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On the Correspondence between Peaks and Valleys in P-V Path Systems of Benzenoids

He Wenjie, He Ying and He Wenchen
Hebei Institute of Technology,
Box 134,Tianjin, 300130, China

Abstract: Each peak-valley P-V path system in a Kekulé hexagonal system H induces a correspondence between the peaks and valleys of H. If H has no hole then this correspondence is the same for all peak-valley path systems, but the converse need not be true. Also, the number of peaks and valleys in holes (called internal peaks and valleys) is discussed.

Key Word: Benzenoid, Coronoid, Hexagonal system, hole, Kekulé structure, Peak, Valley, P-V path system

In this paper , all the terms are applied in consistence with those in[1-7].

A hole in a hexagonal system H is a finite face of H that covers more than one hexagon. The set H_k of all Kekuléan hexagonal systems decomposes into the class B_k of Kekuléan benzenoids (which have no holes) and the class C_k of Kekuléan coronoids (which have some holes).

Consider an $H \in H_k$. It is drawn in a plane such that some of its edges are vertical. A peak of H is a vertex lying above all its first neighbours. And a valley is a vertex lying below all its first neighbours. If a peak (valley) is on the boundary of a hole in H, then it is called an internal one, otherwise an external one. A P-V path of H is a monotone downward path issuing from a peak and terminating in a valley. A P-V path system (also called perfect P-V path system) of H is a system of disjoint P-V paths containing all the peaks and valleys of H.

The concept of P-V paths was proposed by Gordon and Davison in 1952[8]. So far, the P-V path method has become a very useful method to investigate benzenoids and coronoids[9]. In 1984, Sachs proposed the 1-1 correspondence theorem between P-V path systems and Kekulé structures[10]. Now we face an important problem:

"Does the correspondence between peaks and valleys induced by a P-V path system of H depend on the choice of the P-V path system for a given orientation of H ?"

To answer the question by using the P-V matrix method[11] is impossible because the exchange of rows or columns is nothing more then the exchange of their labels and does not change the correspondence between peaks and valleys.

Pierre Hansen and Maolin Zheng in 1991[12] proved the uniqueness for a hexagonal system $H \in B_k$. K.Cameron and H.Sachs also obtained this result (more general) in 1994[13]. Now by using a simple method we investigate this problem and get more results.

Consider a given orientation of a Kekuléan hexagonal system $H \in H_k$. For two P-V path systems of H, the correspondences between peaks and valleys are

$$\begin{pmatrix} p_1, p_2, \cdots, p_p \\ v_1, v_2, \cdots, v_p \end{pmatrix} \text{ and } \begin{pmatrix} p_1, p_2, \cdots, p_p \\ v_{1_0}, v_{2_0}, \cdots, v_{p_0} \end{pmatrix}, \text{ respectively,}$$

where the suffix p is equal to the number of peaks (or valleys) in H.

The change of the correspondences can be expressed by the following permutation of valleys:

$$\begin{pmatrix} v_1, v_2, \cdots, v_p \\ v_{1_0}, v_{2_0}, \cdots, v_{p_0} \end{pmatrix} = (v_{a_1}, v_{a_2}, \cdots, v_{a_n})(v_{b_1}, v_{b_2}, \cdots, v_{b_m})\cdots, \qquad (1)$$

where $n+m+\cdots=p$.

The right hand of (1) is a product of some cycles. It is well known that a permutation can be represented by a product of cycles.

Suppose that a permutation considered is the product of ν_p cycles of length p,$\cdots$,ν_2 cycles of length 2, and ν_1 cycles of length 1 where ν_i's (i=1 to p) are non-negative integers. Then, the permutation is referred to as possessing the cycle structure$(1^{\nu_1}2^{\nu_2}\cdots p^{\nu_p})$, where $1\nu_1+2\nu_2+\cdots+p\nu_p=p$.

Obviously, in the cycle decomposition (1) of a permutation, 1-cycles do not change the correspondence between peaks and valleys. Consider an n-cycle :

$$(v_{a_1}, v_{a_2}, \cdots, v_{a_n}) = \begin{pmatrix} v_{a_1}, v_{a_2}, \cdots, v_{a_n} \\ v_{a_2}, v_{a_3}, \cdots, v_{a_1} \end{pmatrix}, \quad (1 \le n \le p) \qquad (2)$$

We will prove that there exist at least n-1 internal peaks and valleys in H corresponding to the n-cycle, and if $n>1$, then $H \in C_k$.

Before we prove this result, we give a lemma which provides a criterion for a peak or valley to be an internal one.

<u>*Definition*</u> A peak (valley) with its two incident edges is called a peak-arrowhead (valley-arrowhead).

<u>*Lemma*</u> *In an $H \in H_k$, a peak (valley) is an internal one if and only if there exists in H a circuit C such that the peak(valley) belongs to C and its peak-arrowhead (valley-arrowhead) points to the interior of the circuit.*

Proof: Consider an internal peak p_i (valley v_j) in H. According to the definition of internal peak (valley), $p_i(v_j)$ is on the boundary C_0(i.e. a circuit) of a hole in H. Obviously, the peak(valley)-arrowhead of p_i (v_j) points to the interior of the circuit C_0. On the other hand, suppose that a peak p_i (valley v_j) is on a circuit C whose edges and vertices belong to H, and the peak(valley)-arrowhead of $p_i(v_i)$ points to the interior of C. Then in the interior of C and above the peak (below the valley) the two hexagons adjacent to $p_i(v_j)$ are absent. These two hexagons adjacent to each other are shown by shaded lines in Fig.1. and form a part of a hole of H. Thus, $p_i(v_j)$ is on the boundary of the hole. According to the definition of an internal peak (valley), $p_i(v_j)$ is an internal peak (valley). Q.E.D.

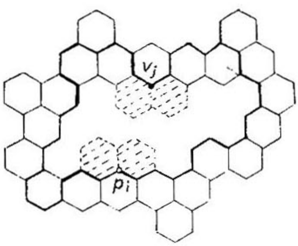


Fig.1 Internal Peak (Valley)

Now we prove, in a more or less sketchy way, that there are at least n-1 internal peaks and valleys corresponding to an n-cycle in the cycle product representation (2) of valley permutation.

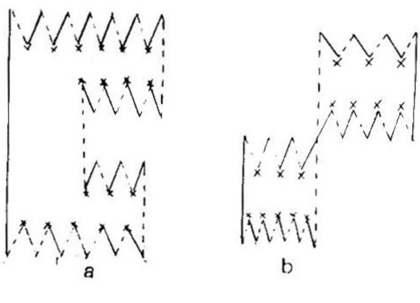


Fig.2

In fact, the paths $p_{a_1}v_{a_1}, p_{a_2}v_{a_2}, \cdots, p_{a_n}v_{a_n} (1 \le n \le p)$ in one P-V path system shown in Fig.2 by heavy lines and the P-V paths $p_{a_1}v_{a_2}, p_{a_2}v_{a_3}, \cdots, p_{a_n}v_{a_1} (1 \le n \le p)$ in the other P-V path system shown in Fig.2 by broken lines form a circuit. Because any two P-V paths belonging to the same P-V path system do not have edges and vertices in common, in the topological graphs (Figs.2a and 2b) only the intersection of lines belonging to different systems is allowed.

First, consider the case in which there is no intersection of the lines belonging to the different systems except for peaks and valleys. As shown in Fig.2a, according to the lemma stated above the peaks and valleys with sign "x" are internal ones. Obviously, the number of these internal peaks and valleys is equal to or greater than n-1. In fact, in the two rows at the top as well as in the two rows at the bottom, the number of vertices with "x" is one less than that of vertices without "x", and in the other rows the number of vertices with "x" is the same as that of vertices without "x". Hence, the number of the vertices with "x" is equal to $(2n-2)/2 = n-1$.

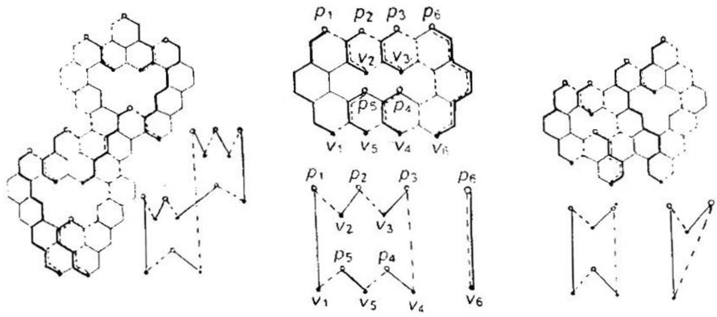
Second, consider the case shown in Fig.2b in which there is only one intersection of a heavy line and a broken line except for peaks and valleys. In this case we have two circuits.And the numbers of their vertices are $2n_1$ and $2n_2$, respectively. $2n_1 + 2n_2 = 2n+2$, at the right hand of which the added two vertices result from the intersection of the two circuits and are neither peaks nor valleys, therefore they have no "x". Thus, we obtain that the number of internal peaks and valleys is equal to or greater than $(n_1 - 1)+(n_2 - 1) = n+1-2 = n-1$.

For the case in which there are k intersections of heavy lines and broken lines except for peaks and valleys, the number of circuits is k+1. Denote by $2n_1, 2n_2, \cdots, 2n_{k+1}$ the number of the vertices of the k+1 circuits, respectively. Obviously, $2n_1 + 2n_2 + \cdots + 2n_{k+1} = 2n+2k$. The number of internal peaks and valleys is equal to or greater than $(n_1 - 1)+(n_2 - 1)+\cdots+ +(n_{k+1} - 1) = n+k-(k+1) = n-1$. Q.E.D.

Thus, we immediately have the following theorem:

<u>Theorem</u> For a given orientation of an $H \in H_k$, if corresponding to two P-V path systems of H, there exists a permutation of valleys $\begin{pmatrix} v_1, v_2, \cdots, v_p \\ v_{1_0}, v_{2_0}, \cdots, v_{p_0} \end{pmatrix}$*, which has a cycle structure* $(1^{\nu_1} 2^{\nu_2} \cdots p^{\nu_p})$*, where* $p = 1\nu_1 + 2\nu_2 + \cdots + p\nu_p$*, then the number m of internal peaks and valleys satisfies* $m \ge \sum_{i=1}^{p}(i-1)\nu_i = p-c$*, where c is the total number of cycles in the cycle structure* $(c = \sum_{i=1}^{p}\nu_i)$*. If* $p-c>0$*, then* $H \in C_k$.

Some examples of the theorem are shown in Fig.3, Fig.4 and Fig.5.



$(1^0 2^0 3^0 4^0 5^0 6^0 7^1)$ $m=p-c=7-1=6$ $(1^1 2^0 3^0 4^0 5^1)$ $m=p-c=6-2=4$ $(1^0 2^1 3^1 4^0 5^0)$ $m=p-c=5-2=3$

Fig 3. Some Examples

If $H \in B_k$, then for any two P-V path systems corresponding to the same orientation of H, the cycle structure of the valley permutation only contains 1-cycles. Hence, we immediately have the following corollary.

Corollary *If $H \in B_k$, then for any orientations of H, all perfect P-V path systems induce the same correspondence between the peaks and valleys of H.*

We have another method of proving this result.

For one of three possible orientations of $H(\in B_k)$, denote by p(H) (v(H)) the number of peaks (valleys) of H.

p(H)=v(H). [14] (3)

Suppose that a P-V path system has a correspondence between peaks and valleys as follows:

$$\begin{pmatrix} p_1, p_2, \cdots, p_p \\ v_1, v_2, \cdots, v_p \end{pmatrix} \tag{4}$$

A P-V path $p_i v_i$ $(1 \le i \le p(H))$ belonging to the P-V path system divides H into two parts. One lies on the left bank of $p_i v_i$ and is denoted by $L(p_i v_i)$ (where $L(p_i v_i)$-$p_i v_i$ may be disconnected) and the other is $R(p_i v_i)$ (where $R(p_i v_i)$-$p_i v_i$ may also be disconnected).

$$L(p_i v_i) \cap R(p_i v_i) = p_i v_i, \quad \text{and} \quad L(p_i v_i) \cup R(p_i v_i) = H. \tag{5}$$

Since both $L(p_i v_i)$ and $R(p_i v_i)$ are Kekuléan,

$$p(L(p_iv_i)) = v(L(p_iv_i)), \quad and \quad p(R(p_iv_i)) = v(R(p_iv_i)). \tag{6}$$

Assume that for another P-V path system the correspondence between peaks and valleys is different from (4): say, the i-th P-V path p_iv_j starts from p_i and ends at v_j $(j \neq i)$. Similar to (6), then we have

$$p(L(p_iv_j)) = v(L(p_iv_j)), \quad and \quad p(R(p_iv_j)) = v(R(p_iv_j)). \tag{7}$$

Without losing generality, put $v_j \in L(p_iv_i)$. Then, obviously,

$$p(L(p_iv_i)) = p(L(p_iv_j)), \quad but \quad v(L(p_iv_i)) > v(L(p_iv_j)). \tag{8}$$

Thus,

$$p(L(p_iv_j)) \neq v(L(p_iv_j)), \quad and \quad p(R(p_iv_j)) \neq v(R(p_iv_j)).$$

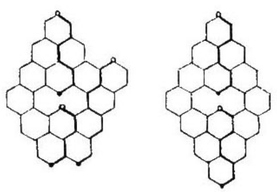
It is in contradiction with (7). Hence, such a P-V path system containing the P-V path p_iv_j does not exist. Q.E.D.

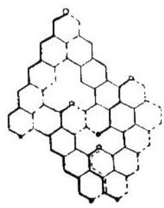
Discussion

1. The theorem stated above indicates that for a given orientation of $H \in H_k$, the violation of uniqueness of the correspondence between peaks and valleys for different P-V path systems results from the holes in H. But the following statement is not true.

If $H \in C_k$, then, for some orientation of H, there are at least two perfect P-V path systems of H inducing different correspondences between peaks and valleys.

Two counterexamples are shown in Fig.4.





$(1^3 2^0 3^0)$ $\quad$ $(1^2 2^0)$ $\quad$ $(1^1 2^0 3^1 4^0)$

$m = 2 > p - c = 3 - 3$ $\quad$ $m = 2 > p - c = 2 - 2$ $\quad$ $m = 3 > p - c = 4 - 2$

Fig.4 $\quad$ *Fig.5*

2. According to the theorem stated above, we have that $m \geq p - c$ where m is the number of internal peaks and valleys in H. For the examples in Fig.3 $m = p - c$; and the examples in Fig.4 and Fig.5 $m > p - c$.

3. For one orientation of $H \in C_k$, the uniqueness of correspondence is violated, while for the other two orientations, the uniqueness may hold. An example is shown in Fig.6.

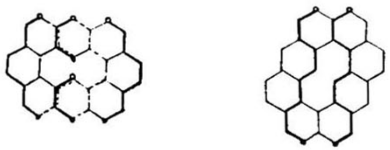


Fig.6

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