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RECOGNIZING KEKULÉAN BENZENOID SYSTEMS BY *C-P-V* PATH ELIMINATION*

Guo XIAOFENG and Zhang FUJI

Department of Mathematics, Xinjiang University, Wulumuqi Xinjiang, People's Rupublic of China

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Abstract

In this paper, we define the concept of a canonical *P-V* path $P(p_i\text{-}v_i)$ on the boundary of a benzenoid system H, and prove that H has a Kekulé structure if and only if $H - P(p_i\text{-}v_i)$ has a Kekulé structure, where $H - P(p_i\text{-}v_i)$ is the graph obtained from H by deleting the vertices on $P(p_i\text{-}v_i)$. It is also proved that there are at least two canonical *P-V* paths in a benzenoid system. By the above results, we give an efficient and simple algorithm, called the canonical *P-V* (C-*P-V*) path elimination, for determining whether or not a given benzenoid system H has Kekulé structures. If H is Kekuléan, the algorithm can find a Kekulé structure of H.

A benzenoid system, or a hexagonal system, is a connected plane graph whose every interior face is a regular hexagon. A Kekulé structure, or a 1-factor, or a perfect matching of a benzenoid system H is an independent edge set in H such that every vertex in H is incident with an edge in the edge set. A benzenoid system is said to be Kekuléan if it possesses a Kekulé structure; otherwise it is said to be non-Kekuléan.

Since the chemical behaviour of Kekuléan and non-Kekuléan benzenoid systems is strikingly different, the existence of Kekulé structures in a benzenoid system is the first fundamental problem in the topological theory of benzenoid systems.

In 1935, Hall [1] found the following theorem:

THEOREM 1

Let G be a bipartite graph with bipartition (X, Y). Then G contains a matching that saturates every vertex in X if and only if $|N(S)| \geq |S|$ for all $S \subseteq X$.

Here, $N(S)$ is the set of all vertices adjacent to the vertices in S, and is called the neighbour set of S.

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Since a benzenoid system is a bipartite graph, theorem 1 can be used to decide whether or not a given benzenoid system has Kekulé structures. However, using theorem 1, we have to examine all subsets of X. This is evidently tedious.

Another early result was given by Dewar and Longuet-Higgins in 1952 [2]:

THEOREM 2

Let A be the adjacent matrix of a benzenoid system H with n vertices, and K the number of Kekulé structures of H. Then $\det(A) = (-1)^{n/2} \cdot K^2$.

Its evident corollary is the following.

COROLLARY 3

A benzenoid system has Kekulé structures if and only if $\det(A) \neq 0$.

Using the theorem and corollary, we need to calculate or treat determinants with high order. This is also troublesome.

Let H be a benzenoid system drawn in a plane such that one of the three edge directions is vertical. A peak (valley) of H is a vertex in H which lies above (below) all its adjacent vertices. A P-V path, or a monotonous path in H, is a path starting from a peak, running monotonously downwards, and terminating in a valley. A perfect P-V path system, or a monotonous path system of H, is a selection of independent P-V paths (monotonous paths) which contain all peaks and valleys of H.

In 1952, the following theorem was discovered by Gordon and Davison [3], and rigorously proved by Sachs [4].

THEOREM 4

(a) The number of Kekulé structures in a benzenoid system is equal to the number of selections of independent monotonous paths.

(b) There is a one-to-one correspondence between the systems of independent monotonous paths and the Kekulé structures.

Theorem 4 implies the following:

COROLLARY 5

A benzenoid system H has Kekulé structures if and only if H has monotonous path systems.

However, it is also difficult to decide whether or not a given benzenoid system has monotonous path systems.

After this, chemists hoped to find some fairly simple necessary and sufficient conditions, or some method for rapid, systematic and reliable recognition. This is why, until 1982–1983, Gutman and Trinajstić pointed out several times [5–7] that the problem of recognizing Kekuléan benzenoid systems was an open problem, and it was thought to be one of the most difficult open problems in the topological theory of benzenoid systems.

In the last few years, some fairly simple necessary and sufficient conditions have been given [8–11], and the results of theorem 2 and corollary 3 have also been improved so that the number of Kekulé structures of a benzenoid system can be calculated by some determinant W with order lower than that of A [12–16]. The above new discoveries are outlined in a synthetical review [17].

On the other hand, some algorithms for determining whether or not a given benzenoid system has Kekulé structures were developed. These algorithms can be used not only for recognizing Kekuléan benzenoid structures, but also for finding a Kekulé structure of a Kekuléan benzenoid system. In ref. [4], Sachs gave such a good algorithm. Another, more economical algorithm, called two-vertex elimination, was suggested by Sheng Rongqin [18]. By theorem 4 and corollary 5, Gutman and Cyvin attempted to derive such an algorithm by deleting the monotonous path at the extreme left (or right) [19]. However, in ref. [29], the same authors pointed out a failure of the proposed "peeling algorithm".

In the present paper, we give an efficient and simple algorithm, called the C-P-V path elimination, for determining whether or not a given benzenoid system has Kekulé structures, or perfect P-V path systems, and we give its rigorous proof. If the given benzenoid system has Kekulé structures, the algorithm can find one of its Kekulé structures or a perfect P-V path system.

In order to derive our algorithm, we need to investigate the P-V paths on the boundary $C(H)$ of a benzenoid system H.

A segment on $C(H)$ is a sequence of adjacent edges. A P-V segment on $C(H)$ is a segment whose one end vertex is a peak and the other is a valley. An elementary P-V segment on $C(H)$ is a P-V segment whose every internal vertex is not a peak or a valley. Let p_i, υ_i be a peak and a valley of H, respectively. A P-V segment on $C(H)$ with end vertices p_i, υ_i is denoted by $S(p_i, \upsilon_i)$. If $S(p_i, \upsilon_i)$ is an elementary P-V segment, it is denoted by $S(p_i\text{-}\upsilon_i)$. If $S(p_i\text{-}\upsilon_i)$ is a P-V path on $C(H)$, it is denoted by $P(p_i\text{-}\upsilon_i)$. A P-P (V-V) segment $S(p_i, p_j)$ ($S(\upsilon_i, \upsilon_j)$), or an elementary P-P (V-V) segment $S(p_i\text{-}p_j)$ ($S(\upsilon_i\text{-}\upsilon_j)$) is defined in a similar way.

Let $n_s(C(H))$ denote the number of elementary P-V segments on $C(H)$, and let $n_p(C(H))$ denote the number of P-V paths on $C(H)$.

LEMMA 6

Let H be a benzenoid system. Then, (1) $n_s(C(H)) \geq 2$, (2) $n_p(C(H)) \geq \frac{1}{2}n_s(C(H)) + 1 \geq 2$.

Proof

(1) Obviously.

(2) Suppose we are running around H, following its boundary just once in a clockwise sense; then the total change of the angle of our movement with respect to a

fixed direction is 2π, where the total change of the angle on a P-P (V-V) segment is $-2k_i\pi$, the total change of the angle on a P-V segment which is not a P-V path is $-\pi - 2k'_j\pi$, the total change of the angle on a P-V path is π, where k_i, k'_j are non-negative integers (see fig. 1). Therefore,

$$n_p(C(H)) \cdot \pi + [n_s(C(H)) - n_p(C(H))] \cdot (-\pi) - 2\pi\left(\sum_i k_i + \sum_j k'_j\right) = 2\pi,$$

implying

$$n_p(C(H)) = \tfrac{1}{2} n_s(C(H)) + 1 + \left(\sum_i k_i + \sum_j k'_j\right) \geq 2.$$

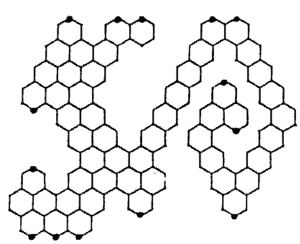


Fig. 1. Illustration for the proof of lemma 6.

DEFINITION 7

Let $P(p_i\text{-}v_i)$ be a P-V path on the boundary $C(H)$ of H. Let v_j be a valley of H such that there exists a P-V path $P(p_i, v_j)$ in H with the P-V segment $S(p_i\text{-}v_i, v_j)$ on $C(H)$ starting from p_i, passing through v_i, terminating in v_j, and being as long as possible. Then $S(p_i\text{-}v_i, v_j)$ is said to be the related segment of $P(p_i\text{-}v_i)$ with respect to p_i, denoted by $S^*(p_i^*\text{-}v_i)$. If there is not any confusion, we simply say that $S^*(p_i^*\text{-}v_i)$ is the related segment with respect to p_i. The complementary of $S^*(p_i^*\text{-}v_i)$ on $C(H)$ is denoted by $\overline{S^*(p_i^*\text{-}v_i)}$. Similarly, we can define the related segment $S^*(p_i\text{-}v_i^*)$ with respect to v_i and its complementary on $C(H)$.

It is easy to determine the related segment of a P-V path $P(p_i\text{-}v_i)$ on $C(H)$ with respect to p_i or v_i, say p_i. If $P(p_i\text{-}v_i)$ starts from p_i, and goes in the first step to the right (left), we make another P-V path $P^*(p_i^*, v_j)$ in H starting from p_i, going monotonously downward and leftward (rightward) as possible, and terminating in the valley v_j. Then the segment $S(p_i\text{-}v_i, v_j)$ on $C(H)$ is the related segment $S^*(p_i^*\text{-}v_i)$ with respect to p_i. The P-V path $P^*(p_i^*, v_j)$ made in this way is said to be the associated P-V path of $P(p_i\text{-}v_i)$ with respect to p_i. The related segment $S^*(p_i\text{-}v_i^*)$ and the associated P-V path $P^*(p_j, v_i^*)$ of $P(p_i\text{-}v_i)$ with respect to v_i can be determined in the same way (see fig. 2).

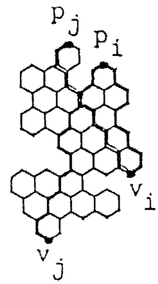


Fig. 2. Illustration for definition 7.

DEFINITION 8

Let $P(p_i\text{-}\upsilon_i)$ be a P-V path on the boundary $C(H)$ of H. If the related segment $S^*(p_i^*\text{-}\upsilon_i)$ $(S^*(p_i\text{-}\upsilon_i^*))$ of $P(p_i\text{-}\upsilon_i)$ contains only one peak p_i (valley υ_i), then $S^*(p_i^*\text{-}\upsilon_i)$ $(S^*(p_i\text{-}\upsilon_i^*)$ is said to be a canonical related segment. If a related segment of $P(p_i\text{-}\upsilon_i)$ is canonical, then $P(p_i\text{-}\upsilon_i)$ is said to be a canonical P-V path.

THEOREM 9

Let $P(p_i\text{-}\upsilon_i)$ be a canonical P-V path of a benzenoid system H, and let $H^* = H - P(p_i\text{-}\upsilon_i)$ be the system obtained from H by deleting the vertices on $P(p_i\text{-}\upsilon_i)$. Then H has a Kekulé structure if and only if H^* has a Kekulé structure.

Proof

Since $P(p_i\text{-}\upsilon_i)$ is canonical, $S^*(p_i^*\text{-}\upsilon_i)$ or $S^*(p_i\text{-}\upsilon_i^*)$, say $S^*(p_i^*\text{-}\upsilon_i)$, contains only one peak p_i of H.

Suppose that H has a Kekulé structure K. Then K corresponds to one P-V path system of H in which every P-V path is a K-alternating path (that is, a path alternately passing through double bonds and single bonds of K, and starting and ending with a double bond). Let $P_K(p_i, \upsilon_j)$ be such a K-alternating P-V path. Then υ_j must be on $S^*(p_i^*\text{-}\upsilon_i)$, and there is no other peak on the segment $S(p_i, \upsilon_j)$ of $S^*(p_i^*\text{-}\upsilon_i)$. So, if $\upsilon_j \neq \upsilon_i$, the perfect P-V path system corresponding to K would not contain υ_i. This is a contradiction. Hence, we have $\upsilon_j = \upsilon_i$. If $P_K(p_i, \upsilon_j)$ and $P(p_i\text{-}\upsilon_i)$ are distinct, then $P_K(p_i, \upsilon_j)\Delta P(p_i\text{-}\upsilon_i)$ (that is, the symmetric difference of their edge sets) is the union of some disjoint K-alternating cycles $C_1, C_2, \ldots, C_t$. Let $K^* = K\Delta C_1 \Delta C_2 \Delta \ldots \Delta C_t$. Then $P(p_i\text{-}\upsilon_i)$ becomes a K^*-alternating path. Therefore, $K^* \backslash E(P(p_i\text{-}\upsilon_i))$ is a Kekulé structure of $H - P(p_i\text{-}\upsilon_i)$. If $P_K(p_i, \upsilon_j) = P(p_i\text{-}\upsilon_i)$, then $P(p_i\text{-}\upsilon_i)$ is a K-alternating path, and $K\backslash E(P(p_i\text{-}\upsilon_i))$ is a Kekulé structure of H^*.

Conversely, suppose H^* has a Kekulé structure K^*. Obviously, $P(p_i\text{-}\upsilon_i)$ has a Kekulé structure K'. Then, $K^* \cup K' = K$ is a Kekulé structure of H.

LEMMA 10

Let H be a benzenoid system, $P(p_i - \upsilon_i)$ a P-V path on $C(H)$. Let $P^*(p_i^*, \upsilon_w)$ ($P^*(p_w, \upsilon_i^*)$) be the associated P-V path of $P(p_i - \upsilon_i)$. Let $P(p_j - \upsilon_j)$ be a P-V path in $S^*(p_i^* - \upsilon_i)$ ($S^*(p_i - \upsilon_i^*)$), and let $P(p_k - \upsilon_k)$ be a P-V path in $\overline{S^*(p_i^* - \upsilon_i)}$ ($\overline{S^*(p_i - \upsilon_i^*)}$), where $\upsilon_k \neq \upsilon_w$ ($p_k \neq p_w$). (1) If the order of p_j, υ_j on $S^*(p_i^* - \upsilon_i)$ ($S^*(p_i - \upsilon_i^*)$) is p_i-υ_i-p_j-υ_j-υ_w (p_w-p_j-υ_j-p_i-υ_i), and the order of p_k, υ_k on $\overline{S^*(p_i^* - \upsilon_i)}$ ($S^*(p_i$-$ui^*)$)*is* υ_w-υ_k-p_k-p_i (υ_i-υ_k-p_k-p_w), then both the associated P-V path of $P(p_j - \upsilon_j)$ with respect to p_j (υ_j) and the associated P-V path of $P(p_k - \upsilon_k)$ with respect to υ_k (p_k) cannot cross over $P^*(p_i^*, \upsilon_w)$ ($P^*(p_w, \upsilon_i^*)$). (2) If the order of p_j, υ_j on $S^*(p_i^* - \upsilon_i)$ ($S^*(p_i - \upsilon_i^*)$) is p_i-υ_i-υ_j-p_j-υ_w (p_w-υ_j-p_j-p_i-υ_i), and the order of p_k, υ_k on $\overline{S^*(p_i^* - \upsilon_i)}$ (S^*(pi-ui*)) is υ_w-p_k-υ_k-p_i (υ_i-p_k-υ_k-p_w), then all the associated paths of $P(p_j - \upsilon_j)$ and $P(p_k$-$\upsilon_k)$ cannot cross over $P^*(p_i^*, \upsilon_w)$ ($P^*(p_w, \upsilon_i^*)$).

Proof

Note that the enclosures in parentheses are the dual cases. We need only consider the case of $P^*(p_i^*, \upsilon_w)$.

From fig. 3, it is not difficult to see that the lemma follows.

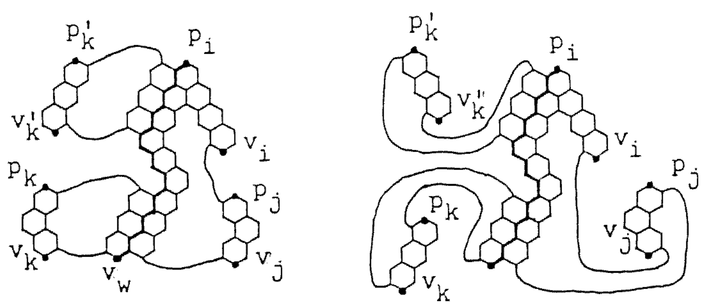


Fig. 3. Illustration for the proof of lemma 10. (a) The associated P-V paths with respect to p_j, υ_k, υ_k' cannot cross over $P^*(p_i^*, \upsilon_w)$. (b) All the associated P-V paths of $P(p_j - \upsilon_j)$, $P(p_k - \upsilon_k)$, $P(p_k', \upsilon_k')$ cannot cross over $P^*(p_i^*, \upsilon_w)$.

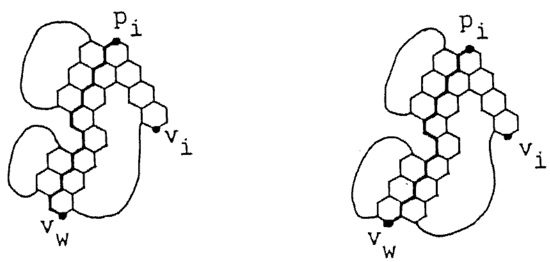
LEMMA 11

Let H be a benzenoid system, $P(p_i - \upsilon_i)$ a P-V path on $C(H)$. Let $P^*(p_i^*, \upsilon_w)$ ($P^*(p_w, \upsilon_i^*)$) be the associated P-V path of $P(p_i - \upsilon_i)$. (1) If $\overline{S^*(p_i^* - \upsilon_i)} \neq P^*(p_i^*, \upsilon_w)$ $\overline{(S^*(p_i - \upsilon_i^*)} \neq P^*(p_w, \upsilon_i^*)$), and in $\overline{S^*(p_i^* - \upsilon_i)}$ ($\overline{S^*(p_i - \upsilon_i^*)}$) there is a valley (peak) other than υ_w (p_w), then there exists a P-V path in $\overline{S^*(p_i^* - \upsilon_i)}$ ($\overline{S^*(p_i - \upsilon_i^*)}$) such that one of its related segments is contained in $\overline{S^*(p_i^*-v_i)}$ ($\overline{S^*(p_i-v_i^*)}$). (2) If $P(p_i-v_i)$ is non–canonical, then there exists a P-V path in $S^*(p_i^*-v_i)$ ($S^*(p_i-v_i^*)$) such that one of its related segments is contained in $S^*(p_i^*-v_i)$ ($S^*(p_i-v_i^*)$).

Proof

By symmetry, we need only discuss the cases of $S^*(p_i^*-v_i)$ and $\overline{S^*(p_i^*-v_i)}$.

Suppose we are running along $S^*(p_i^*-v_i)$ and $P^*(p_i^*, v_w)$ just once, the total change of the angle of our movement on $P^*(p_i^*, v_w)$ is π (see fig. 4), so the total change of the angle on $S^*(p_i^*-v_i)$ is π and the total change of the angle on $\overline{S^*(p_i^*-v_i)}$ is also π. Thus, $n_p(\overline{S^*(p_i^*-v_i)})\cdot\pi + (n_s(\overline{S^*(p_i^*-v_i)}) - n_p(\overline{S^*(p_i^*-v_i)}))\cdot(-\pi) - 2\pi\ \Sigma iki + \Sigma_j k_j') = \pi$, implying $n_p(\overline{S^*(p_i^*-v_i)}) = \frac{1}{2}(n_s(\overline{S^*(p_i^*-v_i)}) + 1) + (\Sigma_i k_i + \Sigma_j k_j') \geq 1$. If $P(p_i-v_i)$ in non-canonical, then $n_s(S(v_i, v_w)) \geq 2$ and $n_p(S(v_i, v_w)) \cdot \pi + (n_s(S(v_i, v_w)) - n_p(S(v_i, v_w))) \cdot (-\pi) - 2\pi(\Sigma_i k_i + \Sigma_j k_j') = 0$, implying $n_p(S(v_i, v_w)) = \frac{1}{2} n_s(S(v_i,$ uw$)) + (\Sigma_i k_i + \Sigma_j k_j') \geq 1$.



(a) (b)

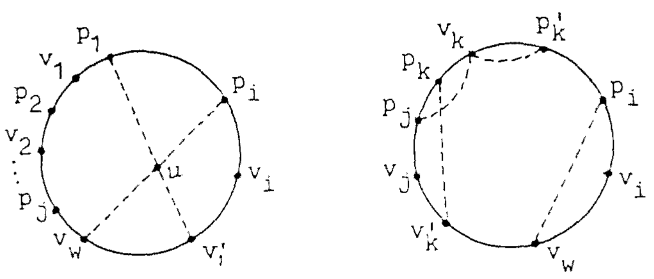
Fig. 4. Illustration for the proof of lemma 11.

(1) By contradiction: Suppose any related segment of any P-V path in $\overline{S^*(p_i^*-v_i)}$ is not contained in $\overline{S^*(p_i^*-v_i)}$.

Since there is a valley other than v_w in $\overline{S^*(p_i^*-v_i)}$, there is a P-V path in $\overline{S^*(p_i^*-v_i)}$ whose valley is not v_w. Otherwise, there is only one P-V path in $\overline{S^*(p_i^*-v_i)}$, say $P(p_j-v_w)$. However, $n_p(S(p_j, p_i)) \cdot \pi + (n_s(S(p_j, p_i)) - n_p(S(p_j,$ pi$)))$ $(-\pi) - 2\pi(\Sigma_i k_i + \Sigma_j k_j') = 0$, implying $n_p(S(p_j, p_i)) = \frac{1}{2} n_s(S(p_j, p_i)) + (\Sigma_i k_i + \Sigma_j k_j') \geq 1$, a contradiction.

In addition, we can assert that there is a P-V path in $\overline{S^*(p_i^*-v_i)}$, say $P(p_k-v_k)$, such that its associated P-V path, say $P^*(p_k^*, v_k')$, is not a P-V path on $C(H)$, and $\overline{S^*(p_k^*-v_k)}$ is contained in $\overline{S^*(p_i^*-v_i)}$ and contains a valley other than v_k'.

Otherwise, let $P(p_1-v_1)$ be a P-V path in $\overline{S^*(p_i^*-v_i)}$, $v_1 \neq v_w$, and let the order of p_1, v_1 on $\overline{S^*(p_i^*-v_i)}$ be v_w-v_1-p_1-p_i. By lemma 10, the asociated P-V path with respect to v_1 cannot cross over $P^*(p_i^*, v_w)$, so it is a P-V path on $\overline{S^*(p_i^*-v_i)}$, say $P(p_2-v_1)$. For the same reason, the associated P-V path with respect to p_2 is also a P-V path on $\overline{S^*(p_i^*-v_i)}$, say $P(p_2-v_2)$. If $v_2 \neq v_w$, then the associated P-V path with respect to v_2 is a P-V path on $S^*(p_i^*-v_i)$, say $P(p_3-v_2)$, and so is $P(p_3-v_3), \ldots$, until $P(p_j-v_w)$ (see fig. 5(a)). Then the total change of the angle on $S(v_w,p_1)$ is $(2j-1)\pi \geq 3\pi$, so $p_1 \neq p_i$. Without loss of generality, we assume that the associated P-V path with respect to p_1, say $P^*(p_1^*, v_1')$, is not a P-V path on $\overline{S^*(p_i^*-v_i)}$ Then $P^*(p_1^*, v_1')$ would cross over $P^*(p_i^*, v_w)$. Let u be their common vertex. Then the path consisting of the segment $S(p_1,u)$ on $P^*(p_1^*, v_1')$ and the segment $S(u, v_w)$ on $P^*(p_i^*, v_w)$ is a P-V path. Thus, the total change of the angle on $S(v_w,p_1)$ is π, contradictory to $(2j-1)\pi \geq 3\pi$.



(a) (b)

Fig. 5. Illustration for the proof of lemma 11(1).

Let $P(p_j-v_j)$ be a P-V path in $\overline{S^*(p_i^*-v_i)}$ such that its associated P-V path, say $P^*(p_j^*, v_k)$, is not a P-V path on $C(H)$, and $\overline{S^*(p_j^*-v_j)}$ is contained in $\overline{S^*(p_i^*-v_i)}$ (see fig. 5(b); if the order of p_j, v_j is opposite, we can discuss it in a similar way). Suppose that there is no valley other than v_k in $\overline{S^*(p_j^*-v_j)}$. Then there is only one P-V path in $\overline{S^*(p_j^*-v_j)}$, say $P(p_k-v_k)$. Let $P^*(p_k^*, v_r)$ and $P^*(p_r, v_k^*)$ be the associated P-V paths with respect to p_k and v_k, respectively. Clearly, p_r must be in $S(v_k,p_i)$. Since there is no valley other than v_k in $\overline{S^*(p_j^*-v_j)}$, $P^*(p_k^*, v_r)$ will cross over $P^*(p_j^*, v_k)$ and v_r must be in $S(v_w, v_j)$ (see fig. 5(b)). However, $P^*(p_k^*, v_r)$ cannot cross over $P^*(p_r, v_k^*)$, so H must be as shown in fig. 6. Clearly, $P^*(p_r, v_k^*)$ is not a P-V path on $C(H)$. If $\overline{S^*(p_k-v_k^*)}$ contains no peak other than p_r, there is only one P-V path in $\overline{S^*(p_k-v_k^*)}$, say $P(p_r-v_s)$. However, the associated P-V path with respect to p_r will terminate in v_k, and $\overline{S^*(p_r^*-v_s)}$ is contained in $\overline{S^*(p_i^*-v_i)}$, a contradiction. Hence, $\overline{S^*(p_k-v_k^*)}$ contains a peak other than p_r, and $P(p_k-v_k)$ is the required P-V path.

Furthermore. let $\overline{S^*(p_k-v_k^*)}$ be minimal. However, for the same reason, there is another P-V path in $\overline{S^*(p_k-v_k^*)}$, say $P(p_t-v_t)$, such that $S^*(p_t^*-v_t)$ or $S^*(p_t-v_t^*)$, say $S^*(p_t^*-v_t)$, contains a valley other than its end vertex and is contained in $\overline{S^*(p_k-v_k^*)}$, contradicting the minimality of $\overline{S^*(p_k-v_k^*)}$.

Now (1) holds.

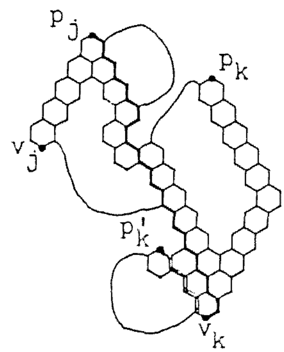


Fig. 6. Illustration for the proof of lemma 11.

(2) Follows from a similar argument as in (1).

THEOREM 12

Let H be a benzenoid system. Then there exist at least two canonical P-V paths on $C(H)$.

Proof

By lemma 6, there are at least two P-V paths on $C(H)$. Let $P(p_i\text{-}\upsilon_i)$ be a P-V path on $C(H)$. If $P(p_i\text{-}\upsilon_i)$ is not canonical, then, by lemma 11(2), in $S^*(p_i^*\text{-}\upsilon_i)$ there is a P-V path such that one of its related segments is contained in $S^*(p_i^*\text{-}\upsilon_i)$. Let $P(p_1\text{-}\upsilon_1)$ be such a P-V path, such that $S^*(p_1^*\text{-}\upsilon_1)$ is contained in $S^*(p_i^*\text{-}\upsilon_i)$ and $S^*(p_1^*\text{-}\upsilon_1)$ is minimal. Then $S^*(p_1^*\text{-}\upsilon_1)$ must be a canonical related segment and so $P(p_1\text{-}\upsilon_1)$ is also canonical.

Let $P^*(p_1^*, \upsilon_2)$ be the associated P-V path with respect to p_1.

If $P^*(p_1^*, \upsilon_2)$ is a P-V path on $C(H)$, then evidently it is also a canonical P-V path.

If $P^*(p_1^*, \upsilon_2)$ is not a P-V path on $C(H)$, and in $\overline{S^*(p_1^*\text{-}\upsilon_1)}$ there is a valley other than υ_2, then, by lemma 11(1), there is a P-V path in $\overline{S^*(p_1^*\text{-}\upsilon_1)}$ such that one of its related segments is contained in $\overline{S^*(p_1^*\text{-}\upsilon_1)}$; so, by lemma 11(2), there is a canonical P-V path in $\overline{S^*(p_1^*\text{-}\upsilon_1)}$. If $\overline{S^*(p_1^*\text{-}\upsilon_1)}$ contains no valley other than υ_2, then there is only one P-V path in $\overline{S^*(p_1^*\text{-}\upsilon_1)}$, say $P(p_2\text{-}\upsilon_2)$. Clearly, $S^*(p_2\text{-}\upsilon_2^*)$ is contained in $\overline{S^*(p_1^*\text{-}\upsilon_1)}$ and contains no valley other than υ_2. So $P(p_2\text{-}\upsilon_2)$ is a canonical P-V path. □

Let H be a benzenoid system, and let $P(p_i\text{-}\upsilon_i)$ be a canonical P-V path of H. We delete from H the vertices on $P(p_i\text{-}\upsilon_i)$, and, successively, the vertices of valency 1 together with their adjacent vertices, until no vertex of valency 1 remains. A component of the resultant graph H' may be an isolated vertex, a benzenoid system, or a generalized

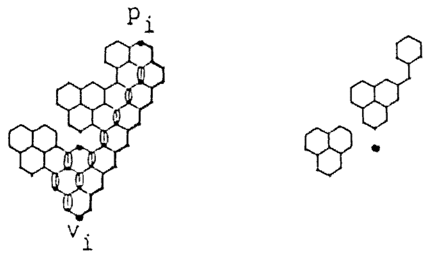


Fig. 7. Illustration for the proof of theorem 12.

benzenoid system which contains cut edges and no vertex of valency 1, and its every interior region is a hexagon (see fig. 7).

DEFINITION 13

A connected subgraph of a benzenoid system which contains no vertex of valency 1 and whose every interior region is a hexagon is said to be a generalized benzenoid system of type T, simply denoted by a TGB. In particular, if a TGB contains no cut edge, it is also a benzenoid system.

Let H^* be a TGB which is not a benzenoid system. Contracting each maximal benzenoid system in H^* to a vertex, we shall obtain a tree $T(H^*)$. An end vertex in $T(H^*)$ corresponds to a maximal benzenoid system H_i^* in H^*, called an end-system, which is incident with only one cut edge of H^*. The vertex in H_i^* incident with the cut edge is called an attachable vertex of H_i^*. Since a nontrivial tree has at least two end vertices, H^* also has at least two end-systems. We denote by $C(H^*)$ the boundary of H^*. Then $C(H^*)$ is a closed walk in which each cut edge of H^* in $C(H^*)$ is traversed twice. If there is a peak or a valley in H^* which is a cut vertex, it will occur twice in $C(H^*)$. Therefore, we need to distinguish proper peaks (valleys) on $C(H^*)$ from improper ones.

DEFINITION 14

Let H^* be a TGB which is not a benzenoid system. Suppose we are running along $C(H^*)$ in a clockwise manner. If we pass through a peak p_i (valley v_i) from the left (right) to the right (left), then p_i (v_i) is said to be a proper peak (valley) on $C(H^*)$, simply said, a peak (valley) on $C(H^*)$, otherwise an improper peak (valley) on $C(H^*)$.

Under this definition, the P-V paths and the P-V segments on $C(H^*)$ possess the same properties as the P-V paths and the P-V segments on the boundary of a benzenoid system. We can also define the concepts of a canonical P-V path on $C(H^*)$, a related segment and an associated path of a P-V path on $C(H^*)$, and prove that the conclusions of lemma 6 and theorems 9 and 12 follow for a TGB. However, for simplicity we prefer to deduce our algorithm from the foregoing results.

THEOREM 15

Let H^* be a TGB which is not a benzenoid system, and let H be an end-system in H^* with the attachable vertex x.

(1) If x is a unique peak or valley of H, then, for any P-V path $P(p_i\text{-}v_i)$ on $C(H)$, H^* has a Kekulé structure if and only if $H^* - P(p_i\text{-}v_i)$ has a Kekulé structure; otherwise:

(2) H contains at least one canonical P-V path $P(p_j\text{-}v_j)$ on $C(H)$, one of whose canonical related segments does not contain x, and H^* has a Kekulé structure if and only if $H^* - P(p_j\text{-}v_j)$ has a Kekulé structure.

Proof

(1) Without loss of generality, we assume that the attachable vertex x of H is a unique valley v_i of H, and $P(p_i\text{-}v_i)$ is a P-V path on $C(H)$.

Suppose that H^* has a Kekulé structure K. The K-alternating P-V path starting from p_i must pass through v_i, for v_i is a unique valley of H. Then we have either that $P(p_i\text{-}v_i)$ is a K-alternating path or that there is another Kekulé structure K^* of H^* such that $P(p_i\text{-}v_i)$ is a K^*-alternating path. So $K \backslash E(P(p_i\text{-}v_i))$ or $K^* \backslash E(P(p_i\text{-}v_i))$ is a Kekulé structure of $H^* - P(p_i\text{-}v_i)$.

Conversely, suppose that $H^* - P(p_i\text{-}v_i)$ has a Kekulé structure K^*. Clearly, $P(p_i\text{-}v_i)$ has a Kekulé structure K'. Then, $K = K^* \cup K'$ is a Kekulé structure of H^*.

(2) We need to consider the following two cases:

Case 1: x is not a peak or a valley of H.

Let $P(p_1\text{-}v_1)$ be a canonical P-V path of H, and let $S^*(p_1^*\text{-}v_1)$ be a canonical related segment. Then either $S^*(p_1^*\text{-}v_1)$ does not contain x or, for the same reason as in the proof of theorem 12, there is a canonical P-V path in $\overline{S^*(p_1^*\text{-}v_1)}$ such that one of its canonical related segments is contained in $\overline{S^*(p_1^*\text{-}v_1)}$, and so does not contain x.

Case 2: x is a peak or a valley, say a valley, of H, but is not a unique valley of H.

It is easy to prove that there is a canonical P-V path $P(p_1\text{-}v_1)$ of H such that $x \neq v_1$. If $S^*(p_1\text{-}v_1^*)$ is a canonical related segment, then it does not contain x. If only $S^*(p_1^*\text{-}v_1)$ is canonical, then $\overline{S^*(p_1^*\text{-}v_1)}$ must contain a valley which is not the end vertex of $\overline{S^*(p_1^*\text{-}v_1)}$ (otherwise $S^*(p_1\text{-}v_1^*)$ would also be canonical, a contradiction). Then either $S^*(p_1^*\text{-}v_1)$ does not contain x or, by lemma 11, in $\overline{S^*(p_1^*\text{-}v_1)}$ there is a canonical P-V path such that one of its canonical related segments is contained in $\overline{S^*(p_1^*\text{-}v_1)}$, and does not contain x.

Now let $P(p_i\text{-}v_i)$ be a canonical P-V path of H, one of whose canonical related segments does not contain x. It is not difficult to see that H^* has a Kekulé structure if and only if $H^* - P(p_i\text{-}v_i)$ has a Kekulé structure.

Now we can give an algorithm for determining whether or not a given benzenoid system H has a Kekulé structure. The algorithm is founded on deleting a canonical P-V path. We call it canonical P-V path elimination, simply C–P-V path elimination. If H is Kekuléan, the algorithm can find a Kekulé structure or a perfect P-V path system of H.

We first give a method for finding a canonical P-V path of a benzenoid system H, or a canonical P-V path $P(p_i\text{-}\upsilon_i)$ of an end-system H of a TGB H^* which satisfies the condition that H^* has a Kekulé structure if and only if $H^* - P(p_i\text{-}\upsilon_i)$ has a Kekulé structure.

PROCEDURE A

Let H be a benzenoid system, and let $P(p_i\text{-}\upsilon_i)$, $i = 1,2,\ldots, n_{\mathrm{p}}(C(H))(\geq 2)$, be P-V paths on $C(H)$.

(1) Set $P(p_i\text{-}\upsilon_i) = P(p_1\text{-}\upsilon_1)$.

(2) Determine $S^*(p_i^*\text{-}\upsilon_i)$ and $S^*(p_i\text{-}\upsilon_i^*)$. If one of them is a canonical related segment of $P(p_i\text{-}\upsilon_i)$, then $P(p_i\text{-}\upsilon_i)$ is a canonical P-V path on $C(H)$, so stop. Otherwise, go to step (3).

(3) Replace $P(p_i\text{-}\upsilon_i)$ by $P(p_{i+1}\text{-}\upsilon_{i+1})$ and go to step (2).

PROCEDURE B

Let H be an end-system of a TGB H^* with the attachable vertex x, and let $P(p_i\text{-}\upsilon_i)$, $i = 1,2,\ldots, n_{\mathrm{p}}(C(H))(\geq 2)$, be P-V paths on $C(H)$.

(1) If x is a unique peak or valley of H, then any P-V path $P(p_i\text{-}\upsilon_i)$ on $C(H)$ satisfies the condition that H^* has a Kekulé structure if and only if $H^* - P(p_i\text{-}\upsilon_i)$ has a Kekulé structure; stop. Otherwise, set $P(p_i\text{-}\upsilon_i) = P(p_1\text{-}\upsilon_1)$ and go to step (2).

(2) Determine $S^*(p_i^*\text{-}\upsilon_i)$ and $S^*(p_i\text{-}\upsilon_i^*)$. If one of them is a canonical related segment of $P(p_i\text{-}\upsilon_i)$, and does not contain x, then $P(p_i\text{-}\upsilon_i)$ satisfies the condition that H^* has a Kekulé structure if and only if $H^* - P(p_i\text{-}\upsilon_i)$ has a Kekulé structure; stop. Otherwise, go to step (3).

(3) Replace $P(p_i\text{-}\upsilon_i)$ by $P(p_{i+1}\text{-}u_{i+1})$ and go to step (2).

By theorems 12 and 15, using procedures A and B, we can surely obtain the required P-V path on $C(H)$.

C–P-V path elimination

Let H be a benzenoid system, and let $p(H)$ and $\upsilon(H)$ be the number of peaks and valleys of H, respectively. If $p(H) \neq \upsilon(H)$, H has no Kekulé structure. Hence, we assume that $p(H) = \upsilon(H)$.

Orient H in the plane so that $p(H)$ is as small as possible. Let $H_1 = H$, and let H_{k+1} be obtained after step k. For $k = 1,2, \ldots,$ do the following operations:

(1) If H_k is a benzenoid system, by using procedure A, find a C–P-V path of H_k and delete it. Then, we colour the edges in the C–P-V path red and blue alternately so that the initial edge is red.

(2) If H_k has a vertex x of valency 1, delete x and its adjacent vertex x'. We colour the edge incident with x red.

(3) If H_k is a TGB, find an end-system H_k' in H_k. Then, by using procedure B, find a canonical P-V path $P(p_i\text{-}v_i)$ on $C(H_k')$ that satisfies the condition that H_k has a Kekulé structure if and only if $H_k - P(p_i\text{-}v_i)$ has a Kekulé structure, and delete it. We colour the edges in the C–P-V path red and blue alternately so that the initial edge is red.

(4) If H_k is not connected, for its one component do the operations.

(5) If H_k has an isolated vertex, stop. Then H has no Kekulé structure.

(6) If all the vertices of H are deleted, then all the red edges are a Kekulé structure of H and all the P-V paths of H, in each of which there is an alternating path of red edges and blue edges with the initial edge red, form a perfect P-V path system of H; stop. Otherwise, return to step (1).

Note that in step (2), H_k has a Kekulé structure if and only if $H_k - x - x'$ has a Kekulé structure, and the reliability of procedures A and B is ensured by theorems 12 and 15. Now the C–P-V path elimination holds rigorously from theorems 9 and 15.

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