Coronoids, Patches and Generalised Altans

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September 22, 2015

Abstract

In this paper we revisit coronoids, in particular multiple coronoids. We consider a mathematical formalisation of the theory of coronoid hydrocarbons that is solely based on incidence between hexagons of the infinite hexagonal grid in the plane. In parallel, we consider perforated patches, which generalise coronoids: in addition to hexagons, other polygons may also be present. Just as coronoids may be considered as benzenoids with holes, perforated patches are patches with holes. Both cases, coronoids and perforated patches, admit a generalisation of the altan operation that can be performed at several holes simultaneously. A formula for the number of Kekulé structures of a generalised altan can be derived easily if the number of Kekulé structures is known for the original graph. Pauling Bond Orders for generalised altans are also easy to derive from those of the original graph.

Keywords: altan, generalised altan, iterated altan, benzenoid, coronoid, patch, perforated patch, Kekulé structure, Pauling Bond Order

Math. Subj. Class. (2010): 92E10, 05C10, 05C90

1 Introduction

The term ‘altan’ was recently coined [30] to describe a particular type of conjugated π-system, defined by a notional expansion of the annulene-like perimeter of a parent hydrocarbon. Mathematical formalisation [19, 20] gives an operation that can be applied to any planar graph to produce the altan of the parent graph, and to predict consequent changes in various properties of mathematical/chemical interest. In a recent paper [1], basic properties of iterated altans were studied. For previous work on altans from both chemical and mathematical perspectives, the reader is referred to [1, 7, 8, 19, 20, 28, 29, 31]. In the present paper we apply successive altan operations, not to a single perimeter (or peripheral root, as it was called in [1]), but to a collection of disjoint perimeters. In particular, a composite operation of this type applies well to general coronoids [5, 21], which, unlike benzenoids, may possess more than one perimeter. In addition to the outer

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perimeter they have a perimeter for each of the holes. We call this operation a *generalised altan*. Owing to its generality it applies to *single* coronoids, i.e., to coronoids possessing exactly one corona hole, and *multiple* coronoids, i.e., coronoids possessing more than one corona hole. It seems that in the past investigations of coronoids mostly *single coronoids* were considered [5, 21].

Finally, we consider Kekulé structures [6] of generalised altans. It turns out to determine the number of Kekulé structures of a generalised altan, if the number of Kekulé structures are known for the original graph.

In a previous paper we shifted attention from benzenoids to the more general subcubic planar graphs that we called *patches*, which generalise the *fullerene patches* of Graver et al. [11, 12, 13, 14, 15, 16]. In this paper, we similarly generalise coronoids to *perforated patches*, i.e., to patches with several disjoint holes.

### 2 Hexagonal Systems, Coronoids and Benzenoids

Traditionally, a *benzenoid* is a collection of hexagons that constitute a simply connected bounded region of the infinite hexagonal grid $H$ in the Euclidean plane. Other equivalent definitions are also possible. For a complete treatment of this topic, see [21]. Many authors consider benzenoids as plane graphs. Take a benzenoid. Note that one of its faces, called the *outer face*, is unbounded. Moreover, every edge is incident to exactly two distinct faces (of which one may be the outer face). Every vertex is incident to 2 or 3 edges. Therefore, a benzenoid graph is 2-connected and 2-edge-connected. In a chemical context, we use terms *atom* and *bond* as synonyms for respective vertex and edge. Intuitively speaking, a *coronoid* is a “benzenoid with holes”, i.e., a benzenoid with some internal bonds and atoms removed. To precisely define the class of coronoids, some additional restrictions are needed. Normally, the resulting structure must be composed entirely of hexagons and connected if it is to be of interest in the theory of conjugated carbon frameworks. Although the two plane graphs on Figure 1 can be obtained from benzenoids by removing vertices and edges, they are not coronoids. This motivates the following mathematical formalisation of coronoids and benzenoids.

In this paper, we will consider the infinite planar hexagonal grid $H$ as a collection of hexagons. Let $a$ and $b$ be two hexagons from $H$. We say that $a$ and $b$ are *adjacent*, and denote this by $a \sim b$, if and only if they are different and share an edge. If two distinct hexagons share an edge we call them *neighbours*. The set of all neighbours of $a$ will be denoted $N(a)$. Note that each hexagon of $H$ has exactly 6 neighbours. Let $K \subseteq H$ be a *hexagonal system*, i.e., an arbitrary collection of hexagons from $H$. $N_K(a)$ will denote the

Figure 1: These two plane graphs are not coronoids. The edge denoted by $a$ (in both examples) is not incident to two distinct faces.
set of those hexagons of $K$ that belong to $N(a)$, i.e., $N_K(a) := N(a) \cap K$. We call them the neighbours of $a$ in $K$. Define equivalence relation $\equiv_K$ as follows: for $a, b \in K$ it holds that $a \equiv_K b$ if there exists a sequence $c_0 = a, c_1, c_2, \ldots, c_m = b$ such that $c_{i-1} \sim c_i$ for $i = 1, 2, \ldots, m$ and $c_i \in K$ for $i = 0, 1, \ldots, m$. In particular, this means that it is possible to move from hexagon $a$ to hexagon $b$ along a pathway composed of adjacent hexagons that all belong to $K$ (see Figure 2). Note that $a \equiv_K b$ if $a \in N_K(b)$ and $b \in K$. Also, it is easy to see that $K \subseteq L$ and $a \equiv_K b$ imply $a \equiv_L b$. Hexagonal system $K$ is naturally decomposed into equivalence classes $\{C_i\}_{i \in C(K)}$, called connected components. Of course, $K = \bigcup_{i \in C(K)} C_i$. If $K$ is finite, the number of its connected components, i.e., the cardinality of $C(K)$, is also finite. A hexagonal system is connected if it comprises only one connected component.

**Lemma 1.** Let $K$ be a hexagonal system and $\{C_i\}_{i \in C(K)}$ its decomposition into equivalence classes. Let $L$ be a connected hexagonal system. If $L \subseteq K$ then $L \subseteq C_i$ for some $i \in C(K)$.

**Proof.** Suppose there exist hexagons $h_i \in L \cap C_i$ and $h_j \in L \cap C_j$. Connectedness of $L$ implies $h_i \equiv_L h_j$. From $L \subseteq K$ it follows that $h_i \equiv_K h_j$. A contradiction. \hfill \Box

**Lemma 2.** Let $K \neq \emptyset$ be an arbitrary hexagonal system and $a \in K$ any of its hexagons. Then hexagon $a$ belongs to some connected component $C_i$ of $K$. Let $b \in N(a)$ be any of the neighbours of $a$ in $H$. Then either $b \in C_i$ or $b \in K^C$. In other words, no hexagon of $C_i$ is adjacent to a hexagon of $C_j$ if $i \neq j$.

**Proof.** Suppose there is a hexagon $b \in C_j$, $i \neq j$, such that $b \in N(a)$. Then $a$ and $b$ are in the same equivalence class by the definition of $\equiv_K$. A contradiction. \hfill \Box

**Lemma 3.** Let $K$ be an arbitrary non-empty hexagonal system that is a proper subset of $H$, i.e., $\emptyset \neq K \subset H$. Let $C_a$ be any connected component of the complement $K^C$. Then there exists a hexagon $\bar{a} \in C_a$ that is adjacent to some hexagon in $K$.

**Proof.** Let $N(R)$ denote the set of all hexagons that are not contained in $R$ and are adjacent to some member of $R$, i.e., $N(R) = (\cup_{r \in R} N(r)) \setminus R$. Let $a \in C_a$ and let $P_0 = \{a\}$. Define $P_k = P_{k-1} \cup N(P_{k-1})$ for $k \geq 1$.

It is clear that $P_0 \subseteq C_a$. Let $n$ be the smallest number such that $P_n \not\subseteq C_a$. Suppose that such a number $n$ exists. Note that $P_{n-1} \subseteq C_a$. Then $P_n$ contains some hexagon $h \not\in C_a$. By Lemma 2, $h \in K$. By construction of family $\{P_k\}_k$, there exists a hexagon $\bar{a} \in P_{n-1}$, such that $\bar{a} \in N(\bar{a})$.

Now suppose that the desired number $n$ does not exist. This means that $P_n \subseteq C_a$ for all $n$. But $\cup_{n=0}^\infty P_n = H$, i.e., for every $h \in H$ there exists some number $m$, s.t. $h \in P_m$. Since $K$ is non-empty there is some hexagon $k \in K \subset H$ and therefore $k \in P_l$ for some number $l$, which is a contradiction. \hfill \Box

Figure 2: A path of hexagons $h_1, h_2, \ldots, h_6$ joining hexagon $a$ to hexagon $b$. 
Definition 4. A finite connected hexagonal system $\mathcal{K}$ is called a (general) coronoid.

Definition 5. A finite connected hexagonal system $\mathcal{K}$ whose complement $\mathcal{K}^c$ is also connected is called a benzenoid.

We prove a useful lemma:

Lemma 6. Let $\mathcal{K}$ be any finite hexagonal system. Then the complement $\mathcal{K}^c$ of $\mathcal{K}$ consists of finitely many, say $d + 1$, $d \geq 0$, connected components:

$$\mathcal{K}^c = C_\infty \sqcup C_1 \sqcup C_2 \sqcup \cdots \sqcup C_d.$$  

All of these components but one, denoted by $C_\infty$, is finite. Each of the finite components $C_i$, $1 \leq i \leq d$, is a coronoid.

Component $C_\infty$ is called the exterior of $\mathcal{K}$ and each $C_i$, $1 \leq i \leq d$, is called a corona hole. In the above expression $\sqcup$ stands for disjoint union. The size of a coronoid $\mathcal{K}$, denoted $|\mathcal{K}|$, is the cardinality of the set $\mathcal{K}$, i.e., the number of hexagons it consists.

Proof. Let $a$ be an arbitrary hexagon of $\mathcal{H}$. Let the family $\{\mathcal{P}_i\}_{i=0}^\infty$ be as defined in the proof of Lemma 3. Since $\mathcal{K}$ is finite, there exists $n \in \mathbb{N}$ such that $\mathcal{K} \subseteq \mathcal{P}_n$. (More precisely, for every $k \in \mathcal{K}$ there exists $n_k$ such that $k \in \mathcal{P}_{n_k}$. Take $n := \max_{k \in \mathcal{K}} n_k$.) The complement of $\mathcal{P} := \mathcal{P}_n$ is contained in $\mathcal{K}^c$. Because $\mathcal{P}^c$ is connected, it is contained in a connected components of $\mathcal{K}^c$. Denote this component by $C_\infty$. Note that this is the infinite component. In addition to $C_\infty$, $\mathcal{K}^c$ may have more connected components. All of them (if there are any) are contained in $\mathcal{P}$. Each is finite, because $\mathcal{P}$ is finite. Their number is bounded by the number of hexagons in $\mathcal{P}$. Therefore, $\mathcal{K}^c$ has finitely many connected components.

The fact that all finite components are coronoids is clear from the definition of coronoids.

The above lemma does not apply to infinite hexagonal systems. (See Figure 3 for examples.)

![Figure 3](image-url)

Figure 3: $\mathcal{K}_1$ consists of infinitely many disjoint infinite lines of hexagons. Its complement has infinitely many connected components that are themselves infinite. $\mathcal{K}_2$ is obtained from $\mathcal{K}_1$ by adding another line of hexagons with a different slope. The hexagonal system $\mathcal{K}_2$ is a connected example. Hexagonal system $\mathcal{K}_3$ (half-plane) is infinite and its complement $\mathcal{K}_3^c$ has a single connected component. In fact, a connected hexagonal system with arbitrary many finite and arbitrary many infinite connected components can be obtained.
Lemma 7. Let \( K \) be a coronoid and let \( C_a \) and \( C_b \) be two connected components of its complement \( K^C \). Let \( a \in C_a \) and \( b \in C_b \). Then \( a \equiv_{K \cup C_a \cup C_b} b \).

Components \( C_a \) and \( C_b \) in the above lemma may be either two corona holes or one corona hole and the exterior of \( K \).

Proof. By Lemma 6 there exists \( \tilde{a} \in C_a \), such that \( \tilde{a} \in N(k_a) \) for some \( k_a \in K \). By the same lemma, there exists \( \tilde{b} \in C_b \), such that \( \tilde{b} \in N(k_b) \) for some \( k_b \in K \). Since \( C_a \) is a connected component, \( a \equiv_{C_a} \tilde{a} \). Similarly, \( b \equiv_{C_b} \tilde{b} \). From \( \tilde{a} \equiv_{K \cup C_a} k_a \), \( \tilde{b} \equiv_{K \cup C_b} k_b \) and \( k_a \equiv_{K} k_b \), it follows that \( a \equiv_{K \cup C_a \cup C_b} b \). \( \square \)

Corollary 8. Let \( K \) be a coronoid and let \( C_a \) be a connected component of its complement \( K^C \). Let \( a \in C_a \) and \( k \in K \). Then \( a \equiv_{K \cup C_a} k \).

Proof. In the proof of Lemma 7 we have already shown the existence of \( \tilde{a} \in C_a \), such that \( \tilde{a} \in N(k_a) \) for some \( k_a \in K \). From \( a \equiv_{C_a} \tilde{a} \), \( \tilde{a} \equiv_{K \cup C_a} k_a \) and \( k_a \equiv_{K} k \), it follows that \( a \equiv_{K \cup C_a} k \). \( \square \)

Theorem 9. Let \( K \) be a coronoid. The complement \( K^C \) of \( K \) has a finite number \( b(K) := d + 1 \), \( d \geq 0 \), of connected components \( B_\infty, B_1, B_2, \ldots, B_d \) such that

\[
K^C = B_\infty \sqcup B_1 \sqcup B_2 \sqcup \cdots \sqcup B_d.
\]

Exactly one component, denoted \( B_\infty \), is infinite and the other \( d \) components are finite, each being a benzenoid. Moreover, \( B_\infty^C \) is also a benzenoid.

Proof. From Lemma 6 it immediately follows that \( K^C = B_\infty \sqcup B_1 \sqcup B_2 \sqcup \cdots \sqcup B_d \), where \( B_\infty \) is an infinite and \( B_i \), \( 1 \leq i \leq d \), are finite connected components. We need to show that each \( B_i \), \( 1 \leq i \leq d \), is a benzenoid.

It only remains to show that the complement \( B_i^C \) of \( B_i \), \( 1 \leq i \leq d \), is connected. From \( \mathcal{H} = K \sqcup K^C = K \sqcup (B_\infty \sqcup B_1 \sqcup B_2 \sqcup \cdots \sqcup B_d) \) it follows that

\[
B_i^C = K \sqcup B_\infty \sqcup B_1 \sqcup B_2 \sqcup \cdots \sqcup B_{i-1} \sqcup B_{i+1} \sqcup \cdots \sqcup B_d.
\]

Hexagonal systems \( K, B_\infty, B_1, \ldots, B_{i-1}, B_{i+1}, \ldots, B_d \) are all connected. By Lemma 7 and Corollary 8 their union is also connected.

To show that \( B_\infty^C \) is a benzenoid, we need to show that \( B_\infty^C \) and \( (B_\infty^C)^C \) are connected and that \( B_\infty^C \) is finite. Since \( (B_\infty^C)^C = B_\infty \), it is clearly connected. Since

\[
B_\infty^C = K \sqcup B_1 \sqcup B_2 \sqcup \cdots \sqcup B_d,
\]

it is connected by the same argument that worked for \( B_\infty^C \) above. Hexagonal systems \( K, B_1, \ldots, B_d \) are all finite and therefore their union \( B_\infty^C \) is also finite. \( \square \)

Definition 10. Let \( K \) be a coronoid. The benzenoid closure of \( K \), denoted \( \overline{K} \), is the intersection of all those benzenoids that include \( K \) as a subset, i.e.,

\[
\overline{K} = \bigcap \{ B \mid B \text{ is benzenoid} \land K \subseteq B \}.
\]

For a coronoid \( K \) we define \( Benz(K) = \{ B \mid B \text{ is benzenoid} \land K \subseteq B \} \). This set will be repeatedly used in several proofs that follow. Using this terminology, \( \overline{K} \) from the above definition can be written in a shorter form as \( \overline{K} = \bigcap Benz(K) \).
Lemma 11. Benzenoid closure $\overline{K}$ of a (general) coronoid $K$ is a benzenoid. Moreover, $\overline{K} = B^c_\infty = K \cup B_1 \sqcup \cdots \sqcup B_d$, where $K^c = B_\infty \sqcup B_1 \sqcup B_2 \sqcup \cdots \sqcup B_d$ as in Theorem 9.

Proof. By Theorem 9, $K^c = B_\infty \sqcup B_1 \sqcup B_2 \sqcup \cdots \sqcup B_d$, where $B_\infty$ is infinite and $B_i$, $1 \leq i \leq d$, are benzenoids. We will show that $\overline{K} = K \cup B_1 \sqcup \cdots \sqcup B_d = B^c_\infty$.

Let $L$ be an arbitrary benzenoid such that $K \subseteq L$. Then $L^c \subseteq K^c$. Because $L^c$ is connected, it is contained in at most one of components $B_\infty, B_1, B_2, \ldots, B_d$. Since $L^c$ is infinite, $L^c \subseteq B_\infty$. Therefore,

$$K \cup B_1 \sqcup B_2 \sqcup \cdots \sqcup B_d = B^c_\infty \subseteq (L^c)^c = L.$$  

This implies $K \cup B_1 \cup B_2 \cup \cdots \cup B_d \subseteq \overline{K}$.

By Theorem 9, $B^c_\infty = K \cup B_1 \sqcup \cdots \sqcup B_d$ is a benzenoid. Thus $\overline{K} \subseteq K \cup B_1 \sqcup \cdots \sqcup B_d$. We have proved that $\overline{K} = K \cup B_1 \sqcup \cdots \sqcup B_d$, where $K \cup B_1 \sqcup \cdots \sqcup B_d$ is a benzenoid. This proves existence, and also uniqueness, of $\overline{K}$. □

In the above proof of Lemma 11 we have also shown how to construct $\overline{K}$ for a given $K$. Reader should note that in general case the intersection of two benzenoids is not necessarily a benzenoid (see Figure 4).

Proposition 12. The benzenoid closure $K \mapsto \overline{K}$ is an operation on the set of all coronoids that satisfies the following three conditions:

(a) $\forall K: K \subseteq \overline{K},$

(b) $\forall K, L: K \subseteq L \implies \overline{K} \subseteq \overline{L}$, and

(c) $\forall K: \overline{K} = K$.

Note that the co-domain of the mapping $K \mapsto \overline{K}$ can be restricted to the set of all benzenoids. This mapping is surjective and the preimage of every benzenoid is a finite set of coronoids.

Proof. By definition, $\overline{K} = \bigcap Benz(K)$. From the definition it follows directly that $K \subseteq \overline{K}$.

Let us now show that $\overline{K} = \overline{\overline{K}}$. By definition, $\overline{K} = \bigcap Benz(K)$. Therefore $\overline{K} \subseteq \overline{K}$. Since $\overline{K}$ is a benzenoid, $\overline{K} \in Benz(\overline{K})$. Therefore, $\overline{K} \subseteq \overline{K}$.

Finally, we will show that $K \subseteq L \implies \overline{K} \subseteq \overline{L}$. By definition, $\overline{K} = \bigcap Benz(K)$ and $\overline{L} = \bigcap Benz(L)$. From $K \subseteq L$ it follows that every element of $Benz(L)$ is also an element of $Benz(K)$, i.e., $Benz(L) \subseteq Benz(K)$. Therefore, $\overline{K} \subseteq \overline{L}$. □

We define another closure operation.

Definition 13. An alternative benzenoid closure $\overline{K} \mapsto \widetilde{K}$ is a mapping on the set of all coronoids that satisfies the following three conditions:

(i) $\forall K: \widetilde{K}$ is benzenoid,

(ii) $\forall K: K \subseteq \widetilde{K}$, and

(iii) $\forall K: \forall$ benzenoid $L: K \subseteq L \implies \widetilde{K} \subseteq L$. 

6
The following lemma tells us that this corresponds to an alternative definition of the benzenoid closure operation.

**Lemma 14.** Let \( K \) be a general coronoid. Then \( \tilde{K} = \overline{K} \). With other words, benzenoid closure operation and the alternative benzenoid closure operation coincide.

**Proof.** First, we will prove existence of \( \tilde{K} \) by proving that \( K \) satisfies the three conditions of Definition 13.

By Lemma 11, \( K \) is a benzenoid, so (i) holds. Proposition 12 tells us that \( K \subseteq \overline{K} \), so (ii) also holds. It only remains to see that \( K \subseteq L \implies \overline{K} \subseteq L \) for every benzenoid \( L \).

Let \( L \) be any benzenoid such that \( K \subseteq L \). By definition, \( L \in \text{Benz}(K) \). It is clear that \( L \in \text{Benz}(K) \) implies \( \overline{K} = \bigcap \text{Benz}(K) \subseteq L \).

In principle, there could exist some other benzenoid, different from \( K \), which would also satisfy the three conditions in Definition 13. We will show that this is not the case by proving that every \( \tilde{K} \) from Definition 13 is \( K \).

Let \( L \) be any element of \( \text{Benz}(K) \). Condition (iii) implies that \( \tilde{K} \subseteq L \). Therefore \( \tilde{K} \subseteq \bigcap \text{Benz}(K) = \overline{K} \). By condition (i) and (ii), \( \tilde{K} \) is a benzenoid such that \( K \subseteq \tilde{K} \). This means that \( \tilde{K} \) is a member of \( \text{Benz}(K) \). Clearly, \( \overline{K} = \bigcap \text{Benz}(K) \subseteq \tilde{K} \). From \( \tilde{K} \subseteq \overline{K} \) and \( \tilde{K} \subseteq \overline{K} \) it follows that \( \tilde{K} = \overline{K} \) which completes the proof. \( \square \)

![Figure 4: The intersection of two benzenoids is not necessarily a benzenoid.](image)

**Lemma 15.** The intersection of two benzenoids is the disjoint union of finitely many benzenoids.

**Proof.** Let \( L_a \) and \( L_b \) be two benzenoids and let \( L = L_a \cap L_b \). Because \( L_a \) and \( L_b \) are finite, \( L \) is also finite. It consists of finitely many (possibly 0) finite connected components. That allows us to write \( L = K_1 \sqcup K_2 \sqcup \cdots \sqcup K_d \). To complete the proof, we have to show that each \( K_i \) is connected.

By Lemma 6, \( K_i^c = C_\infty \sqcup C_1 \sqcup C_2 \sqcup \cdots \sqcup C_m \). From \( K_i \subseteq L \subseteq L_a \) we obtain \( L_a^c \subseteq K_i^c \). Since \( L_a^c \) is connected and infinite, \( L_a^c \subseteq C_\infty \). In addition to \( C_\infty \), \( K_i^c \) may have 0 or more other connected components. Suppose \( m \geq 1 \).

By Lemma 3, there exists \( h \in C_1 \) which is adjacent to some \( k \in K_i \). Then \( h \notin L_a \) or \( h \notin L_b \). If \( h \) belonged to both \( L_a \) and \( L_b \), then \( h \in K_j \) for some \( j \). From \( h \in C_1 \subseteq K_i^c \), it follows that \( j \neq i \). But this contradicts Lemma 2, so \( h \) indeed belongs to at most one of \( L_a \) or \( L_b \). Without loss of generality, we can assume \( h \notin L_a \). In other words, \( h \in L_b^c \subseteq C_\infty \). This contradicts the fact that \( h \in C_1 \).

This means that \( m = 0 \), implying \( K_i^c = C_\infty \), and the proof is complete. \( \square \)
Look at Figure 5. Benzenoids $K_1 = \{h_1, h_2, h_3, h_4\}$ and $K_2 = \{h_5, h_6, h_7, h_8\}$ are equivalent. Benzenoids $K_1$ and $K_2$ are not equal, i.e., $K_1 \neq K_2$. For instance, $h_1 \in K_1$ but $h_1 \notin K_2$. If one would draw them on a piece of paper and cut them out, they would coincide. This notion of coincidence can be precisely defined. Let $\text{Aut}(\mathcal{H})$ be the group of symmetries of the hexagonal grid, i.e., isometries of the plane that map hexagons to hexagons. (For more details on this topic see [17].) If the coordinate system is placed so that the origin is in the centre of a chosen hexagon and if hexagons have sides of unit length then isometries $\phi_1, \phi_2, \phi_3, \phi_4 : \mathbb{R}^2 \to \mathbb{R}^2$, where

$$
\begin{align*}
\phi_1(x, y) &= (x + \sqrt{3}, y), \\
\phi_2(x, y) &= (x + \frac{\sqrt{3}}{2}, y + \frac{3}{2}), \\
\phi_3(x, y) &= (-x, y), \quad \text{and} \\
\phi_4(x, y) &= (x \cdot \cos \frac{\pi}{3} - y \cdot \sin \frac{\pi}{3}, x \cdot \sin \frac{\pi}{3} + y \cdot \cos \frac{\pi}{3})
\end{align*}
$$

generate the group $\text{Aut}(\mathcal{H})$. Now, we can define:

**Definition 16.** Hexagonal systems $\mathcal{K}$ and $\mathcal{L}$ are equivalent, denoted $\mathcal{K} \cong \mathcal{L}$, if there exists an isometry $\psi \in \text{Aut}(\mathcal{H})$, such that $\psi(\mathcal{K}) = \mathcal{L}$.

Let $\mathcal{K}$ be a (general) coronoid. From Lemma [11] it follows that

$$\overline{\mathcal{K}} \setminus \mathcal{K} = B_1 \sqcup \cdots \sqcup B_d \quad (d \geq 0),$$

where each $B_i$ is a benzenoid. The benzenoids $B_i$ are called corona holes. They consist of one or more hexagons. The (general) coronoids (a) and (b) in Figure 6 have two corona holes each, whilst coronoid (c) has only one. Examples (b) and (c) are special in a sense. A general coronoid is called degenerate if one of its corona holes is a single hexagon. This is because such a corona hole has no interpretation in chemistry. Otherwise it is called non-degenerate. Corona holes of size 1 will be called degenerate corona holes.

**Definition 17.** Let $\mathcal{K}$ be any coronoid. Non-degenerate closure of $\mathcal{K}$, denoted $\text{NonDeg}(\mathcal{K})$, is the smallest non-degenerate coronoid which includes $\mathcal{K}$.

It is not hard to see that $\text{NonDeg}(\mathcal{K})$ can be obtained from $\mathcal{K}$ by adding to it exactly its degenerate corona holes. Later in this paper, where we consider applications of this theory in chemistry, by the word coronoid we will always mean a non-degenerate coronoid.

The definition of coronoids includes benzenoids as a special case. A proper coronoid is one that is not also a benzenoid. Using the terminology of topology one may say that the only difference between benzenoids and proper coronoids is that both are connected, but the former are also simply connected. To give a precise meaning to this, one has to consider benzenoids as surfaces with a boundary. Plane graphs on their own are not
sufficient model for coronoids. Some faces have to be labelled as “not present”. We will call them 
holes. In this context, the outer face of a coronoid is merely one of its holes. Chemists do not always 
distinguish between the two models (coronoids as plane graphs and coronoids as surfaces with 
boundary); for them, exactly those faces of length strictly greater than 6 are holes. In other words, 
they do not recognise degenerate corona holes. As we will see later, when we generalise coronoids to 
perforated patches, some care should be taken over this distinction.

We defined coronoids (and benzenoids) as subsets of hexagons in the Euclidean plane. We may 
consider them as 2-dimensional cell complexes \[24\]. In what follows, we will adopt some topological 
terminology and notation. The infinite hexagonal grid \(\mathcal{H}\) can be obtained by embedding the 
infinite cubic graph called hexagonal lattice \[22\] in the Euclidean plane. Vertices of the hexagonal 
lattice are 0-cells, edges are 1-cells and faces are 2-cells. Every edge of the hexagonal lattice is 
incident to exactly two distinct hexagonal faces. Any two distinct faces can either share a single 
edge or nothing at all.

Let \(K\) be a coronoid. By our definition it is a collection of 2-cells. We can assign to \(K\) the 
smallest subcomplex of the hexagonal grid which includes all hexagons (2-cells) of \(K\). Note that a 
subcomplex contains the closure of each of its cells. Its 1-skeleton is a graph that is a subgraph of 
the hexagonal lattice consisting of those vertices and edges which are incident with at least one hexagon of \(K\). We will denote this graph by \(G(K)\) and call it a skeleton in the general setting and a 
coronoid graph when we deal with coronoids. Note that if \(\mathcal{H}\) denotes the hexagonal grid, then 
\(G(\mathcal{H})\) is the hexagonal lattice. Note that \(\text{Aut}(G(\mathcal{H}))\) acts transitively on vertices of 
\(G(\mathcal{H})\). Elements of \(\text{Aut}(G(\mathcal{H}))\) are graph automorphisms.

Consider the three examples of coronoids on Figure 6. As in the case of benzenoids, every edge is 
incident to exactly two distinct faces of which one may be a hole, but not both. Every vertex is 
incident to either 2 or 3 edges. A coronoid graph is a 2-connected and 2-edge-connected graph.

The edges of a coronoid graph are naturally divided into two types: internal and boundary. An 
edge belonging to two (adjacent) hexagons is internal and an edge belonging to only one hexagon is 
a boundary edge. Vertices of a coronoid graph can also be divided into internal and boundary. Internal 
vertices are incident with 3 internal edges. All other vertices of \(G(K)\) are called boundary. Boundary 
vertices can be further divided into two types: those of degree 2 and those of degree 3. A hexagon \(h\) of 
a coronoid \(K\) is internal if \(|N_K(h)| = 6\). Otherwise it is a boundary hexagon. In other words, an internal
hexagon is surrounded by 6 internal edges. The subgraph of $G(K)$ that consists of all boundary vertices and edges will be called border of $K$ and denoted $\partial K$. When $K = \{k\}$ is a singleton, we will write $\partial k$. A benzenoid is called catacondensed if it has no internal vertices, and pericondensed otherwise. Pericondensed benzenoids can be further divided into two groups: those with internal hexagons which we call corpulent benzenoids and those without internal hexagons which we call gaunt benzenoids.

**Proposition 18.** The girth of the infinite hexagonal lattice is 6, i.e.,

$$\text{girth}(G(H)) = 6.$$

Let $C$ be an arbitrary cycle of $G(H)$. Then $|C| = 6$ if and only if there exists a hexagon $h \in H$ such that $C = \partial h$.

**Proof.** Let $h \in H$ be any hexagon. Then $\partial h \cong C_6$. We will show that there are no shorter cycles and also that all 6-cycles are the borders of hexagonal faces of the hexagonal grid.

The distance between vertices $u$ and $v$ of a graph $G$ is the length of the shortest path between $u$ and $v$ in $G$. We will denote it by $d_G(u,v)$.

Owing to symmetry, to investigate the structural properties of cycles of $G(H)$ it is enough to investigate cycles that contain a given vertex $u$. Up to symmetries of $G(H)$ there is only one path of length 2. See Figure 7. Vertices $u$ and $v$ are not adjacent, so there are no triangles in $G(H)$. There are two possible paths of length 3 (see Figure 8). In both the endpoints are not adjacent, so there are no rectangles in $G(H)$. Both paths of length 3 can be extended in two ways yielding four paths of length 4 (see Figure 9). In all cases their endpoints are non-adjacent, so there are no 5-cycles in $G(H)$. In cases (i), (ii) and (iii) we have that $d(u,v) = 4$. Therefore, these paths cannot form 6-cycles. The case (iv) can be extended to a 5-path in two ways (see Figure 10). In case (b), we have that $d(u,v) = 3$, which means that no 6-cycle can be formed. In case (a), vertices $u$ and $v$ are adjacent and therefore form a 6-cycle. We have examined all options and no other 6-cycles arise, which means that all of them can be obtained as borders of hexagons. □

Note that every vertex of $G(K)$ belongs to one, two or three 6-cycles and that every edge of $G(K)$ belongs to one or two 6-cycles. Because $G(K) \subseteq G(H)$, every 6-cycle of $G(K)$ is
also a 6-cycle of $G(\mathcal{H})$. Therefore, for every 6-cycle $C$ in $G(K)$ there exists some $h \in \mathcal{H}$, such that $C = \partial h$. Let $u$ be an arbitrary vertex of $G(K)$. It is incident with 3 hexagons, say $h_1, h_2$ and $h_3$, of $\mathcal{H}$. By definition of skeleton, at least one of those hexagons must also be in $\mathcal{K}$. Without loss of generality $h_1 \in \mathcal{K}$. Therefore, $u$ belongs to 6-cycle $\partial h_1$. It may also happen that $h_2 \in \mathcal{K}$ and/or $h_3 \in \mathcal{K}$. Let $e$ be an arbitrary edge of $G(K)$. There exist $h_1 \in \mathcal{H}$ and $h_2 \in \mathcal{H}$ such that $e \in \partial h_1$ and $e \in \partial h_2$. By definition of skeleton at least one of them also belongs to $\mathcal{K}$. It may also happen that both of them belong to $\mathcal{K}$. The following proposition is also obvious:

**Proposition 19.** Let $K \subseteq \mathcal{H}$ be an arbitrary coronoid. Then the following statements are true:

(a) Graph $G(K)$ is connected.

(b) For every edge $e \in E(G(K))$ there exists $h \in K$ such that $e \in \partial h$.

(c) For every cycle $C \subseteq G(K)$ the inequality $|C| \geq 6$ holds. The equality is attained if and only if there exists a hexagon $h \in \mathcal{H}$ such that $C = \partial h$. Moreover, if $K$ is non-degenerate then $h \in K$.

**Proof.** To show that $G(K)$ is connected, we will find a $(u, v)$-path for any pair of vertices $u, v \in V(G(K))$. We already know that there exist $h_u$ and $h_v$ such that $u \in \partial h_u$ and $v \in \partial h_v$. There exists a sequence of hexagon $h_0 = h_u, h_1, \ldots, h_n = h_v$ such that $h_i$ and $h_{i+1}$ are adjacent for all $i$. If two hexagons $h$ and $k$ are adjacent, there exists a path from any vertex of $\partial h$ to any vertex of $\partial k$. On every hexagon $h_i$, $1 \leq i < n$, choose a vertex $v_i$. Let $v_0 = v$ and $v_n = u$. There exist paths $P_i$ with endvertices $v_i$ and $v_{i+1}$. Concatenation of paths $P_0, P_1, \ldots, P_{n-1}$ is a $(u, v)$-walk.

Statement (b) was already in the discussion above.

If $H \subseteq G$, then $\text{girth}(H) \geq \text{girth}(G)$. The fact that $G(K) \subseteq G(\mathcal{H})$ and Proposition 18 give us the inequality. Those cycles which attain the equality are characterized by Proposition 18. Now suppose that $h \notin K$ and that $K$ is non-degenerate. Hexagon $h$ is surrounded by 6 hexagons $h_1, h_2, \ldots, h_6$ of $\mathcal{H}$. By definition of $G(K)$, at least one of $h$ or
Proposition 20. For any coronoid \( K \), the subgraph \( \partial K \) forms a collection of \( b(K) \geq 1 \) cycles. A coronoid is a benzenoid if \( b(K) = 1 \) and is a proper coronoid with \( b(K) - 1 \) corona holes if \( b(K) > 1 \).

Proof. Look at Figure 11. There are two types of boundary vertex: the one in Figure 11(a) is incident with only one hexagon of \( K \); the one in Figure 11(b) is incident with 2 hexagons of \( K \). We consider the subgraph containing boundary vertices and edges. In the first case vertex \( v \) is incident with edges \( e \) and \( e' \) and has degree 2. In the second case, \( v \) is incident with \( e \) and \( e'' \) and also has degree 2. Therefore, the subgraph containing boundary vertices and edges is a 2-regular graph which is a union of vertex-disjoint cycles. By the Jordan curve theorem, every cycle splits the plane into two disconnected regions. Consider a hexagon \( h \in K \). It is contained in a region that is surrounded by one of the cycles. No member of \( K \) is inside this region, because a pathway of hexagons cannot enter the region elsewhere but through the perimeter. Therefore, perimeters separate corona holes from the coronoid \( K \). By Theorem 9 there must be the same number of cycles as there are corona holes (including the outer face).

For two graphs \( G \) and \( H \) by \( H \hookrightarrow G \) we denote embedding (injective homomorphism) of graph \( H \) into \( G \). Note that graph \( G(K) \) is not a plane graph and does not possess any geometric information. Let \( \mathcal{A} \) be anthracene. From Figure 12, it is clear that \( G(\mathcal{A}) \) can be drawn in the plane in many different ways.

![Figure 11: Two types of boundary vertices. Shaded hexagons are present in the coronoid. Vertex \( v \) is of degree 2 in the first case and of degree 3 in the second case. Boundary vertices and edges are emphasized.](image)

![Figure 12: Different drawings of the anthracene graph \( G(\mathcal{A}) \) in the Euclidean plane.](image)
The most appropriate drawing of anthracene for chemical purposes is the left-most. It is the only one that can be obtained from the hexagonal grid \( \mathcal{H} \). There is an embedding of a coronoid graph into the hexagonal grid \( \mathcal{H} \) called the natural embedding. Recall that \( G(\mathcal{K}) \) was obtained from \( \mathcal{K} \) by taking all 0-cells and 1-cells of corresponding subcomplex. The natural embedding just sends the graph back to its place of birth. We have the following theorem to tell us that there is only one drawing up to symmetries of the hexagonal grid:

**Theorem 21.** Let \( \mathcal{K} \) be a coronoid and let \( C \subseteq G(\mathcal{K}) \) be a cycle of length 6 (\(|C| = 6\)). Then \( C \hookrightarrow G(\mathcal{H}) \) can be extended to \( G(\mathcal{K}) \hookrightarrow G(\mathcal{H}) \) in an unique way.

**Proof.** Let \( e = uv \in E(C_6) \). Then \( e \hookrightarrow G(\mathcal{H}) \) can be extended to \( C_6 \hookrightarrow G(\mathcal{H}) \) in two different ways.

The distance between hexagons \( h \) and \( k \) in \( \mathcal{K} \), \( d(h,k) \), is the smallest \( n \) for which a sequence \( h_0 = h, h_1, \ldots, h_n = k \) of sequentially adjacent hexagons of \( \mathcal{K} \) exist. Let \( \mathcal{K} = \{h_1, h_2, \ldots, h_d\} \). Suppose that \( C = \partial h_1 \) and that \( d(h_1, h_i) \leq d(h_1, h_{i+1}) \). We start with \( C \hookrightarrow G(\mathcal{H}) \) and extend it step by step. On \( i \)-th step we find images of those vertices of \( \partial h_i \) that are not already embedded. For \( h_i \) there exists some \( h_{ij}, j < i \), such that \( \partial h_j \) was already embedded and \( h_i \) shares an edge \( e_i \) with \( h_j \). If vertices of \( \partial h_i \) were already embedded, there is nothing left to do. Otherwise, \( e_i \hookrightarrow G(\mathcal{H}) \) can be extended to \( \partial h_i \hookrightarrow G(\mathcal{H}) \) in two ways. As we are constructing an injective homomorphism, images of \( \partial h_j \) and \( \partial h_i \) may not overlap. Therefore, only one option remains.

This constructive proof gives rise to an algorithm for embedding an arbitrary coronoid graph \( G \) into the hexagonal lattice. If anything goes wrong during this procedure, that means that the input graph \( G \) was not a valid coronoid graph. If the graph \( G \) is a valid coronoid graph, the algorithm will always finish successfully.

Theorem 21 no longer holds, if we permit arbitrary subgraphs of \( G(\mathcal{H}) \). (See the examples given in Figure 13, Figure 14 and Figure 15.)

![Figure 13](https://via.placeholder.com/150)

Figure 13: A graph that consists of two hexagons that are connected by a path of length 3 can be embedded in the hexagonal lattice in more than one way, even when the hexagon denoted by \( a \) is fixed.

**Lemma 22.** Let \( \mathcal{K} \) be a coronoid and let \( G := G(\mathcal{K}) \). Then there exists (up to symmetry of \( \mathcal{H} \)) exactly one non-degenerate coronoid \( \mathcal{N} \) such that \( G = G(\mathcal{N}) \). Moreover, \( \mathcal{N} \cong \text{NonDeg}(\mathcal{K}) \).

**Proof.** Choose some hexagon \( h \in \mathcal{H} \) and choose an arbitrary 6-cycle \( C \) in \( G \). Let \( \phi: C \hookrightarrow G(\mathcal{H}) \) be an embedding such that \( \phi(C) = \partial h \). By Theorem 21 \( \phi \) can be extended to \( \Phi: G \hookrightarrow G(\mathcal{H}) \) in a unique way. Let \( \mathcal{N} = \{h \in \mathcal{H} \mid \partial h \subseteq \Phi(G)\} \). For every 6-cycle \( C \) in \( \Phi(G) \) there exists some \( h_C \in \mathcal{N} \) such that \( \Phi(C) = \partial h_C \).
Figure 14: Another example of a non-coronoid subgraph of the lattice that can be embedded in two different ways.

Figure 15: An example of a 2-connected non-coronoid graph that can be embedded in more than one way. (Not all embeddings are listed.)

First we show that $N$ is non-degenerate. Suppose that it has a corona hole of size 1, i.e., there exists $\tilde{h} \in N^c$ which is surrounded by $h_1, h_2, \ldots, h_6 \in N$. Every edge of cycle $\partial h$ is present in $\Phi(G)$ because all hexagons $h_1, \ldots, h_6$ are present in $N$. But then, by definition of $N$, also $\tilde{h} \in N$. A contradiction.

Now, we show that $N \cong \text{NonDeg}(K)$. Without loss of generality, we can assume that $\Phi$ is the natural embedding. If $k \in K$ then from the definition of $G(K)$ we conclude that $\partial k \in G(K)$. Therefore, $k \in N$. This means that $K \subseteq N$.

Let $h \in N \setminus K$. Let $\tilde{h} \in N(h)$ and suppose that $\tilde{h} \notin K$. We know that $h$ and $\tilde{h}$ share an edge $e$ which does not belong to $G(K)$, because neither $h$ nor $\tilde{h}$ belongs to $K$. But $e \in G(K)$ by definition of $N$. This is a contradiction. Therefore, $\tilde{h} \in K$ for every $\tilde{h} \in N(h)$. With other words, $h$ is a degenerate corona hole inside $K$. That means that $N$ is obtained from $K$ by adding degenerate corona holes. \hfill \Box

We use the terminology of Gutman and Cyvin [21]. Each boundary cycle is called a perimeter. In a proper coronoid there is one outer perimeter and one or more inner perimeters. It may happen that one of the inner perimeters is longer than the outer perimeter (see Figure 16). Nevertheless, the cycle of a coronoid graph that belong to the outer perimeter can be easily recognised. By Theorem 21 a coronoid can be embedded

Figure 16: The outer perimeter of this single coronoid is of length 48 whilst the inner perimeter is of length 58.
in the hexagonal lattice in a unique way (up to symmetry). Then the left-most vertex of the coronoid belongs to the outer perimeter.

A corona hole is a unique benzenoid that can fill the interior of an inner perimeter. An inner perimeter of a coronoid may be viewed as the (outer) perimeter of the corresponding corona hole. The roles of boundary vertices of degrees 2 and 3 are interchanged when we make this change of viewpoint. A corona hole of a non-degenerate coronoid has at least 2 hexagons and the corresponding inner perimeter has at least two vertices of degree 2. A typical coronoid is schematically illustrated in Figure 17.

![Figure 17: Schematic illustration of a typical coronoid. The outer perimeter has at least 6 vertices of degree 2 and any inner perimeter has at least 2 vertices of degree 2.](image)

There are exactly two vertices of degree 2 on the inner perimeter in the case of a naphthalene corona hole. For all other corona holes the number of such vertices is strictly greater than 2. A lower bound can easily be obtained from the equations in [21].

**Proposition 23.** Let $h$, $n$, $m$ and $n_i$ denote, respectively, the number of hexagons, vertices, edges and internal vertices in a corona hole. The number of boundary vertices of degree 3, which correspond to vertices of degree 2 on the inner perimeter, is

$$2h - 2 - n_i = n - 2h - 4 \geq \sqrt{12h - 3} - 3.$$

**Proof.** Let $\nu$ denote the number of boundary vertices of degree 3 that belong to the corona hole (those vertices are exactly degree-2 vertices of the corresponding inner perimeter). In [21] one can find the following equation:

$$\nu = 2h - 2 - n_i.$$  \hspace{1cm} (1)

Using $n = 4h + 2 - n_i$ [21], we can eliminate variable $n_i$ from (1) to obtain $\nu = n - 2h - 4$. Then apply $2h + 1 + \sqrt{12h - 3} \leq n$ [21] to get $\nu \geq \sqrt{12h - 3} - 3$. \hfill \Box
3 Patches and Perforated Patches

First we generalise benzenoids and coronoids to patches and perforated patches, respectively. Essentially, a patch is a (2-connected) plane graph similar to a benzenoid in which various polygons may be used instead of hexagons alone. All internal vertices are of degree 3, whilst boundary vertices are of degree 2 or 3 (see example in Figure 18).

![Figure 18: A patch.](image)

We will present a mathematical formalisation which is based on the treatment of coronoids and benzenoids in the previous section of this paper. As we will see later, our definition of a fullerene patch is compatible with Graver’s definition [12, 13]. There is also a notion of a \((m,k)\)-patch which received a lot of attention in the past years [2, 3, 11, 18]. By our definition, faces may have a range of different degrees, but \(m = 3\).

Our point of departure is a finite plane cubic (simple) graph \(G\), which divides the Euclidean plane \(\mathbb{R}^2\) into several regions called faces. The collection of all faces is denoted \(\mathcal{F}_G\). One face is unbounded and the rest are bounded. Two examples of plane cubic graphs are in Figure 19. Note that in the previous section, the role of graph \(G\) was taken by an infinite cubic graph with all faces hexagons which we called hexagonal lattice. Here we restrict our attention to finite graphs \(G\). Later on, we will compare finite and infinite versions of this theory.

![Figure 19: Two examples of cubic plane graphs.](image)

The hexagonal lattice has additional nice properties. First of all, no two faces of \(H\) share more than one edge; the graph in Figure 19(b) does not have that property. Also, no face of \(H\) is incident with itself; the graph in Figure 19(a) does not have that property, since one if its edges is incident to only one face (the outer face). Here, we also permit graphs which are not 2-connected, such as the one on Figure 19(a).

Let \(P \subseteq \mathcal{F}_G\) be some arbitrary subcollection of faces and let \(a, b \in P\). We say that \(a\) and \(b\) are adjacent, \(a \sim b\), if they share an edge. We define relation \(\equiv_P\) in exact same way.
as before, i.e., $a \equiv_P b$ if there is a sequence $c_0 = a, c_1, c_2, \ldots, c_m = b$ such that $c_{i-1} \sim c_i$ and $c_i \in \mathcal{P}$. $\mathcal{P}$ is connected if $a \equiv_P b$ for any $a, b \in \mathcal{P}$. Set $\mathcal{P}$ is naturally decomposed into connected components.

**Definition 24.** Let $G$ be any finite plane cubic graph. A proper subset $\mathcal{P} \subset \mathcal{F}_G$ is called a perforated patch if it is connected.

**Definition 25.** Let $G$ be any finite plane cubic graph. A proper subset $\mathcal{P} \subset \mathcal{F}_G$ is called a patch if $\mathcal{P}$ is connected and $\mathcal{P}^\mathcal{C} = \mathcal{F}_G \setminus \mathcal{P}$ is also connected.

Observe that finiteness of set $\mathcal{K}$ in Definitions 4 and 5 implies that $\mathcal{K}$ is a proper subset of $\mathcal{H}$. In this finite version of those two definitions we had to make that explicit.

Most observations of the previous section about coronoids and benzenoids are also true for their corresponding generalisations, namely perforated patches and patches. In some cases the proof remains essentially the same and in some cases it slightly simplifies, since we do not have to deal with infinity anymore. We will transcribe results of the previous section into this new language and omit the proofs. When appropriate, we will give some clarifications. For our considerations, only the combinatorial data is relevant (adjacency between faces and the cyclic ordering of edges incident to a common vertex). Geometric details of the drawing are unimportant. Moreover, the outer face does not play a special role. The graph $G$ could also be embedded on the sphere $S^2$, where all faces would be bounded. All the combinatorial information would, of course, remain exactly the same.

**Lemma 26.** Let $G$ be any finite plane cubic graph and let $\emptyset \neq \mathcal{P} \subset \mathcal{F}_G$. Let $a$ be any of its faces. Then every element of $\mathcal{P}$ belongs to some connected component $C_i$ of $\mathcal{P}$. Let $b \in N(a)$. Then either $b \in C_i$ or $b \in \mathcal{P}^\mathcal{C}$.

**Lemma 27.** Let $G$ be any finite plane cubic graph and let $\emptyset \neq \mathcal{P} \subset \mathcal{F}_G$. Let $C_a$ be any connected component of its complement $\mathcal{P}^\mathcal{C}$. Then there exists a face $\bar{a} \in C_a$ that is adjacent to some face in $\mathcal{P}$.

**Lemma 28.** Let $G$ be any finite plane cubic graph and let $\emptyset \neq \mathcal{P} \subset \mathcal{F}_G$. Let $\mathcal{C}_a$ be a connected component of its complement $\mathcal{P}^\mathcal{C}$, $a \in \mathcal{C}_a$ and $p \in \mathcal{P}$. Then $a \equiv_{\mathcal{P} \cup \mathcal{C}_a} p$. Let $\mathcal{C}_b$ be another connected component of $\mathcal{P}^\mathcal{C}$. Then $a \equiv_{\mathcal{P} \cup \mathcal{C}_a \cup \mathcal{C}_b} b$.

The above Lemma 28 corresponds to both Lemma 7 and Corollary 8.

**Lemma 29.** Let $G$ be any finite plane cubic graph and let $\emptyset \neq \mathcal{P} \subset \mathcal{F}_G$. Then the complement $\mathcal{P}^\mathcal{C}$ of $\mathcal{P}$ consists of finitely many connected components:

$$\mathcal{P}^\mathcal{C} = \mathcal{C}_1 \sqcup \mathcal{C}_2 \sqcup \cdots \sqcup \mathcal{C}_d.$$  

Each of the components $\mathcal{C}_i$, $i \geq 1$, is a perforated patch. If $\mathcal{P}$ is a perforated patch, then each $\mathcal{C}_i$ is a patch.

The above Lemma 29 corresponds to both Lemma 6 and Theorem 9. Since we do not have to deal with an infinite number of faces, the proof becomes trivial. The definition of the benzenoid closure was natural. Here, one should be slightly more careful:

**Definition 30.** Let $\mathcal{P}$ be a perforated patch. The closure of $\mathcal{P}$ with respect to $p \in \mathcal{P}^\mathcal{C}$, denoted $Cl(\mathcal{P}, p)$ is the intersection of all those patches which include $\mathcal{P}$ as a subset and do not contain $p$ among their faces, i.e.,

$$Cl(\mathcal{P}, p) = \bigcap \{ \mathcal{Q} \mid \mathcal{Q} \text{ is patch } \land \mathcal{P} \subseteq \mathcal{Q} \land p \notin \mathcal{Q} \}.$$
Let us investigate what happens if the extra condition, i.e., exclusion of a designated face \( p \), is omitted. By Lemma 29, \( \mathcal{P} = C_1 \sqcup C_2 \sqcup \cdots \sqcup C_d \) where each \( C_i \) is a patch. Define \( \mathcal{P}_i := \mathcal{P} \sqcup C_1 \sqcup \cdots \sqcup C_{i-1} \sqcup C_{i+1} \sqcup \cdots \sqcup C_d \). It is easy to see that each \( \mathcal{P}_i \), \( 1 \leq i \leq d \), is a patch. Clearly, \( \mathcal{P} \subseteq \mathcal{P}_i \) for each \( i = 1, \ldots, d \). But \( \bigcap \{ \mathcal{P}_i | 1 \leq i \leq d \} = \mathcal{P} \). Without that extra condition the definition would not make sense. In most cases this “forbidden” face \( p \) can be chosen in advance and one can deal with only those perforated patches which do not include face \( p \). Then we can write \( \text{Cl}(\mathcal{P}) \) instead of \( \text{Cl}(\mathcal{P}, p) \) without introducing any ambiguity. The most natural candidate for the forbidden face is, of course, the outer face. Let us denote \( \text{Pat}(\mathcal{P}, p) = \{ Q | Q \text{ is patch} \land \mathcal{P} \subseteq Q \land p \notin Q \} \) for convenience. Lemma 11 and Proposition 12 give rise to the following analogue in the theory of perforated patches:

**Lemma 31.** Let \( \mathcal{P} \) be a perforated patch and \( p \in \mathcal{P}^c \) a face in its complement. Let \( \mathcal{P} = C_1 \sqcup C_2 \sqcup \cdots \sqcup C_d \) as in Lemma 29. Then the closure of \( \mathcal{P} \) with respect to \( p \) is

\[
\text{Cl}(\mathcal{P}, p) = \mathcal{P} \sqcup C_1 \sqcup \cdots \sqcup C_{j-1} \sqcup C_{j+1} \sqcup \cdots \sqcup C_d,
\]

where \( \mathcal{P}_j \) is the connected component of \( \mathcal{P} \) which includes \( p \) among its faces, i.e., \( p \in \mathcal{C}_j \). Moreover, the closure with respect to \( p \) is an operation on the set of perforated patches without \( p \) that satisfies the following conditions:

\begin{enumerate}
  \item \( \mathcal{P} \subseteq \text{Cl}(\mathcal{P}, p) \),
  \item \( \mathcal{P} \subseteq \mathcal{Q} \implies \text{Cl}(\mathcal{P}, p) \subseteq \text{Cl}(\mathcal{Q}, p) \), and
  \item \( \text{Cl}(\text{Cl}(\mathcal{P}, p), p) = \text{Cl}(\mathcal{P}, p) \).
\end{enumerate}

\[\square\]

The following lemma is an analogue to Definition 13 and Lemma 14 from the theory of corondoid hydrocarbons:

**Lemma 32.** Let \( \mathcal{P} \) be a perforated patch such that \( p \notin \mathcal{P} \). Let \( \mathcal{P} \subseteq \mathcal{F}_G \) satisfy the following conditions:

\begin{enumerate}
  \item \( \mathcal{P} \) is a patch without \( p \),
  \item \( \mathcal{P} \subseteq \mathcal{P} \), and
  \item \( \mathcal{P} \subseteq \mathcal{Q} \implies \mathcal{P} \subseteq \mathcal{Q} \) for every patch \( \mathcal{Q} \) without \( p \).
\end{enumerate}

There exists a unique \( \mathcal{P} \) with given properties and \( \mathcal{P} = \text{Cl}(\mathcal{P}, p) \).

\[\square\]

Some caution should be used in making the analogy with Lemma 15, as seen in Figure 20, the intersection of two patches may be a perforated patch. However, the following is true:

**Lemma 33.** Let \( \mathcal{P} \) and \( \mathcal{Q} \) be two patches such that their complements share a face, i.e., \( \mathcal{P}^c \cap \mathcal{Q}^c \neq \emptyset \). Then the intersection of patches \( \mathcal{P} \) and \( \mathcal{Q} \) is disjoint union of patches.

\[\square\]

To obtain a perforated patch we choose a set of faces of the plane cubic graph \( G \) that constitute a connected region. Sometimes we talk about “removing faces”. This means that we select members of the complement, i.e., faces that will not be present in the perforated patch.
Figure 20: The intersection of two patches may be a perforated patch.

Figure 21: Two distinct perforated patches with the same skeleton. The faces that we removed, i.e., the faces in the complement, are indicated by shading and the corresponding hole is also shaded.

Given a perforated patch as a plane graph it is not possible to detect (in the general case) which faces are corona holes and which not. An example is given in Figure 21. Therefore, plane graphs do not give a sufficient model for perforated patches. One has to indicate which faces are actually present, and which are not. This means that Lemma 22 has no equivalent in this theory.

A patch is called $k$-connected when its skeleton is $k$-connected. A face which is incident to an edge from both sides is called an ill-behaved face. The following proposition precisely characterizes 2-connected patches:

**Proposition 34.** A patch $\mathcal{P}$ is 2-connected if and only if it contains no ill-behaved faces.

**Proof.** An ill-behaved face means there is a bridge (cut-edge) so it is not 2-connected. If there are no ill-behaved faces: start with a single face. Its skeleton is a cycle which is 2-connected. Then iteratively add adjacent faces. The newly added edges form one
or more paths that are connected to the existing graph. In this way we construct ear-decomposition.

It is possible to generalise this theory for the case when the cubic planar graph $G$ is infinite. The standard embedding of the hexagonal lattice is such an example. If one tries to use an arbitrary infinite cubic graph, problems of topological nature may arise. Some remarks must therefore be made. Hexagonal grid, as we will see, has certain nice properties. In the proof of Lemma 3 we use the fact that $\bigcup_{n=0}^{\infty} P_n = \mathcal{H}$ without proving it. This holds when there exists a finite pathway of faces between any two faces of the plane graph. With other words, the distance between every two vertices of the dual graph is finite. Hexagonal grid is an example. If this was not the case, the proof of Lemma 3 would fail. Another important building block of this theory is Lemma 6. In its proof, when we claim that $P_\mathcal{C}$ is connected, we implicitly use the Jordan curve theorem. This renowned theorem seems obvious at the first sight, but its proof happens to be involved. Another sensitive part of the proof is when we claim that $P_n$ contains finitely many faces. A nifty topologist could construct such an example where this would fail. Luckily, every bounded region of the infinite hexagonal grid contains finitely many faces. This is another condition on the infinite plane graph $G$ that has to be met.

4 Altans, Generalised Altans and Iterated Altans

We will start by making a small extension of the definition of an altan as presented previously [1]. Let $G$ be a graph and let $C$, the perimeter, be a cycle in $G$ having $k \geq 2$ vertices of degree 2. Then $A(G, C)$ will be the altan as defined in [1] with respect to the degree-2 vertices of $C$. Those edges which connect degree-3 vertices on the new cycle with $C$ will be called spokes.

**Example 35.** See Figure 22

![Diagram](image)

(a) $G, C = (1, a, 2, b, 3, c, 4, d, 5, e)$

(b) $G' = A(G, C), C' = (1', 1'', 2', 2'', 3', 3'', 4', 4'', 5', 5'')$

Figure 22: A graph $G$ with a designated perimeter $C$ (on the left), and its altan $A(G, C)$ (on the right).

A generalised altan is obtained by selecting a collection of cycles $C_1, C_2, \ldots, C_k$ in $G$ with the property that any degree-2 vertex of $G$ appears on at most one cycle and that each of the cycles $C_i$ contains at least 2 vertices of degree 2. We call $(G; C_1, \ldots, C_k)$ an
admissible structure. In addition we select a non-empty subset of indices $J \subseteq \{1, 2, \ldots, k\}$ and perform the altan operation on all cycles $C_j$, $j \in J$. We define

$$A(G; C_1, \ldots, C_k; \emptyset) = (G; C_1, C_2, \ldots, C_k),$$

and

$$A(G; C_1, \ldots, C_k; J) = A(G'; C_1, \ldots, C_{j-1}, C'_j, C_{j+1}, \ldots, C_k; J \setminus j),$$

for $J \neq \emptyset$, where $j = \min J$. Graph $G'$ is obtained from $G$ by adding a new copy, denoted $C'_j$, of a cycle on $2d$ vertices, where $d$ is the number of degree-2 vertices on cycle $C_j$. Every second vertex on cycle $C'_j$ is attached to a degree-2 vertex on $C_j$. Usually we take either $|J| = 1$ or $|J| = k$. In the former case we are dealing with the ordinary altan operation. In the latter case all perimeters are used.

**Example 36.** Let $G$ be the subdivided cube in Figure 23. Let $C_1 = (1, 2, 3, 4, 7, 6, 5)$, $C_2 = (1, 5, 9, 10, 14, 8)$ and $C_3 = (10, 11, 12, 13, 16, 15, 14)$. Then $(G; C_1, C_2, C_3)$ is an admissible structure. Note that cycles $C_1, \ldots, C_k$ of an admissible structure need not be disjoint as long as no degree-2 vertex lies on a shared part. The generalised altan $A(G; C_1, C_2, C_3; \{1, 2, 3\})$ is on the right in Figure 23.

We may apply the generalised altan operation iteratively. The order in which we apply individual “local” altan operations is irrelevant.

### 4.1 Iterated generalised altans

Let $(G; C_1, C_2, \ldots, C_k)$ be an admissible structure. Let $n = (n_1, n_2, \ldots, n_k)$ be an integer vector with $n_i \geq 0$. Then

$$A^n(G; C_1, \ldots, C_k)$$

denotes the generalised iterated altan. Let $n^\dagger = (n_1^\dagger, n_2^\dagger, \ldots, n_k^\dagger)$ where

$$n_i^\dagger = \begin{cases} n_i - 1, & \text{if } n_i > 0 \\ 0, & \text{otherwise.} \end{cases}$$

Moreover, let $J_n^\dagger = \{i \mid n_i > 0\}$. Then iterated generalised altan can be defined in terms of the generalised altan in the following way

$$A^n(G; C_1, \ldots, C_k) = A^{n^\dagger}(A(G; C_1, \ldots, C_k; J_n^\dagger)).$$

Naturally, $A^0(G; C_1, \ldots, C_k) = (G; C_1, \ldots, C_k)$ where $0 = (0, 0, \ldots, 0)$. 
Example 37. Consider admissible structure $(G; C_1, C_2, C_3)$ from Example 36. Iterated generalised altan $A^{(1,0,2)}(G; C_1, C_2, C_3)$ is shown in Figure 24.

Figure 24: The iterated generalised altan $A^{(1,0,2)}(G; C_1, C_2, C_3)$.

4.2 Altans of coronoids and perforated patches

From now on, by a coronoid we mean a non-degenerate coronoid. Each coronoid $K$ with its perimeters is an admissible generalised altan structure. Hence, $A^n(K)$ is well-defined as soon as we label its perimeters. Note that the cycles are exactly perimeters and they are disjoint. When $n \neq 0$, we call $A^n(K)$ a proper generalised altan.

Example 38. Let $K$ be the coronoid in Figure 24 (the part consisting of dotted faces). Let $C_1$ denote the left inner perimeter, $C_2$ the right inner perimeter and $C_3$ the outer perimeter. Generalised altan $A^{(2,3,0)}(K)$ consists of shaded and dotted faces in Figure 25.

Figure 25: $A^{(2,3,0)}(K)$.

Proposition 39. A proper generalised altan of a coronoid is not a coronoid.

Proof. In the case of a benzenoid, we restate Gutman’s observation [20] on the structural features of altan-benzenoids. Every benzenoids contains a $(2, 2)$-edge, i.e., an edge
connecting two degree-2 vertices. Figure 26(a) shows a fragment of a benzenoid with a (2,2)-edge. This gives rise to a pentagon in its altan. (The new vertices that are obtained by the altan operation are distinguished by shading.)

![Figure 26: The altan of a coronoid is no longer a coronoid.](image)

In the case of a coronoid, the same proof works for the outer perimeter. For an inner perimeter, one can observe that it must contain at least one (3,3)-edge which corresponds to a (2,2)-edge in its corona hole. This means that there are at least two vertices of degree 3 between some pair of degree-2 vertices. This give rise to a heptagon or an even larger face (see Figure 26(b)).

However, Gutman has shown [20] that when the altan is performed on a convex benzenoid [4], degrees of the newly obtained faces are limited to 5 and 6. Traditionally, a patch is defined as a subcubic plane graph that has all its degree-2 vertices on its outer perimeter. Clearly, the skeleton \( G(P) \) of a patch \( P \) is such a graph. The following result shows that our definition actually coincides with the traditional one:

**Proposition 40.** Let \( G \) be a plane subcubic graph with all the degree-2 vertices on its outer perimeter. Then there exists a plane cubic graph \( \tilde{G} \), such that \( G \subseteq \tilde{G} \), all inner faces of \( G \) are also faces of \( \tilde{G} \) and there exists patch \( \mathcal{P} \subseteq \mathcal{F}_{\tilde{G}} \) such that \( G = G(\mathcal{P}) \). Moreover, if \( G \) is 2-connected with at least two degree-2 vertices, then there exists a 2-connected graph \( \tilde{G} \).

**Proof.** If \( G \) contains three or more degree-2 vertices, choose \( C \) to be the outer perimeter of \( G \) and make altan \( A(G, C) \). Then remove all the newly obtained degree-2 vertices and reconnect its neighbours (reverse operation to subdivision) as shown in Figure 27. It is trivial to verify that this graph is indeed the desired \( \tilde{G} \). If \( G \) was 2-connected then

![Figure 27: Obtaining \( \tilde{G} \) from \( G \) with three or more degree-2 vertices.](image)

its ear-decomposition can easily be extended to include the newly obtained edges. This shows that \( \tilde{G} \) is also 2-connected.

If \( G \) had only two degree-2 vertices, then the above procedure would yield a multigraph. It can be fixed by subdiving its edges on the new outer perimeter to obtain 3 or more...
Figure 28: Obtaining $\tilde{G}$ from $G$ with two degree-2 vertices. Again, it is not hard to see that this yields the desired $\tilde{G}$ and that the ear-decomposition of $G$ can be extended to $\tilde{G}$.

Figure 29: A “cherry”.

If $G$ has only one degree-2 vertex, there is no hope of obtaining 2-connected $\tilde{G}$. Graph $\tilde{G}$ can be obtain from $G$ by attaching a “cherry” (see Figure 29) to its degree 2 vertex.

We can say more:

**Proposition 41.** Let $G$ be a plane subcubic bipartite graph with all degree-2 vertices on its outer perimeter. Then there exists a plane cubic bipartite graph $\tilde{G}$, such that $G \subseteq \tilde{G}$, all faces of $G$ are also faces of $\tilde{G}$ and there exists a patch $\mathcal{P} \subseteq \mathcal{F}_{\tilde{G}}$ such that $G = G(\mathcal{P})$. Moreover, if $G$ was 2-connected then there exists a 2-connected graph $\tilde{G}$ with desired properties.

**Proof.** Suppose there are at least two degree-2 vertices of the same colour, i.e., belong to the same set of the bipartition, in graph $G$ and denote those two vertices by $u$ and $v$. Without loss of generality, we can assume they are coloured black. Those two vertices can be chosen in such way that there are no other black vertices between them when we traverse the perimeter from $u$ to $v$ in the clockwise direction (see Figure 30(a)). However, there may be 0 or more white vertices on that path. Say there are one or more white

![Figure 30: A step in obtaining bipartite $\tilde{G}$ from bipartite $G$.](image)
vertices. Label those vertices \( w_1, w_2, \ldots, w_l \), where \( l \geq 1 \). Make an altan of \( G \) with vertices \((u, w_1, \ldots, w_l, v)\) as its peripheral root. Label the newly obtained neighbours of vertices \( u \) and \( v \) with \( u' \) and \( v' \), respectively. Then make a reverse subdivision operation which removes all degree-2 vertices in the neighbourhood of \( u' \) and \( v' \). Also, remove the edge \( u'v' \) to obtain the graph in Figure \ref{fig30}(a). If there are no white vertices between \( u \) and \( v \), add a new vertex to the graph and connect it to \( u \) and \( v \) as shown in Figure \ref{fig30}(b). In both cases, this graph is clearly bipartite and 2-connected if the graph \( G \) was 2-connected. Also, two black degree-2 vertices and \( l \) white degree-2 vertices have disappeared and \( l + 1 \) new white degree-2 vertices have emerged. The total number of degree-2 vertices is therefore decreased by one.

This procedure terminates when there are only two vertices left, which have to be of different colours. (The situation with only one degree-2 vertex, say a white vertex, cannot occur. The number of edges should be divisible by 3, because every black vertex has degree 3. On the other hand, there is one white vertex of degree 2 and the rest have degree 3, which implies that the number of edges is congruent 2 modulo 3, a contradiction.) If those

![Figure 31: The final step in obtaining bipartite \( \tilde{G} \) from bipartite \( G \).](image)

final two vertices (which have to be of different colour) are non-adjacent, connect them by an edge as shown in Figure \ref{fig31}(a). If they are adjacent, we would create a multigraph. In that case, use the construction shown in Figure \ref{fig31}(b) to avoid the multigraph.

A perforated patch with pentagonal and hexagonal faces is called a perforated fullerene patch. Similarly, a patch with pentagonal and hexagonal faces is called a fullerene patch. One should be aware that the restriction to hexagonal and pentagonal faces applies within the patch \( P \); other faces of the cubic graph \( G \) from which the patch was derived may be of other sizes. If such a graph \( G \) with exclusively pentagonal and hexagonal faces exists, then the patch (or perforated patch) can be extended to a fullerene. It is not easy to verify the existence of such \( G \).

**Example 42.** Figure \ref{fig32} shows that various possibilities can occur when we apply the altan operation to a fullerene patch. In first case (left-hand side of Figure \ref{fig32}), the altan contains a 7-gon. In the second case (right-hand side), the altan is again a fullerene patch (which may or may not extend to a fullerene).

There is another viewpoint we can take when dealing with (perforated) patches. In addition to the skeleton \( G(P) \), one can also obtain a planar pre-graph, denoted \( P(P) \). It can be obtained from the plane graph \( G \) by removing all vertices that are not incident to any face of \( P \), together with all semiedges that are incident to removed vertices. In addition, edges incident to two faces from \( P^b \) are also removed and replaced with two half edges (as if the edge was cut in the middle). An example is given in Figure \ref{fig33}.
Figure 32: Altans of fullerene patches.

Figure 33: A pre-graph of a patch. Half edges are “without vertices” on one end, i.e., they are “dangling”.

Theorem 43. The generalised altan of a perforated patch $\mathcal{P}$ is a perforated patch. Moreover, if $G(\mathcal{P})$ is 2-connected then $G(A^n(\mathcal{P}))$ is also 2-connected.

Proof. The pre-graph of a perforated patch $\mathcal{P}$ is schematically illustrated in Figure 34. Each hole corresponds to a void space that can be filled with an open disc. There are also half edges (attached to degree-2 vertices of $G(\mathcal{P})$) which are drawn inside those holes. When we perform an altan operation on that perforated patch, a cycle is drawn inside every hole on which the altan operation is performed and an annulus of new faces (bounded by the new and the old perimeter) is added to the patch. See Figure 35 for an illustration. New holes have the same number of half edges as they had before the
operation. The parts that were removed from $G$ can be reattached to form the plane cubic graph.

![Figure 35: Pre-graph of an altan of a perforated patch.](image)

It is clear that $G(A^n(P))$ is 2-connected if $G(P)$ is 2-connected. The ear decomposition of $G(P)$ can easily be extended to include the newly obtained edges. \hfill \Box

The following corollary obviously follows from Theorem 43:

**Corollary 44.** The generalised altan of a patch $P$ is a patch. Moreover, if $G(P)$ is 2-connected then $G(A^n(P))$ is also 2-connected.

## 5 Kekulé Structures and Pauling Bond Orders

It is not hard to see that iteration of the generalised altan operation on coronoids and perforated patches grows tubes on each perimeter, i.e., we can visualize an embedded version in a way that is reminiscent of the classic ruled surface of the graph in which some central planar perforated patch has tubular towers growing out of it (in either up or down directions). See Figure 37.

![Figure 36: Pants resulting from a disk with two holes by applying iterated altan operation. If the disk has $K$ Kekulé structures then the pants have $K' = 2^{n_1+n_2+n_3}K$ Kekulé structures.](image)

The *binary boundary code* for benzenoids is described in [32]. (This code is also known as PC-1 [25].) The binary boundary code of a benzenoid is a sequence of degrees of consecutive vertices along its perimeter. Cyclic shifts and reversal of the sequence are considered as equivalent codes. Traditionally, ones and zeroes were used, but we will use...
3s and 2s instead. To each perimeter $C_i$ of an admissible structure $(G; C_1, \ldots, C_k)$ we will assign a binary boundary code, denoted $BBC(C_i)$. Boundary-edges codes for benzenoids, introduced in [23], are useful on many occasions [26], but in this case binary boundary codes are more natural.

**Example 45.** The first coronoid in Figure 6 has three perimeters. Let $C_\infty$ denote the outer perimeter and $C_1$ and $C_2$ the inner perimeters. Then

$$\text{BBC}(C_\infty) = 3232223322332232232323232323223232232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232323232
Figure 37: Iteration of the altan construction leads to a carbon nanostructure in which nanotubes grow out of the original holes of the coronoid. A given tube may grow up or down, as a ‘chimney-stack’ or a ‘mine-shaft’ on the graphene-like landscape, leading to isomeric structures that share a common molecular graph.

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