AN IMPROVEMENT OF THE CANONICAL $P-V$ PATH ELIMINATION FOR RECOGNIZING KEKULÉAN BENZENOID SYSTEMS*

Guo XIAOFENG and Zhang FUJI
Department of Mathematics, Xinjiang University, Wulumuqi Xinjiang, P.R. of China

Received 1 November 1990

Abstract

The canonical $P-V$ path elimination for recognizing Kekuléan benzenoid systems has been given in ref. [1]. In this paper, we give a new definition of a canonical $P-V$ path of a benzenoid system which is an improvement of the definition in ref. [1], so that the canonical $P-V$ paths can be more easily recognized. By the new definition, we give an improved canonical $P-V$ path elimination.

A benzenoid system is a connected plane with no cut vertex whose every interior face is bounded by a regular hexagon. A connected subgraph of a benzenoid system is said to be a generalized benzenoid system. A generalized benzenoid system is said to be type T, denoted by TGB, if it contains no vertex of valency one and each of its interior faces is bounded by a hexagon. Particularly, if a TGB contains no cut edge, it is also a benzenoid system.

Let H be a TGB 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 $P(p_i-v_i)$ in H is a path starting from a peak p_i, running monotonously downward, and terminating in a valley v_i. A (perfect) $P-V$ path system of H is a selection of independent $P-V$ paths which contain all peaks and valleys of H. The numbers of peaks and valleys in H are denoted by $p(H)$ and $v(H)$, respectively.

A Kekulé structure of a TGB H is an independent edge set in H such that every vertex in H is incident with an edge in the edge set. H 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 fundamental problem in the topological theory of benzenoid systems.

In the last few years, some necessary and sufficient conditions for recognizing Kekuléan benzenoid systems have been given [2,3]. On the other hand, some algorithms for determining whether or not a given benzenoid system has Kekulé structures as

*This project was supported by NSFC.

well as for finding a Kekulé structure of a Kekuléan benzenoid system have also been developed. In ref. [4], Sachs gave such a good algorithm. Another, more economical, algorithm, called two-vertex elimination, was suggested by Sheng Rongqin [5]. Based on a one-to-one correspondence between $P-V$ path systems and Kekulé structures of a benzenoid system, Gutman and Cyvin attempted to derive a peeling algorithm [6] by deleting a $P-V$ path at the extreme left (or right). However, in ref. [7], the same authors pointed out a failure of the proposed peeling algorithm. Hence, an efficient algorithm, called the canonical $P-V$ path elimination, was founded by us [1]. In refs. [8,9], He Wenchen and He Wenjie proposed a $P-V$ path network flow method based on the algorithm for maximizing the flow in a network. The method is not a greedy algorithm. Using the method, one needs to approach the maximum flow one by one from the zero flow. However, all the algorithms in refs. [1,4,5] are greedy.

The canonical $P-V$ path elimination given in [1] is based on the following definitions of a canonical $P-V$ path of a benzenoid system H.

DEFINITION 1

Let $P(p_i-v_i)$ be a $P-V$ path on the boundary $C(H)$ of a benzenoid system 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 $S(p_i-v_i, v_j)$ on $C(H)$ starting from p_i, passing through v_i, terminating in v_j, and being as long as possible. Then $P(p_i, v_j)$ is said to be the associated $P-V$ path of $P(p_i-v_i)$ with respect to (simply w.r.t.) p_i, denoted by $P^*(p_i^*-v_i)$, and $S(p_i-v_i, v_j)$ is said to be the related segment of $P(p_i-v_i)$ w.r.t. p_i, denoted by $S^*(p_i^*-v_i)$. Similarly, the associated $P-V$ path and the related segment of $P(p_i-v_i)$ w.r.t. v_i are denoted by $P^*(p_i-v_i^*)$ and $S^*(p_i-v_i^*)$, respectively.

The associated $P-V$ path and the related segment of a $P-V$ path $P(p_i-v_i)$ w.r.t. p_i or v_i, say p_i, can be easily determined in the following way.

If $P(p_i-v_i)$ starts from p_i, and goes in the first step to the right (left), we make the $P-V$ 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 $P(p_i, v_j)$ is the associated $P-V$ path of $P(p_i-v_i)$ w.r.t. p_i, and the segment $S(p_i-v_i, v_j)$ on $C(H)$ is the related segment of $P(p_i-v_i)$ w.r.t. p_i.

DEFINITION 2 [1]

Let $P(p_i-v_i)$ be a $P-V$ on the boundary $C(H)$ of a benzenoid system H. If the related segment $S^*(p_i^*-v_i)$ $(S^*(p_i-v_i^*))$ of $P(p_i-v_i)$ contains only one peak p_i (valley v_i), then $S^*(p_i^*-v_i)$ $(S^*(p_i-v_i^*))$ is said to be a canonical related segment. If a related segment of $P(p_i-v_i)$ is canonical, then $P(p_i-v_i)$ is said to be a canonical $P-V$ path of H.

Recently, we found that the canonical $P-V$ path elimination can be further improved by giving a new definition of a canonical $P-V$ path of a benzenoid system.

DEFINITION 3

Let $P(p_i-v_i)$ be a $P-V$ path on the boundary $C(H)$ of a benzenoid system H. If the associated $P-V$ paths $P^*(p_i^*-v_i)$ and $P^*(p_i-v_i^*)$ have a vertex in common, then $P(p_i-v_i)$ is said to be a canonical $P-V$ path of H.

PROPOSITION 4

A canonical $P-V$ path $P(p_i-v_i)$ of a benzenoid system H under definition 2 must be a canonical $P-V$ path of H under definition 3.

Proof

Since $P(p_i-v_i)$ is canonical under definition 2, one of its related segments, say $S^*(p_i^*-v_i)$, is canonical. Then, since in $S^*(p_i^*-v_i)$ there is no peak other than p_i, the associated $P-V$ path $P^*(p_i-v_i^*)$ must cross over $P^*(p_i^*-v_i)$ or terminate in p_i, so $P^*(p_i^*-v_i)$ and $P^*(p_i-v_i^*)$ must have a common vertex and $P(p_i-v_i)$ is also canonical under definition 3.

However, the contrary of proposition 4 is not true, that is, a canonical $P-V$ path under definition 3 need not be a canonical $P-V$ path under definition 2. Figure 1 shows a benzenoid system H in which $P(p_i-v_i)$ is a $P-V$ path on $C(H)$

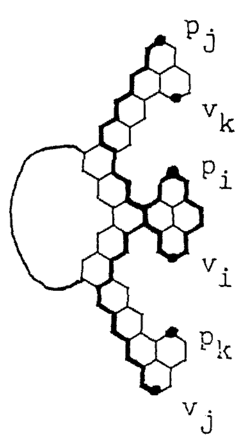

Fig. 1.

whose two associated $P-V$ paths have a common vertex, so it is a canonical $P-V$ path of H under definition 3, but two related segments of $P(p_i-v_i)$ are not both canonical, so $P(p_i-v_i)$ is not a canonical $P-V$ path of H under definition 2.

This means that definition 3 is more universal than definition 2, and the canonical $P-V$ paths under definition 2 are only a particular case of the canonical $P-V$ paths under definition 3. On the other hand, to determine whether or not a $P-V$ path $P(p_i-v_i)$ on $C(H)$ is canonical under definition 3, we need only determine whether two associated $P-V$ paths of $P(p_i-v_i)$ have a common vertex, but need not consider the related segments of $P(p_i-v_i)$. Therefore, the canonical $P-V$ paths on $C(H)$ under definition 3 can be more easily recognized than those under definition 2, and we can give an improved $C-P-V$ path elimination from the definition.

From now on, we call a canonical $P-V$ path (simply $C-P-V$ path) of H implying that it is one under definition 3.

THEOREM 5

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

Proof

By theorem 12 in ref. [1], there exist at least two $C-P-V$ paths on $C(H)$ under definition 2. So, by proposition 4, they are also canonical under definition 3.

THEOREM 6

Let $P(p_i-v_i)$ be a $C-P-V$ path on the boundary $C(H)$ of a benzenoid system H. Then H has Kekulé structures if and only if $H-P(p_i-v_i)$ has Kekulé structures, where $H-P(p_i-v_i)$ is the graph obtained from H by deleting the vertices on $P(p_i-v_i)$.

Proof

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 with the initial edge being a double bond of K. Let $P(p_i,v_j)$ be such a K-alternating $P-V$ path that passes through p_i. Then we have that $v_j=v_i$. Otherwise, $P(p_i,v_j)$ would cross over $P^*(p_i-v_i^*)$ and, since in the region surrounded by $P(p_i-v_i)$, $P(p_i,v_j)$, and $P^*(p_i-v_i^*)$ there is no peak other than p_i, the K-alternating $P-V$ path passing through v_i would also cross over $P(p_i,v_j)$. This contradicts that the $P-V$ path system of H corresponding to K is a collection of independent $P-V$ paths which contain all peaks and valleys of H. Now assume that $P(p_i,v_j)$ $(=P(p_i,v_i))$ and $P(p_i-v_i)$ are distinct. Then $P(p_i,v_j)\Delta P(p_i-v_i)$ (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 $P(p_i-v_i)$ becomes a K^*-alternating path, and $K^*\setminus E(P(p_i-v_i))$ is a Kekulé structure of $H-P(p_i-v_i)$.

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

For a TGB which is not a benzenoid system, we call a maximal benzenoid system in H an end-system if it is incident with only one cut edge of H. The vertex in an end-system incident with a cut edge of H is called the attachable vertex of the end-system. Clearly, H has at least two end-systems.

THEOREM 7

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

(1) If x is a unique peak or valley of H_x, then, for any $P-V$ path $P(p_i-v_i)$ on $C(H_x)$, H has Kekulé structures if and only if $H - P(p_i-v_i)$ has Kekulé structures; otherwise:

(2) H_x contains at least one canonical $P-V$ path $P(p_j-v_j)$ on $C(H_x)$ which does not contain x, and H has Kekulé structures if and only if $H - P(p_j-v_j)$ has Kekulé structures.

Proof

(1) follows from theorem 15(1) in ref. [1].

(2) In this case, x is not a unique peak or valley of H_x. By theorem 15(2) in ref. [1], H_x contains at least one $C-P-V$ path $P(p_j-v_j)$, one of whose canonical related segments does not contain x, and H has Kekulé structures if and only if $H - P(p_j-v_j)$ has Kekulé structures. Clearly, $P(p_j-v_j)$ is contained in each of its related segments, so $P(p_j-v_j)$ also does not contain x.

Now we can give an improved $C-P-V$ path elimination for determining whether or not a given benzenoid system H has Kekulé structures.

We first give a method for finding a $C-P-V$ path of a benzenoid system H, or a $C-P-V$ path of an end-system H_x of a TGB, which does not contain the attachable vertex x of H_x.

PROCEDURE A

Let H (H_x) be a benzenoid system (an end-system of a TGB with the attachable vertex x), and let $P(p_i-v_i)$, $i = 1, 2, \ldots, t$, be $P-V$ paths on $C(H)$ ($C(H_x)$, each of which does not contain x).

(1) Set $P(p_i-v_i) = P(p_1-v_1)$.

(2) Determine $P^*(p_i^*-v_i)$ and $P^*(p_i-v_i^*)$. If $V(P^*(p_i^*-v_i)) \cap V(P^*(p_i-v_i^*)) \neq \emptyset$, then $P(p_i-v_i)$ is a $C-P-V$ path on $C(H)$ ($C(H_x)$), so stop. Otherwise, go to step (3).

(3) Replace $P(p_i-v_i)$ by $P(p_{i+1}-v_{i+1})$ and go to step (2).

$C-P-V$ PATH ELIMINATION

Let H be a benzenoid system with $p(H) = v(H)$ (if $p(H) \neq v(H)$, H has no Kekulé structure).

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 on $C(H_k)$ and delete it. Then colour the edges on the $C-P-V$ path red and blue alternately so that the initial edge is red.

(2) If H_k has a vertex v of valency one, delete it and its adjacent vertex v', and colour the edge vv' red. Repeat the operation until the resultant graph has no vertex of valency one.

(3) If H_k is a TGB, find an end-system H_k^* of H_k. If the attachable vertex x of H_k^* is a unique peak or valley of H_k^*, take a $P-V$ path on $C(H_k^*)$, and delete it; otherwise, by using procedure A, find a $C-P-V$ path on $C(H_k^*)$ which does not contain x, and delete it. Then colour the edges on the deleted $P-V$ 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 form a Kekulé structure of H and all the $P-V$ paths of H, each of which is an alternating path of red and blue edges with the initial edge red, form a perfect $P-V$ path system of H, stop. Otherwise, return to step (1).

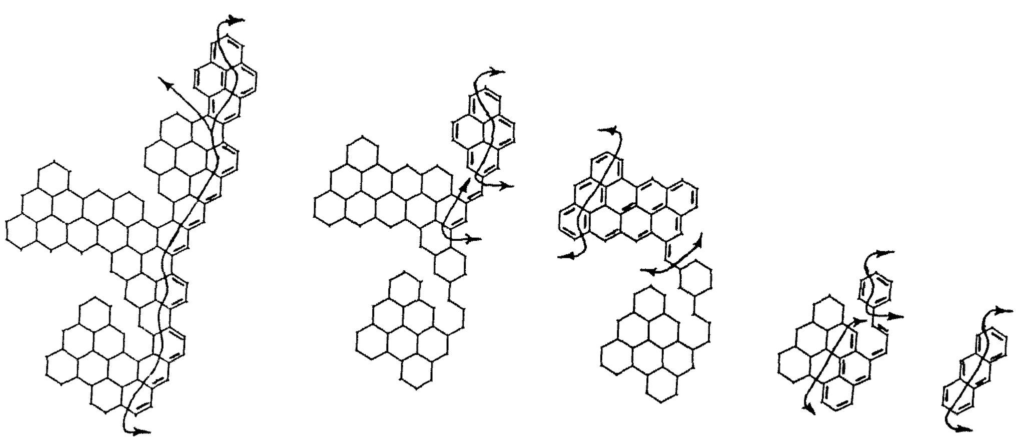

Fig. 2.

An example for finding a Kekulé structure of a Kekuléan benzenoid system by $C-P-V$ elimination is shown in fig. 2.

Remarks

Let H be a TGB, and let H_x be an end-system of H with the attachable vertex x.

(1) If x is a unique peak or valley of H_x and $p(H_x) \neq v(H_x)$, then, after deleting a $P-V$ path on $C(H_x)$ and the vertices of valency one successively, there is an isolated vertex in the resultant graph of H_x, implying that H has no Kekulé structure.

(2) If x is a unique peak or valley of H_x and $p(H_x) = v(H_x) = 1$, then, after deleting a $P-V$ path on $C(H_x)$ and the vertices of valency one successively, there is no vertex of H_x left, implying that H has Kekulé structures if and only if $H - V(H_x)$ has Kekulé structures, and the maximum independent edge set in a $P-V$ path of H_x together with all the vertical edges not in the $P-V$ path form a Kekulé structure of H_x.

(3) If $P(p_i-v_i)$ is a $C-P-V$ path of H_x which does not contain x, then, after deleting $P(p_i-v_i)$ and the vertices of valency one successively, the resultant graph has a smaller number of peaks and valleys than H.

(4) If H is a benzenoid system and $P(p_i-v_i)$ is a $C-P-V$ path of H, then, after deleting $P(p_i-v_i)$ and the vertices of valency one successively, the resultant graph has a smaller number of peaks and valleys than H.

Note that in implementing $C-P-V$ path elimination, the cases in remarks (1) and (2) can be rapidly treated, and for the cases in remarks (3) and (4), we need to eliminate at most $p(H)$ $C-P-V$ paths. Therefore, the $C-P-V$ path elimination is a fairly efficient and rapid algorithm.

References

[1] Guo Xiaofeng and Zhang Fuji, J. Math. Chem. 5(1990)157.

[2] Zhang Fuji and Guo Xiaofeng, MATCH 2(1988)229.

[3] Zhang Fuji, Guo Xiaofeng and Chen Rongsi, in: *Advances in the Theory of Benzenoid Hydrocarbons, Topics in Current Chemistry*, Vol. 153, ed. I. Gutman and S.J. Cyvin (Springer, Berlin–Heidelberg, 1990), pp. 181–193.

[4] H. Sachs, Combinatorica 4(1984)89.

[5] Sheng Tongqin, Chem. Phys. Lett. 142(1987)196.

[6] I. Gutman and S.J. Cyvin, J. Mol. Struct. (THEOCHEM) 138(1986)325.

[7] S.J. Cyvin and I. Gutman, J. Mol. Struct. (THEOCHEM) 164(1988)183.

[8] He Wenjie and He Wenchen, in: *Graph Theory and Topology in Chemistry*, ed. R.B. King and D.H. Rouvray, *Studies in Physical and Theoretical Chemistry*, Vol. 51 (1987), p. 476.

[9] He Wenchen and He Wenjie, *Topics in Current Chemistry*, Vol. 153 (1990), p. 195.