MATHEMATICAL PROPERTIES AND STRUCTURES OF SETS OF SEXTET PATTERNS OF GENERALIZED POLYHEXES*

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Abstract

Several definitions of sextet patterns and super sextets of (generalized) polyhexes have been given, first by He Wenjie and He Wenchen [1], later by Zhang Fuji and Guo Xiaofeng [2], and by Ohkami [3], respectively. The one-to-one correspondence between Kekulé and sextet patterns has also been proved by the above authors using different methods. However, in a rigorous sense, their definitions of sextet patterns and super sextets are only some procedures for finding sextet patterns and super sextets, not explicit definitions. In this paper, we give for the first time such an explicit definition from properties of generalized polyhexes, and give a new proof of the Ohkami–Hosoya conjecture using the new definition. Furthermore, we investigate mathematical properties and structures of sets of generalized polyhexes, and prove that the s-sextet rotation graph $R_s(G)$ of the set of sextet patterns of a generalized polyhex G is a directed tree with a unique root corresponding to the g-root sextet pattern of G.

1. Introduction

From a purely empirical standpoint, Clar found that various electronic properties of polycyclic aromatic hydrocarbons can be predicted by appropriately defining an aromatic sextet for their Kekulé patterns [4]. According to Clar's aromatic sextet theory, the Clar formula of a polyhex G (the molecule model of a polycyclic aromatic hydrocarbon) is a set of mutually resonant sextets with the maximum cardinal number. The sextet polynomial $B_G(x)$ of a polyhex G was first introduced by Hosoya and Yamaguchi [5] as follows:

$$B_G(x) = \sum_{i=0}^{m} r(G,i)x^i, \tag{1}$$

where $r(G, i)$ is the number of ways in which i mutually resonant sextets are chosen from G (called a sextet pattern), and m is the maximum number of i. It was also

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found that Clar's aromatic sextet theory and the resonant theory are closely related through the following expressions [5]:

$$B_G(1) = k(G), \tag{2}$$

$$B'_G(1) = \sum_s K(G-s), \tag{3}$$

where s is a hexagon of G. However, for a long period, these mathematical relations were proved only for catacondensed and some pericondensed polyhexes [6,7,21]. For pericondensed polyhexes, neither (2) nor (3) are generally valid. In order to extend the applicability of expression (2), Hosoya and Yamaguchi [5] introduced the concept of "super ring" or "super sextet". However, in spite of certain attempts [6], a precise definition of super sextets was still missing. It was pointed out by Gutman [8] that this seemed to be one of the most significant open problems in the topology theory of polyhexes.

Expression (2) implies that for any polyhex G with Kekulé patterns, there exists a one-to-one correspondence between Kekulé and sextet patterns of G. This is also called the *Ohkami–Hosoya conjecture* [9].

In 1986, He Wenjie and He Wenchen first gave a definition of sextet patterns and super sextets by a procedure [1]. They also claimed to prove the one-to-one correspondence between Kekulé and sextet patterns. However, their proof has some errors. The existence of the root Kekulé pattern was asserted only by sextet rotations and the finiteness of a generalized polyhex (that is, a polyhex with holes). But this is an incorrect argument, and hence the other results in ref. [1] were not placed on a confident foundation. Later, in ref. [2] (submitted in 1988), Zhang Fuji and Guo Xiaofeng investigated mathematical properties and structure of the set of Kekulé patterns of a generalized polyhex G, introduced the concept of generalized proper (improper) sextets of G (simply, g-sextets), and proved that in the g-sextet rotation graph $R_g(G)$ of the set of Kekulé patterns of G there is no directed cycle. It was also proved that $R_g(G)$ is a directed tree with a unique root corresponding to the unique g-root Kekulé pattern G. These results just repaired the defect of ref. [1], and a new proof of the Ohkami–Hosoya conjecture was also given in ref. [2]. In both ref. [1] and ref. [2], the concepts of sextet patterns and super sextets were defined from Kekulé patterns. In other words, in order to find a sextet pattern, one needs first to find a Kekulé pattern, and for obtaining the sextet polynomial of G, one must draw all the Kekulé patterns of G. In ref. [3], Ohkami first pointed out that in this sense these definitions do not match the theory of the sextet polynomial. In addition, Ohkami gave a new definition of sextet patterns and super sextets by a procedure based on properties of (generalized) polyhexes with no fixed bond, not from Kekulé patterns. She also gave a new proof of the Ohkami–Hosoya conjecture. We should say that Ohkami's results are formally graceful. However, there are still some problems which also should be pointed out. In the first step of Ohkami's procedure, one needs to find the sets of i mutually resonant rings from a free polyhex G for every i. If $i > 1$, one must check whether or not any i disjoint rings are mutually resonant, that is, whether or not the resultant graph obtained from G by deleting the i rings is Kekuléan. However, the resultant graph consists of some generalized polyhexes or polyhex fragments (arbitrary subgraph in the hexagonal lattice), and recognizing a generalized Kekuléan polyhex and finding a Kekulé pattern of it have nearly the same complexity. In the second step of Ohkami's procedure, one needs to choose a sextet pattern S_i for which the resultant graph, obtained from G by deleting all resonant rings in S_i and then deleting all fixed bonds of the remaining parts, has a component which is a holed polyhex (that is, a generalized polyhex with no fixed bond). When all resonant rings in S_i are deleted, the remaining parts are also some generalized polyhexes or polyhex fragments. One must first find their fixed bonds. However, recognizing fixed bonds of a generalized polyhex G is an open problem, although some algorithms and criteria for recognizing fixed bonds of a polyhex have been made [11–14]. For a GP G, when a Kekulé pattern or a perfect $P-V$ path system of G has been given, we can give an algorithm for finding all fixed bonds of G. But it is still a difficult open problem to recognize fixed bonds of G not from a Kekulé pattern or a perfect $P-V$ path system of G. So, for the efficient use of Ohkami's procedure, we propose the following open problems.

PROBLEM 1

How to find the set of i mutually resonant rings of a polyhex for every i?

PROBLEM 2

How to recognize fixed bonds of a generalized polyhex G not from a Kekulé pattern of G?

It is easy to see that problem 1 depends on problem 2. In addition, in a rigorous sense, the two types of definitions of sextet patterns and super sextets given in refs. [1–3] are only some procedures for finding sextet patterns and super sextets, not explicit definitions. On the other hand, mathematical properties and structures of sets of sextet patterns of generalized polyhexes have still not been investigated so far.

In the present paper, we first give an explicit definition of sextet patterns and super sextets from properties of generalized polyhexes, and then give a new simple proof of the Ohkami–Hosoya conjecture by our new definition. Furthermore, for the first time we investigate mathematical properties and structures of sets of sextet patterns of generalized polyhexes, and prove that the s-sextet rotation graph $R_s(G)$ of sextet patterns of a generalized polyhex G is a directed tree with a unique root corresponding to the unique root sextet pattern of G.

Based on the directed tree structure of the set of sextet patterns of a generalized polyhex G, we can establish an efficient algorithm for generating both all sextet patterns and all Kekulé patterns of G in the same process, which will be given in another paper.

2. Some related definitions and results

DEFINITION 2.1

A polyhex fragment (PF) is a connected subgraph in the hexagonal lattice. A PF is said to be a generalized polyhex (GP) if it is 2-connected. A ring in a GP G is the boundary of an interior face of G. A GP G is said to be a polyhex if every ring of G is a hexagon. A GP (PF) with Kekulé patterns is simply denoted by KGP (KPF). A GP (a polyhex) with no fixed bond is denoted by FGP (FP). For a KPF G, a cut edge of G is obviously a fixed bond of G, called a trivial fixed bond. The graph obtained from G by deleting all trivial fixed double bonds successively is called the GP-subgraph of G, denoted by $[G]^*$ (see fig. 1).

Throughout this paper, a GP (PF) is always placed on a plane so that a pair of edges of every hexagon are parallel to the vertical line.

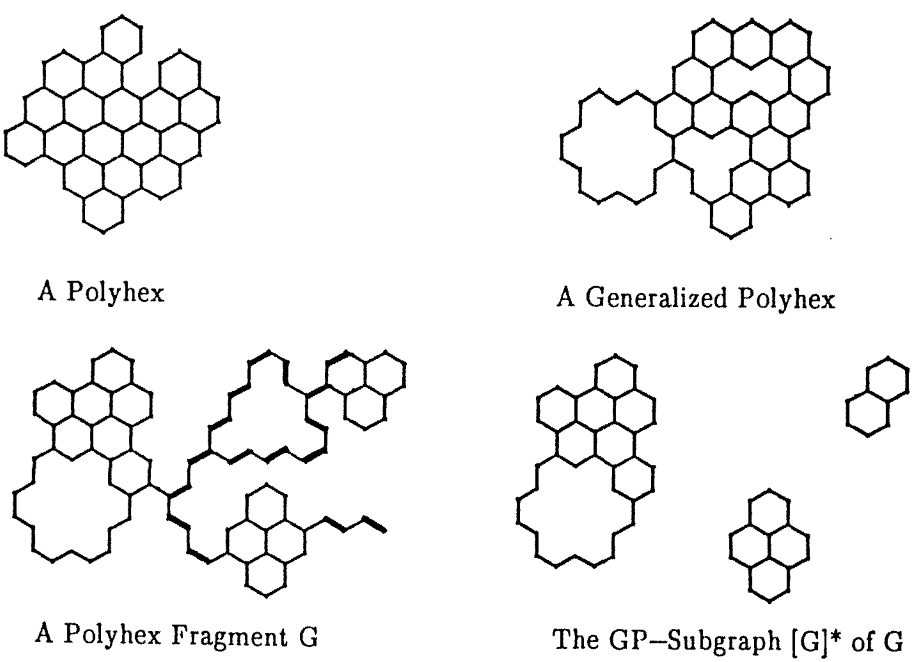
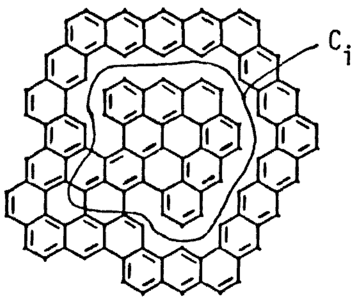


Fig. 1.

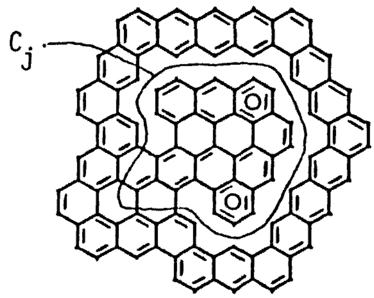
DEFINITION 2.2

For a Kekulé pattern K_i of a KGP (KPF) G, a K_i-alternating cycle is said to be a proper (improper) cycle of K_i if the extreme right (left) vertical edge of it is a K_i-double bond. A proper (improper) cycle C of K_i of G is said to be a generalized proper (improper) sextet, or simply proper (improper) g-sextet if there is no other proper (improper) cycle of K_i whose interior is contained in the interior of C.

Particularly, if a proper (improper) g-sextet C is a ring of G, it is also called a proper (improper) ring; if C is a hexagon, it becomes a proper (improper) sextet (see fig. 2).



A Proper g–Sextet C_i



A Minimal Proper Cycle C_j

Fig. 2.

DEFINITION 2.3

A generalized root Kekulé pattern K_i of a KGP (KPF) G, simply a g-root Kekulé pattern, is the Kekulé pattern with no proper g-sextet. If G is a polyhex, K_i is also a root Kekulé pattern of G. A g-root Kekulé pattern of a disconnected polyhex fragment graph consists of g-root Kekulé patterns of connected components of it. Similarly, we can define an improper g-root Kekulé pattern of G.

THEOREM 2.4 [2]

Let C be a proper (improper) g-sextet of a Kekulé pattern of a KGP G. Then, either C is a hexagon or there is a ring with length greater than six, i.e. a hole, whose interior is contained in the interior of C.

THEOREM 2.5 [2]

For any KGP G, there is exactly one g-root Kekulé pattern of G.

For a cycle C_i in a GP G, all edges with an end vertex on C_i and the other in the interior of C_i are called the interior incident edges of C_i.

THEOREM 2.6 [10]

Let C be a proper (improper) g-sextet of a Kekulé pattern K_i of a KGP G. Then, if C is neither a hexagon nor a hole, all the interior incident edges of C are fixed single bonds of G.

THEOREM 2.7 [2]

Let K be a Kekulé pattern of a KGP G, and C_i and C_j two distinct proper (improper) g-sextets of K. Then, C_i with its interior and C_j with its interior are disjoint.

Let G be a GP and G_i a subgraph of G. For convenience, we denote by $G - G_i$ the graph obtained from G by deleting all vertices of G with all incident edges of them.

3. An explicit definition of sextet patterns and super sextets of generalized polyhexes, and a proof of the Ohkami–Hosoya conjecture

As stated above, several given definitions of sextet patterns and super sextets in fact are only some procedures for finding sextet patterns and super sextets. We restate them as follows.

PROCEDURE 3.1 [1,2]

Let K be a Kekulé pattern of a KGP G.

(1) Let S_0 be the set of all proper (improper) g-sextets of K.

(2) For each component G_j', $j = 1, 2, \ldots$, of $G - S_i$, take the set S_j' of all proper (improper) g-sextets of K, and then set $S_{i+1} = S_i \cup \{\cup_{j \geq 1} S_j'\}$.

(3) If in any component of $G - S_{i+1}$ there exist proper (improper) g-sextets of K, set $i + 1 \to i$, go to (2).

(4) End.

When the procedure ends, S_{i+1} is a proper (improper) sextet pattern of G corresponding to K, and a proper (improper) cycle in S_{i+1} which is not a ring is said to be a proper (improper) super sextet of G corresponding to K. If we draw a closed curve in each proper (improper) g-sextet and each proper (improper) super sextet in S_{i+1} and delete all the double bonds, a sextet pattern and some super sextets corresponding to K are obtained.

PROCEDURE 3.2 [3]

Let G be an FP. The set S_G of sextet patterns of G is obtained as follows:

(1) Choose a set of mutually resonant rings from G, and draw circles in these rings to obtain a sextet pattern. Let S_G be the set of all these sextet patterns.

(2) Choose a sextet pattern $S_i \in S_G$ for which a component of $G - [A_i]$ is a GP with holes and without fixed bond, where A_i is the set of all aromatic rings and cycles in S_i, $G - [A_i]$ denotes the graph obtained from G by deleting all

the rings and cycles in A_i and then all fixed bonds in $G - A_i$. If there is no such sextet pattern, go to (4).

(3) Choose a ring r of $G - [A_i]$ which is not a ring in G, and draw a circle in the cycle r and in every ring or cycle in A_i to obtain a sextet pattern S_j. If $S_j \notin S_G$, then add S_j to S_G, and set $A_j = A_i + r$. Go to (2).

(4) End.

A cycle in S_G which is not a ring in G is called a super sextet of G.

Now we give an explicit definition of sextet patterns and super sextets of a KGP G from properties of G.

DEFINITION 3.3

A proper (improper) cycle C_i of a Kekulé pattern K_i in a KGP G is said to be minimal if there is no such proper (improper) cycle of K_i which has a common edge with C_i and whose interior is contained in the interior of C_i.

THEOREM 3.4

A proper (improper) cycle C_i of a Kekulé pattern K_i in a KGP G is minimal if and only if all the interior incident edges of C_i are fixed single bonds of G.

Proof

The sufficiency is obvious. We need only to prove the necessity. Suppose that C_i is minimal, but there is an interior incident edge e of C_i which is not a fixed single bond of G. Then there is a Kekulé pattern K_j of G such that e is a K_j-double bond. In $K_i \Delta K_j$, there is a $K_i(K_j)$-alternating cycle C_j which contains the edge e. Let $ve \ldots v'$ be the segment on C_j which contains e and has only its end vertices v and v' on C_i. Then the segment and some segment $v \ldots v'$ on C_i form a proper cycle whose interior is contained in the interior of C_i, a contradiction. □

Note that a minimal proper (improper) cycle C_i is not necessarily a proper (improper) g-sextet, since in the interior of C_i there may be a proper (improper) cycle, but a proper (improper) g-sextet is certainly a minimal proper (improper) cycle (see fig. 2).

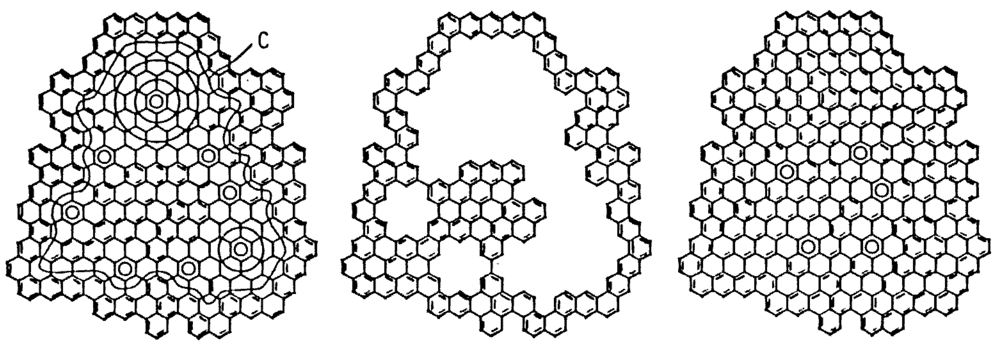
Since the property that all the interior incident edges of a minimal proper (improper) cycle of a Kekulé pattern of a KGP G are fixed single bonds of G is independent of Kekulé patterns of G, we also have the following definition.

DEFINITION 3.5

A cycle C_i in a KGP G is said to be a minimal cycle if all the interior incident edges of C_i are fixed single bonds of G.

DEFINITION 3.6

Let G be a KGP. Let $S = \{C_1, C_2, \ldots, C_t\}$ be a set of t (≥ 0) mutually resonant cycles in G. For a cycle C_j in S, let $S(C_j)$ denote the set of cycles in S which are contained in the interior of C_j (possibly, $S(C_j) = \varnothing$). S is said to be a sextet pattern of G if any cycle C_j in S is minimal in $G - S(C_j)$ (see fig. 3). A cycle in a sextet pattern S of G is said to be a super sextet if it is not a ring in G. A sextet pattern with no cycle of G is said to be a root sextet pattern of G.



A Sextet Pattern S of G   G−S(C) $\Pi_s(S)=S^*$

Fig. 3.

DEFINITION 3.7

Let S_G and K_G be the sets of sextet and Kekulé patterns of a KGP G, respectively. We define mappings f (or $\bar{f}$) and g (or $\bar{g}$) as follows:

f (or $\bar{f}$): $K_G \to S_G$: For any Kekulé pattern $K \in K_G, f(K)$ ($\bar{f}(K)$) is determined by procedure 3.1.

g (or $\bar{g}$): $S_G \to K_G$: For any sextet pattern $S \in S_G$, $g(S)$ ($\bar{g}(S)$) is determined by the following procedure:

(1) Let all cycles in S be proper (improper) cycles.

(2) Let every component of $G - S$ have a (an improper) g-root Kekulé pattern.

PROPERTY 3.8

Let S_i be a sextet pattern of a KGP G and C_i a cycle in S_i. Let K_j be a Kekulé pattern of G.

(1) If C_i is a super sextet with $S_i(C_i) = \varnothing$, then C_i is a proper (improper) g-sextet of $g(S_i)$ ($\bar{g}(S_i)$); if C_i is a super sextet with $S_i(C_i) \neq \varnothing$, then C_i is a proper (improper) g-sextet of $g(S_i) \setminus E(S_i(C_i))$ ($\bar{g}(S_i) \setminus E(S_i(C_i))$) in $G - S_i(C_i)$.

(2) $K_j \setminus E(f(K_j))$ ($K_j \setminus E(\bar{f}(K_j))$) is a proper (improper) g-root Kekulé pattern of $G - f(K_j)$ ($G - \bar{f}(K_j)$).

Proof

By the definition of g and $\bar{g}$, (1) obviously holds.

(2) Suppose that $K_j \setminus E(f(K_j))$ is not a g-root Kekulé pattern of $G - f(K_j)$. In $G - f(K_j)$ there is a proper cycle C_j of $K_j \setminus E(f(K_j))$, and so there is also a proper g-sextet whose interior is contained in the interior of C_j, contradicting the definition of f. The case of $K_j \setminus E(\bar{f}(K_j))$ is similar. □

THEOREM 3.9

f and g are mutually inverse mappings, that is, $f^{-1} = g$ and $g^{-1} = f$.

Proof

For a Kekulé pattern K of a KGP G, by theorem 2.7 and procedure 3.1, $f(K)$ ($\bar{f}(K)$) is uniquely determined, and is obviously a set of mutually resonant cycles in G. For any cycle r in $f(K)$ ($\bar{f}(K)$), by property 3.8 and theorem 2.6, r satisfies the conditions of definitions 3.5, 3.6. So $f(K)$ ($\bar{f}(K)$) is a unique sextet pattern of G corresponding to K, implying that f (or $\bar{f}$) is a mapping from K_G to S_G.

For a sextet pattern S of G, by theorem 2.5, $g(S)$ ($\bar{g}(S)$) is a unique Kekulé pattern of G corresponding to S, implying that g (or $\bar{g}$) is a mapping from S_G to K_G.

Suppose that f and g are not mutually inverse mappings, that is, $g(f(K)) = K^* \neq K$. Then, $f(K)$ is a set of proper cycles of both K and K^*, and $K \setminus E(f(K))$ and $K^* \setminus E(f(K))$ are two g-root Kekulé patterns of $G - f(K)$, respectively, by definition 3.7 and property 3.8. So, by theorem 2.5, $K \setminus E(f(K)) = K^* \setminus E(f(K))$, and so $K = K^*$, a contradiction.

Now it follows that $f^{-1} = g$ and $g^{-1} = f$. Similarly, we have that $\bar{f}^{-1} = \bar{g}$ and $\bar{g}^{-1} = \bar{f}$. □

Theorem 3.9 implies that f ($\bar{f}$) and g ($\bar{g}$) are mutually inverse one-to-one mappings, that is, there exists a one-to-one correspondence between Kekulé and sextet patterns of a KGP, and the Ohkami–Hosoya conjecture is thus proved.

4. The directed tree structure of the set of sextet patterns of a generalized polyhex

Many investigations of mathematical properties and structures of sets of Kekulé patterns of polyhexes and GPs have been carried out in recent years [2,5,6,10,15–20]. However, up to now, mathematical properties and structures of sets of sextet patterns of GPs have not been investigated. In the following, we give some results.

DEFINITION 4.1

Let S_i be a sextet pattern of a KGP G and $g(S_i)$ the Kekulé pattern corresponding to S_i. A simultaneous rotation of all the proper g-sextets and super sextets of $g(S_i)$ into improper g-sextets and super sextets to give another Kekulé pattern $g(S_j) = g(S_i) \Delta S_i$ (the symmetry difference of their edge sets) and the corresponding sextet pattern S_j of G is called a super sextet rotation, simply s-sextet rotation, denoted by $R_s(S_i) = S_j$ and $R_s(g(S_i)) = g(S_j)$ (see fig. 3).

DEFINITION 4.2

The s-sextet rotation graph $R_s(G)$ of a KGP G is a directed graph whose vertex set is the set of sextet patterns of G and there is an arc from a vertex S_i to another vertex S_j if and only if $R_s(S_i) = S_j$.

DEFINITION 4.3

Let f be an interior face of a GP G, and let $c(f)$ and $c(G)$ be the boundaries of f and G, respectively. The distance of f from $c(G)$, denoted by $d(f)$, is defined as follows:

(1) If $c(G) \cap c(f) \neq \emptyset$, then $d(f) = 0$.

(2) Let $F_n = \{f_i \mid d(f_i) \leq n\}$. If $f \notin F_n$ and there is an $f_i \in F_n$ such that $c(f) \cap c(f_i) \neq \emptyset$, then $d(f) = n + 1$.

DEFINITION 4.4

Let C be a cycle of a GP G; then the distance of C from the boundary $c(G)$ of G, denoted by $d(C)$, is determined by

$$d(C) = \min\{d(f) \mid f \text{ is any interior face in the interior of } C\}.$$

THEOREM 4.5

Let G be a KGP. Then there is no directed cycle in the s-sextet rotation graph $R_s(G)$ of G.

Proof

By contradiction. Suppose that there is a directed cycle in $R_s(G)$. Let the sextet patterns $S_1, S_2, \ldots, S_t$ be on the directed cycle and $R_s(S_i) = S_{i+1}$, for $i = 1, 2, \ldots, t-1$, $R_s(S_t) = S_1$.

Let C^* be a cycle in $\cup_{i=1}^{t} S_i$ such that the distance $d(C^*)$ from $c(G)$ is the smallest. Without loss of generality, we assume that C^* is a cycle in S_1.

If $d(C^*) = 0$, then there is an edge e^* on $C^* \cap c(G)$. Since C^* is a proper cycle of $g(S_1)$, and $g(S_2) = R_s(g(S_1))$, so C^* must be an improper cycle of $g(S_2)$. Let f^* be an interior face in the interior of C^* whose boundary $c(f^*)$ contains e^*. Since e^* is on $c(G)$, any cycle containing e^* must have its interior contain f^*. So e^* must not belong to any proper cycle of $g(S_i)$ for $i = 3, 4, \ldots, t$. Thus, if e^* is a double (single) bond of $g(S_1)$, then e^* must be a single (double) bond of $R_s(g(S_t))$. This implies that $R_s(S_t) \neq S_1$, contradicting our assumption.

Now suppose that $d(C^*) > 0$. Since every $g(S_1)$-double(single) bond on C^* changes to a $g(S_2)$-single(double) bond after the s-sextet rotation $R_s(S_1) = S_2$, they will be changed back to double (single) after some s-sextet rotation $R_s(S_i) = S_{i+1}$, $2 \leq i \leq t-1$, or $R_s(S_t) = S_1$. Thus, each edge C^* must be on a cycle in some S_i, $2 \leq i \leq t$. On the other hand, by the definition of the distance of a cycle from $c(G)$, in the exterior of C^* there is an interior face $\bar{f}$ of G such that $c(\bar{f})$ and C^* have an edge in common and $d(\bar{f}) < d(C^*)$. Let $\bar{e}$ be an edge on $C^* \cap c(\bar{f})$. Then $\bar{e}$ must also be on a cycle in some S_i, $2 \leq i \leq t$, say C_i. It is not difficult to see that the interior of C_i must contain the interior of $c(\bar{f})$. This implies that $d(C_i) < d(C^*)$, contradicting the choice of C^*. □

COROLLARY 4.6

Let S_i be a sextet pattern of a KGP G. Then in $R_s(G)$ there is a finite directed path from S_i to some root sextet pattern of G.

THEOREM 4.7

For any KGP G, there is exactly one root sextet pattern.

Proof

The conclusion of the theorem follows from theorem 2.5 and the one-to-one correspondence between Kekulé and sextet patterns. □

Now we are in the position to give the following theorem of the mathematical structure of the set of sextet patterns of a KGP which is the immediate consequence of theorems 4.5, 4.6, and 4.7.

THEOREM 4.8

Let G be a KGP. Then the s-sextet rotation graph $R_s(G)$ of G is a directed tree with a unique root corresponding to the unique g-root Kekulé pattern of G.

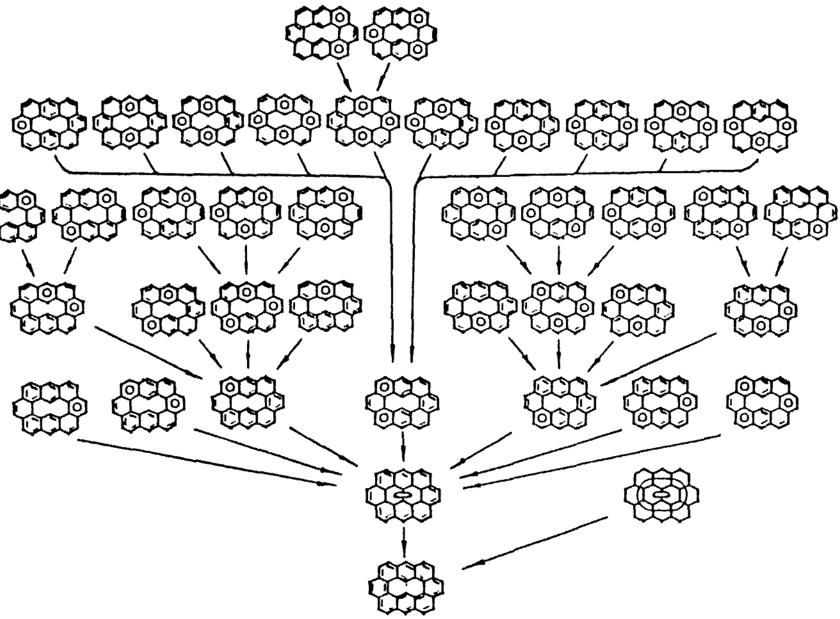


Fig. 4. A GP G and the s-sextet rotation graph $R_s(G)$.

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