same size as I and contains u, i.e. one more leaf than I,
- if $v \notin I$, then the set $I \cup \{u\}$ is an independent set of size bigger than the size of I.

In both cases, we obtain a contradiction that establishes the lemma. ■

In the next lemma an upper bound for the independence number is shown.

Lemma 3.2 *Let T be a subcubic tree on $n \geq 1$ vertices with independence number $\alpha(T)$. Then*

$$\alpha(T) \leq \left\lceil \frac{2n+1}{3} \right\rceil .$$

Proof. Let VC be a vertex cover of smallest size and let $|\mathrm{VC}| = \tau(T)$. Since any edge of T is incident with at least one vertex from VC, we have $|E(T)| \leq \sum_{v \in \mathrm{VC}} \deg(v)$. Moreover, $|E(T)| = n - 1$, since T is a tree, and $\sum_{v \in \mathrm{VC}} \deg(v) \leq 3\tau(T)$ since T is subcubic. Hence, $\tau(T) \geq \frac{n-1}{3}$. Substituting this to the Gallai identity $\alpha(T) + \tau(T) = n$ (see [8]) we get $\alpha(T) + \frac{n-1}{3} \leq n$, which can be rearranged to the desired form. ■

To state the main result of this section, one definition is needed.

Definition 3.3 *Let $k \geq 2$ be an integer. The tree T_k is composed of the path on vertices $v_1, \ldots, v_{2k+1}$ with $k-2$ additional leaves which are attached to the vertices $v_4, v_6, \ldots, v_{2k-2}$ (see Figure 1).*

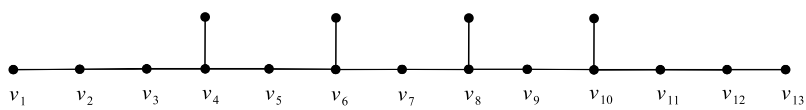

Figure 1. Tree T_6 from Definition 3.3.

In the following theorem we investigate subcubic trees for which the independence number attains the upper bound from Lemma 3.2.

Theorem 3.4 *Let T be a subcubic tree on $n \geq 3$ vertices with independence number $\left\lceil \frac{2n+1}{3} \right\rceil$. Then exactly one of the following statements holds:*

(i) T is a tree T_k with $k \geq 2$.

(ii) T has a vertex that is adjacent to (at least) two leaves.

Proof. Suppose that T satisfies the conditions of the theorem and that T does not have a vertex adjacent to (at least) two leaves. Denote by $\alpha(T)$ the independence number of T. Moreover, denote by ℓ the number of leaves of T. Each of these leaves has a unique neighbour, and by assumption all these neighbours are pairwise distinct. We will denote the set of all these neighbours by S. Moreover, let ℓ_1 be the number of vertices in the set S with degree two and let ℓ_2 be the number of vertices in the set S with degree three. Now, let T' be the forest obtained from T by removing all the leaves and their neighbours. Note that T' has $n' = n - 2\ell$ vertices and denote by r the number of connected components of T'. It is obvious that $r \leq \ell_2 + 1$. We will denote these components by $C_1, \ldots, C_r$ (see Figure 2). Also, let $|V(C_i)| = n_i$ for any $i \in \{1, \ldots, r\}$.

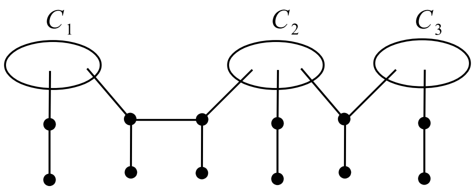

Figure 2. Tree T with $\ell = 6$, $\ell_1 = 3$, $\ell_2 = 3$ and connected components C_1, C_2, C_3 of T'.

Since any C_i is a tree, it follows by Lemma 3.2 that

$$\alpha(C_i) \leq \frac{2n_i + 1}{3}$$

for any $i \in \{1, \ldots, r\}$. Hence, we obtain

$$\alpha(T') \leq \sum_{i=1}^{r} \frac{2n_i + 1}{3} = \frac{2n' + r}{3} \leq \frac{2n' + \ell_2 + 1}{3}.$$

Moreover, by Lemma 3.1 it is easy to observe that

$$\alpha(T) = \alpha(T') + \ell. \tag{1}$$

Therefore, we have

$$\left\lceil \frac{2n+1}{3} \right\rceil \leq \frac{2n'+\ell_2+1}{3} + \ell = \frac{2n-\ell+\ell_2+1}{3}.$$

Since $\ell_1 = \ell - \ell_2$, we get

$$\left\lceil \frac{2n+1}{3} \right\rceil \leq \frac{2n-\ell_1+1}{3}. \tag{2}$$

In the following we first show that $\ell_1 \geq 2$. Let T'' be a tree obtained from T by removing all the leaves of T. Obviously, T'' has more than one vertex (otherwise T has less than three vertices or has a vertex with two leaves, which gives a contradiction in both cases) and therefore, it has at least two leaves. Since it is easy to see that the number of leaves in T'' is exactly ℓ_1, it follows that $\ell_1 \geq 2$. If $\ell_1 \geq 3$, we obtain a contradiction with (2) and therefore, $\ell_1 = 2$.

Next, we show that any connected component of T' is a path. Since we already know that the number of leaves in T'' is exactly ℓ_1, it follows that T'' has exactly two leaves. Therefore, T'' is a path. Since T' is obtained from T'' by removing some vertices, it is obvious that every connected component of T' is a path.

Suppose that T' has m isolated vertices ($0 \leq m \leq r \leq \ell_2+1$). Therefore, it has $r-m$ connected components isomorphic to a path on more than one vertex. It is obvious that $\alpha(\overline{K_m}) = m$, where $\overline{K_m}$ denotes the empty graph on m vertices, and $\alpha(P_j) \leq 2j/3$ for any $j \geq 2$, where P_j denotes the path on j vertices. Hence, we obtain

$$\alpha(T') \leq m + \frac{2}{3}(n-2\ell-m) = \frac{2n-4\ell+m}{3}$$

and by (1) it follows

$$\left\lceil \frac{2n+1}{3} \right\rceil \leq \frac{2n-\ell+m}{3}.$$

Obviously, if $\ell \geq m+2$ we obtain a contradiction with the previous inequality and therefore, $\ell \leq m+1$. Since $m \leq \ell_2+1 = \ell-1$ we also get $\ell \geq m+1$ and we deduce $\ell = m+1$. Hence, T' has $m = \ell-1 = \ell_2+1$ isolated vertices and since the number of connected components of T' is at most ℓ_2+1, the graph T' has exactly ℓ_2+1 connected components and all of them are isolated vertices. Therefore, T'' is a path on $2\ell-1$ vertices and finally, we can conclude that the original tree T can be obtained from a path of length $2\ell-1$ by attaching a leaf to every second vertex, starting with the first one, i.e., T is isomorphic to T_ℓ. Hence, the case (i) of the theorem holds and the proof is complete. ■

Lemma 3.5 *Let $k \geq 2$. Then for the tree T_k the independence number attains the upper bound from Lemma 3.2. Moreover, the maximum independent set is unique and contains vertices $v_1, v_3, \ldots, v_{2k-1}, v_{2k+1}$ and all the additional leaves.*

Proof. Let I be the set of vertices $v_1, v_3, \ldots, v_{2k-1}, v_{2k+1}$ and all the additional leaves. It is easy to check that I contains $2k-1$ vertices and that T_k has exactly $3k-1$ vertices. Therefore,

$$\alpha(T_k) = 2k - 1 = \left\lceil \frac{2(3k-1)+1}{3} \right\rceil$$

and we have shown that I is the maximum independent set and that for the tree T_k the independence number attains the upper bound from Lemma 3.2.

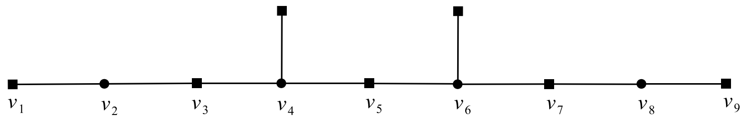

Figure 3. Tree T_4. Vertices in I are denoted with a square.

To prove the second part, suppose that I' is another maximum independent set in T_k. Since $I' \neq I$ there is some $u \in I'$ such that $u \notin I$. We consider two cases.

(a) *u is a vertex of degree 3.* Let T_k' be the graph obtained from T_k by removing u and all its neighbours. Obviously, T_k' has two connected components and we will denote them by C_0 and C_1. Let $I_j = I \cap V(C_j)$ for $j \in \{0, 1\}$. It is easy to check that I_j is a maximum independent set for C_j where $j \in \{0, 1\}$. Therefore, $|I'| = 1 + \alpha(C_0) + \alpha(C_1)$. On the other hand, we know that $|I| = 3 + \alpha(C_0) + \alpha(C_1)$. Since I' and I are both maximum independent sets, it holds $|I| = |I'|$ and we get a contradiction.

(b) *$u = v_2$ or $u = v_{2k}$.* Let T_k' be the graph obtained from T_k by removing u and all its neighbours. Let $I'' = I \cap V(T_k')$. It is easy to check that I'' is a maximum independent set for T_k'. Therefore, $|I'| = 1 + \alpha(T_k')$. On the other hand, we know that $|I| = 2 + \alpha(T_k')$. Since I' and I are both maximum independent sets, it holds $|I| = |I'|$ and we get a contradiction.

Since we get a contradiction in every case it follows that I is the unique maximum independent set for T_k. ∎

4 Catacondensed benzenoid graphs with large Clar number

In this section we prove an upper bound for the Clar number of catacondensed benzenoid graphs and characterize those graphs that attain this bound.

The *dualist* graph of a given benzenoid graph B consists of vertices corresponding to hexagons of B; two vertices are adjacent if and only if the corresponding hexagons have a common edge. Obviously, the dualist graph of B is a tree if and only if B is catacondensed. If B has n hexagons, then this tree has n vertices and none of its vertices have degree greater than 3 (so it is a subcubic tree). For a catacondensed benzenoid graph B we will denote its dualist tree by $T(B)$. For an example see Figure 4.

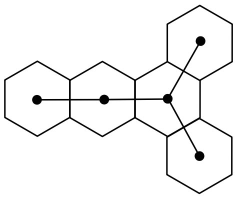

Figure 4. Benzenoid graph B with the dualist tree $T(B)$.

Lemma 4.1 *Let B be a catacondensed benzenoid graph with n hexagons. Then*

$$\mathrm{Cl}(B) \leq \left\lceil \frac{2n+1}{3} \right\rceil .$$

Proof. Let C be a Clar set for B and let $T(B)$ be a dualist tree of B. Obviously, the vertices corresponding to the hexagons of C form an independent set in $T(B)$. Therefore, by Lemma 3.2 we have

$$\mathrm{Cl}(B) \leq \alpha(T(B)) \leq \left\lceil \frac{2n+1}{3} \right\rceil .$$

■

A hexagon h of a benzenoid graph B adjacent to exactly two other hexagons possesses two vertices of degree 2. If these two vertices are adjacent, then h is *angularly connected*, for short we say that h is *angular*. If these two vertices are not adjacent, then h is *linearly connected*, and we say that h is *linear*.

To characterize graphs that attain the upper bound we need the following lemma.

Lemma 4.2 *Let B be a catacondensed benzenoid graph with n hexagons such that $T(B) \simeq T_k$ for some $k \geq 2$. Then* $\mathrm{Cl}(B) = \left[\frac{2n+1}{3}\right]$ *if and only if the two hexagons corresponding to vertices v_2 and v_{2k} are both angular.*

Proof. First suppose that the two hexagons corresponding to vertices v_2 and v_{2k} are both angular and we denote these hexagons by h and h'. It is obvious that any vertex of T_k different from v_2 and v_{2k} is either in the unique maximum independent set or has degree 3. We need to find a perfect matching M for B with exactly $\left[\frac{2n+1}{3}\right]$ independent M-alternating hexagons. Let M' be a matching containing exactly 3 edges from all the hexagons that correspond to the vertices in the unique maximum independent set of T_k. Moreover, let e and e' be the edges of h and h', respectively, with both end-vertices of degree 2. Finally, we define $M = M' \cup \{e, e'\}$ (see Figure 5). It is easy to check that M is a perfect matching for B and by Lemma 3.5 it has exactly $\left[\frac{2n+1}{3}\right]$ independent M-alternating hexagons. Therefore, $\mathrm{Cl}(B) = \left[\frac{2n+1}{3}\right]$.

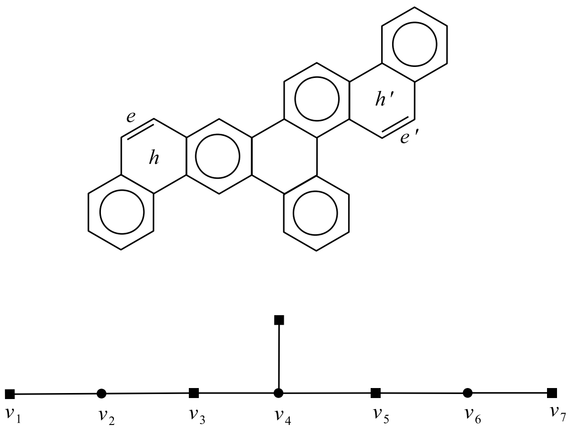

Figure 5. Benzenoid graph with a perfect matching M and the corresponding dualist tree T_3.

To show the other direction, suppose that $\mathrm{Cl}(B) = \left[\frac{2n+1}{3}\right]$. Hence, there is a Clar set C for B with exactly $\left[\frac{2n+1}{3}\right]$ hexagons. The vertices of $T(B) \simeq T_k$ corresponding to the hexagons from C form an independent set I of T_k. Since $|I| = \left[\frac{2n+1}{3}\right]$, set I is uniquely defined by Lemma 3.5. Let M be a perfect matching for B that gives Clar set C. Since $v_1, v_3 \in I$, the hexagons corresponding to the vertices v_1 and v_3 are M-alternating hexagons. If the hexagon corresponding to vertex v_2 is not angular, there are two vertices in this hexagon that are not incident with an edge from M, which is a contradiction. Therefore, the hexagon corresponding to v_2 is angular. In a similar way we can show that the hexagon corresponding to v_{2k} is also angular and the proof is complete. ■

Next, we define family $\mathcal{B}$ of catacondensed benzenoid graphs as follows:

(i) The benzenoid graph with one hexagon belongs to $\mathcal{B}$ and the benzenoid graph with two hexagons belongs to $\mathcal{B}$. If B_1 is a catacondensed benzenoid graph with three hexagons such that the hexagon adjacent to two other hexagons is angular, then B_1 belongs to $\mathcal{B}$ (see Figure 6).

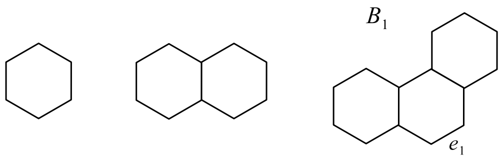

Figure 6. Benzenoid graphs from case (i).

(ii) Let B be a catacondensed benzenoid graph such that $T(B) \simeq T_k$ for some $k \geq 2$ and such that the two hexagons corresponding to vertices v_2 and v_{2k} are both angular. Then B belongs to $\mathcal{B}$.

(iii) Let B' be a catacondensed benzenoid graph from $\mathcal{B}$ and let e' be any edge of B' with both end-vertices of degree 2. Moreover, let B_1 be the benzenoid graph from Figure 6 and let e_1 be the edge of the angular hexagon with both end-vertices of degree 2. We define B to be a benzenoid graph obtained from B' and B_1 by identifying edges e' and e_1 (see Figure 7). Then B belongs to $\mathcal{B}$.

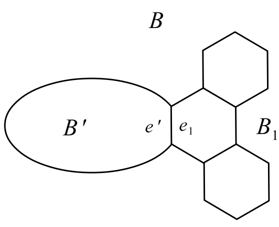

Figure 7. Benzenoid graph B obtained from $B' \in \mathcal{B}$ and B_1.

We notice that family $\mathcal{B}$ is defined inductively. Cases (i) and (ii) represent the basis and Case (iii) represents the inductive step. It is easy to observe that $\mathcal{B}$ contains only catacondensed benzenoid graphs. In Figure 8 we can see all catacondensed benzenoid graphs with five hexagons that belong to $\mathcal{B}$. The first two graphs are obtained using Case (i) and (iii), the other graphs are obtained from Case (ii). However, when we increase the number of hexagons, the number of such graphs in $\mathcal{B}$ becomes much higher.

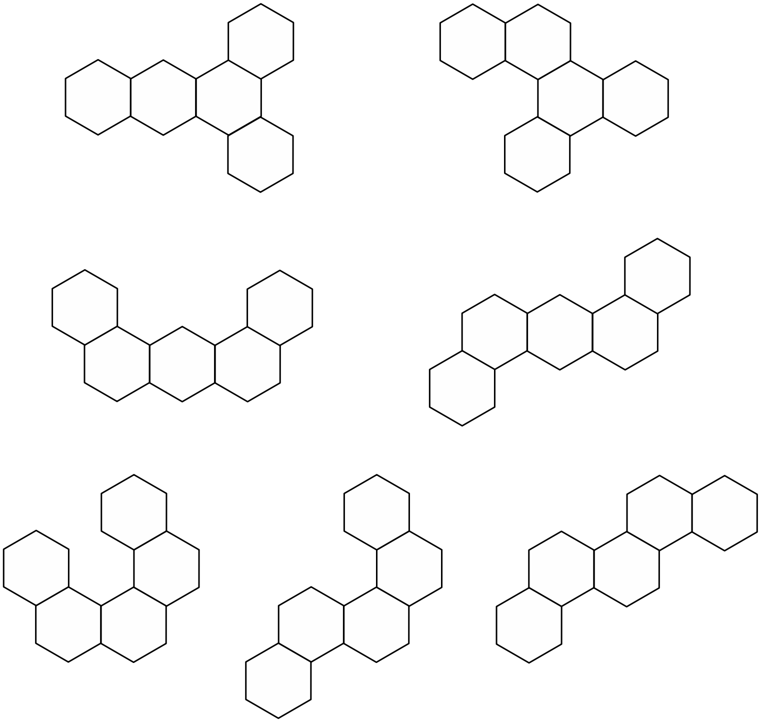

Figure 8. All graphs in $\mathcal{B}$ with exactly five hexagons.

Finally, we are able to prove the main result of this paper.

Theorem 4.3 *Let B be a catacondensed benzenoid graph with n hexagons. Then*

$$\mathrm{Cl}(B) \leq \left[\frac{2n+1}{3}\right]$$

and equality holds if and only if B belongs to $\mathcal{B}$.

Proof. The inequality follows by Lemma 4.1.

First, suppose that a benzenoid graph B with n hexagons belongs to $\mathcal{B}$. We will show that the Clar number of B attains the upper bound. Consider the following cases:

(i) If B has one hexagon, then $\mathrm{Cl}(B) = 1 = \left[\frac{2\cdot 1+1}{3}\right]$. If B has two hexagons, then $\mathrm{Cl}(B) = 1 = \left[\frac{2\cdot 2+1}{3}\right]$. Also, for B_1 it holds $\mathrm{Cl}(B_1) = 2 = \left[\frac{2\cdot 3+1}{3}\right]$.

(ii) If B is a catacondensed benzenoid graph such that $T(B) \simeq T_k$ for some $k \geq 2$ and such that the two hexagons corresponding to vertices v_2 and v_{2k} are both angular, then the Clar number of B attains the upper bound by Lemma 4.2.

(iii) Let B be obtained from $B' \in \mathcal{B}$ and B_1 by identifying edges e' and e_1 (see Figure 7). We use induction to prove that the Clar number of B attains the upper bound. The base step is proved in Case (i) and Case (ii). For the induction step, assume that B' has n' hexagons and that the Clar number of B' attains the upper bound, i.e. $\mathrm{Cl}(B') = \left[\frac{2n'+1}{3}\right]$. Hence, let M' be a perfect matching of B' with $\mathrm{Cl}(B')$ independent M'-alternating hexagons. Moreover, let M'' be a perfect matching of B_1 with two independent M''-alternating hexagons. Obviously, edge e_1 of B_1 belongs to M''. Finally, we define $M = M' \cup (M'' \setminus \{e_1\})$. Obviously, M is a perfect matching of B with exactly $\mathrm{Cl}(B') + 2$ independent M-alternating hexagons. Hence, we obtain

$$\mathrm{Cl}(B) \geq \mathrm{Cl}(B') + 2 = \left[\frac{2n'+1}{3}\right] + 2 = \left[\frac{2(n'+3)+1}{3}\right].$$

Since B has $n' + 3$ hexagons, by Lemma 4.1 we get

$$\mathrm{Cl}(B) = \left[\frac{2(n'+3)+1}{3}\right].$$

We have shown that if B belongs to $\mathcal{B}$, then the Clar number of B attains the upper bound.

For the other direction, suppose that B has n hexagons and that $\mathrm{Cl}(B) = \left[\frac{2n+1}{3}\right]$. We have to prove that B belongs to $\mathcal{B}$. Let C be a Clar set of B and let I be the set of vertices in $T(B)$ that correspond to the hexagons from C. Obviously, by Lemma 3.2, $\alpha(T(B)) = |I| = \left[\frac{2n+1}{3}\right]$. We consider two cases:

(a) *$T(B)$ does not have a vertex that is adjacent to (at least) two leaves.* By Theorem 3.4, $T(B)$ has at most two vertices or $T(B) \simeq T_k$ for some $k \geq 2$. In the last case, by Lemma 4.2, the two hexagons corresponding to vertices v_2 and v_{2k} are both angular. In both cases, B belongs to $\mathcal{B}$.

(b) *$T(B)$ has a vertex that is adjacent to (at least) two leaves.* If $T(B)$ has three vertices, then B has three hexagons and the hexagon adjacent to two other hexagons is angular (otherwise the Clar number does not attain the upper bound). Therefore, $B = B_1$ and B belongs to $\mathcal{B}$.

Now, suppose that $T(B)$ has more than three vertices. Then we have the situation from Figure 9. Let M be a perfect matching of B that gives the Clar set C. We will show that $h_2, h_3 \in C$. We will also denote by B_1 the subgraph of B composed of hexagons h_1, h_2, and h_3. Consider the following cases:

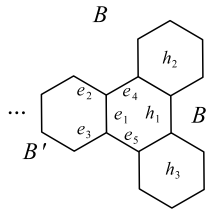

Figure 9. Benzenoid graph B with edges e_1, e_2, e_3, e_4, and e_5.

1. If $e_2, e_5 \in M$ or $e_3, e_4 \in M$, then we can easily see that M can not be a perfect matching, so this case can not happen.
2. If $e_4, e_5 \in M$, then hexagons h_2, h_3 are not M-alternating and perfect matching M can be changed to $\overline{M}$ (in subgraph B_1) so that h_2, h_3 are $\overline{M}$-alternating. Therefore, $\overline{C} = (C \setminus \{h_1\}) \cup \{h_2, h_3\}$ is a set of independent $\overline{M}$-alternating hexagons and $|\overline{C}| > |C|$, which is a contradiction.
3. If $e_1 \in M$ or $e_2, e_3 \in M$, then h_2, h_3 are M-alternating and $h_2, h_3 \in C$ (otherwise C is not a Clar set).

Since cases 1. and 2. can not happen, it follows that h_2, h_3 are M-alternating and $h_2, h_3 \in C$. We define B' to be the graph obtained from B by removing hexagons h_2 and h_3 and all the edges incident to h_2 or h_3. Moreover, let $M' = M \cap E(B')$. Obviously, $C' = C \setminus \{h_2, h_3\}$ is a set of independent M'-alternating hexagons and therefore,

$$\mathrm{Cl}(B') \geq \left\lceil \frac{2n+1}{3} \right\rceil - 2 = \left\lceil \frac{2(n-3)+1}{3} \right\rceil .$$

We know that B' has exactly $n-3$ hexagons and hence, by Lemma 4.1, $\mathrm{Cl}(B') = \left\lceil \frac{2(n-3)+1}{3} \right\rceil$. If $T(B')$ does not have a vertex that is adjacent to two leaves, then by Case (a) B' belongs to $\mathcal{B}$ and therefore, by definition of $\mathcal{B}$, also B belongs to $\mathcal{B}$. If $T(B')$ has a vertex that is adjacent to two leaves, then we can repeat the above procedure (at every step we remove 3 hexagons) until we get B'' such that $T(B'')$ does not have a vertex that is adjacent to two leaves. Again, it follows that B belongs to $\mathcal{B}$.

Since in every case we get that B belongs to $\mathcal{B}$, the proof is finished. ■

We conclude this section with two additional results.

Lemma 4.4 *Let B be a catacondensed benzenoid graph and h_0 a hexagon that is adjacent to at most one other hexagon. Moreover, let B' be a benzenoid graph obtained from B by adding k, $k \geq 1$, linearly connected hexagons to h_0 such that h_0 is also linearly connected (or adjacent only to h_1), see Figure 10. Then* $\mathrm{Cl}(B') = \mathrm{Cl}(B)$.

Proof. Denote the added hexagons by $h_1, \ldots, h_k$ and let C be a Clar set for B. See Figure 10.

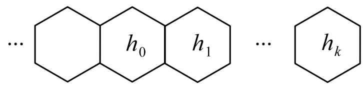

Figure 10. Adding hexagons $h_1, \ldots, h_k$.

Obviously, there is a perfect matching M' of B' such that C is an independent set of M'-alternating hexagons. Therefore, it follows $\mathrm{Cl}(B') \geq \mathrm{Cl}(B)$.

To show the equality, let C' be a Clar set for B'. Since hexagons $h_0, h_1, \ldots, h_k$ are linearly connected, at most one of these hexagons belongs to C'. Consider two cases.

- If one of hexagons $h_1, \ldots, h_k$ belongs to C', then it is possible to find a Clar set C'' for B' such that $h_0 \in C''$. Obviously, C'' is also a Clar set for B and $\mathrm{Cl}(B') = \mathrm{Cl}(B)$.
- If none of hexagons $h_1, \ldots, h_k$ belongs to C', then C' is also a Clar set for B and $\mathrm{Cl}(B') = \mathrm{Cl}(B)$.

In both cases we get $\mathrm{Cl}(B') = \mathrm{Cl}(B)$ and the proof is complete. ■

Next result follows by Lemma 4.4 and the main theorem.

Theorem 4.5 *Let n be a positive integer. Then for every $c \in \left\{1, 2, \ldots, \left[\frac{2n+1}{3}\right]\right\}$ there exists a catacondensed benzenoid graph B with n hexagons and with Clar number* $\mathrm{Cl}(B) =$ *c.*

Proof. Let n be a positive integer and $c \in \left\{1, 2, \ldots, \left[\frac{2n+1}{3}\right]\right\}$. If $c = \left[\frac{2n+1}{3}\right]$, then such a graph exists by Theorem 4.3. Now suppose that $c \leq \left[\frac{2n+1}{3}\right] - 1$. Then we obtain $c \leq \frac{2n-2}{3}$.

Let B' be a catacondensed benzenoid graph with n' hexagons such that $c = \left[\frac{2n'+1}{3}\right]$. Hence, $c > \frac{2n'-2}{3}$ and $n' < \frac{3c+2}{2}$. Finally, we get

$$n' < \frac{3c+2}{2} \leq \frac{3 \cdot \frac{2n-2}{3} + 2}{2} = n.$$

Therefore, we add $n - n'$ linearly connected hexagons to one hexagon (which corresponds to a vertex of degree at most one in $T(B')$) of B' to obtain B. Obviously, B has n hexagons and by Lemma 4.4, $\mathrm{Cl}(B) = c$. ■

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