match no. 24 pp. 323-332 1989

THE CONSTRUCTION METHOD OF KEKULÉAN HEXAGONAL SYSTEMS WITH EACH HEXAGON BEING RESONANT

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(Received: May 1988)

ABSTRACT

In this paper we give a recursive method to construct all the Kekuléan hexagonal systems with each hexagon being resonant. This paper can be regarded as a continuation of Gutman's work [2].

It is known that the skeletons of benzenoid hydrocarbon molecules can be represented by Kekuléan hexagonal systems. A hexagonal system is obtained by arranging congruent regular hexagons in the plane so that two hexagons are either disjoint or possess a common edge. A hexagonal system with Kekulé structures is called a Kekuléan hexagonal system. A Kekulé structure is known in graph theory under the name "perfect matching".

As Gutman pointed out in [2], resonance theory is one of the significant topological theories in hexagonal systems. Gutman gave a class of Kekuléan hexagonal system with each hexagon being resonant [1]. In this paper we are devoted to construct all the Kekuléan hexagonal systems with the property that each hexagon is resonant.

If a hexagonal system is drawn so that some of its edges are vertical, then we call a vertex a peak if it lies above all its first neighbours and a valley if all its first neighbours lie above it. We define four graph operations as follows.

Op.1: Let H_i (i=1,2) be a hexagonal system and v_1, v_2 (v_1', v_2') be adjacent vertices with degree two on the boundary of H_1 (H_2). Let edge v_1v_2 be identified with the edge $v_1'v_2'$. If no overlap occurs (except v_1v_2 and $v_1'v_2'$), then we denoted the resultant graph by $H=H_1O_1H_2$ (see Fig. 1).

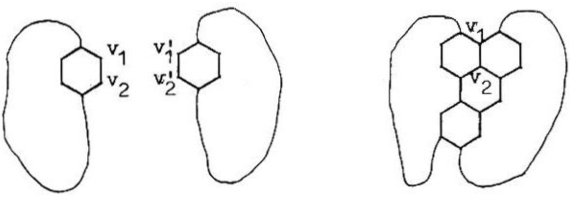

Fig.1

Op.2: Let H be a hexagonal system, v_1, v_2, v_3 and v_4 be successive vertices on the boundary of H such that v_2 and v_3 are of degree three and v_1 and v_4 are of degree two. Let $v_1', v_2', v_3', v_4', v_5'$ and v_6' be six vertices of benzene s Ho_2s is defined to be the graph obtained by identifying v_i with v_i', i=1,2,3,4 (see Fig.2)

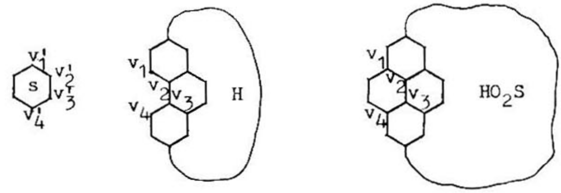

Fig.2

Op.3: Let H_i(i=1,2) be hexagonal systems, $v_1, v_2(v_3, v_4)$ be adjacent vertices of $H_1(H_2)$ and s be a benzene. Identify edge v_1v_2 with $v_1'v_2'$, and edge v_3v_4 with $v_3'v_4'$. If no overlap occurs, then we define the resultant graph as $H=H_1o_3H_2$ (see Fig.3).

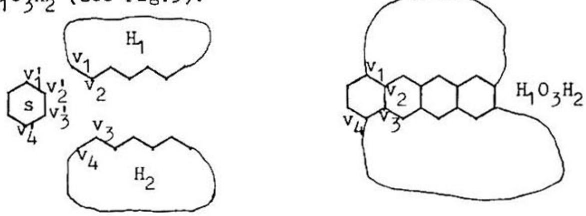

Fig.3

Op.4: Let H_1 be a hexagonal chain (see Fig.4) with the lower boundary $v_0'v_1'...v_{2h}'$. Let H_2 be a hexagonal system with upper boundry $v_1v_2...v_{2h}$. The vertex v' is of degree two and the vertices v_{2h+1} and v_{2h+2} are of degree three and two, respectively. We define graph $H_1o_4H_2$ to be the graph obtained from H_1 and H_2 by identify $v_1v_2...v_{2h+2}$ with $v_1'v_2'...v_{2h+2}'$ if no overlap occurs(see Fig.4).

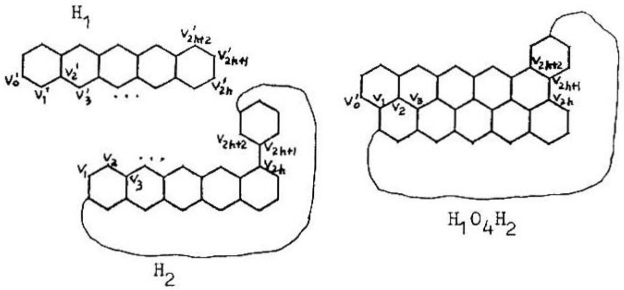

Fig.4

Let M be a Kekulé structure (perfect matching) of hexagonal system H. An M-alternating cycle in H is a cycle whose edges are alternately in M and E-M where E is the set of edges of H.

Lemma 1. [3] Let H be a hexagonal system. Then each hexagon of H is resonant if and only if there exist a Kekulé structure M of H such that the boundary of H is an M-alternating cycle.

Theorem 2. Let H_o be a hexagonal chain, $H_i (i=1,2)$ be hexagonal systems with each hexagon being resonant. S be a benzene. Then $H_1 o_1 H_2$, $H_1 o_2 s$, $H_1 o_3 H_2$ and $H_o o_4 H_1$ are hexagonal systems with each hexagon being resonant.

Proof. By Lemma 1 let $M_1 (M_2)$ be a Kekulé structure of $H_1 (H_2)$ such that the boundary of $H_1 (H_2)$ is an $M_1 (M_2)$-alternating cycle and $v_1 v_2 \notin M_1, (v_1' v_2' \in M_2)$(see Fig.1). Then $M' = M_1 \cup M_2 - \{v_1' v_2'\}$ is a Kekulé structure of $H_1 o_1 H_2$ and the boundary of $H_1 o_1 H_2$ is an M'-alternating cycle. Thus $H_1 o_1 H_2$ is a hexagonal system with each hexagon being resonant(Lemma.1).In a similar way,we can verify that $H_1 o_2 s$ is a hexagonal system with each hexagon being resonant.

Let M_i be a Kekulé structure of $H_i (i=1,2)$ such that the boundary of H_i is an M_i-alternating cycle and $v_1 v_2$ $(v_3 v_4) \notin M_1 (M_2)$. Then $M' = M_1 \cup M_2 \cup \{v_5' v_2'\}$ is a Kekulé structure of $H_1 o_3 H_2$ and the boundary of $H_1 o_3 H_2$ is an M'-alternating cycle of it. Thus $H_1 o_3 H_2$ is a hexagonal system with each hexagon being resonant. Now let M_1 be a Kekulé structure of H_1 such that the boundary of H_1 is an M-alternating cycle and $v_1 v_2 \notin M$. Finally, $M_1 \cup \{v_{2h+3} v_{2h+4} \cdots v_{4h-1} v_{4h} v_{4h+1} v_o\}$ is a Kekulé structure such that the boundary of $H_o o_4 H_1$ is an alternating cycle. Therefore, by Lemma 1 $H_o o_4 H_1$ is a hexagonal system with each hexagon being resonant.

Let m(H) be the number of hexagons of H. We have the following theorem.

Theorem 3. Let H be a hexagonal system with each hexagon being resonant and $m(H) > 1$. Then at least one of the following occurs, where $H_i (i=0,1,2)$ is a hexagonal system with each hexagon being resonant, and $m(H) > m(H_i)$.

(i) $H=H_1 o_1 H_2$

(ii) $H=H_1 o_2 s$

(iii) $H=H_1 o_3 H_2$

(iv) $H=H_0 o_4 H_1$

Proof. For any hexagonal system with $m(H) > 1$ there is at least a pair of adjacent vertices with degree two (2) and at most four successive vertices of degree two. We distinguish three cases.

Case 1. There are four successive vertices of degree two, say v_1, v_2, v_3 and v_4, on the boundary of H. By Lemma 1 there is a Kekulé structure M of H such that the boundary of H is an M-alternating cycle. It is not difficult to see that $H=H_1 o_1 s$ where $H_1=H-\{v_1, v_2, v_3, v_4\}$.

Case 2. There are four successive vertices v_1, v_2, v_3 and v_4 of H such that v_1 and v_2 are of degree two and v_3 and v_4 are of degree three. We consider the following subcases.

Subcase 2.1 $H-\{v_1,v_2\}$ is a hexagonal system. By Lemma 1 H has a Kekulé structure M such that the boundary of H is an M-alternating cycle and $v_1v_2 \in M$. Let $e_1,e_2,\ldots e_t$ be the edges intersected by the horizontal line C and e_t lies on the boundary of H. If $e_i \notin M(i=1,\ldots t)$, then delete all the edges intersected by C. We obtain two hexagonal systems H_1 and H_2 (see Fig.5). It is not difficult to see that $H=H_1o_3H_2$. Otherwise at least one edge of H intersected by the perpendicular bisector of v_1v_2 belongs to M. Then either the boundary of $H-\{v_1,v_2\}$ is an M-alternating cycle or we can find an M-alternating cycle G such that $M'=M\Delta G$ is also a Kekulé structure of H and the boundary of $H_1=H-\{v_1,v_2\}$ is an M'-alternating cycle (see Fig.6). It is not difficult to see that $H=H_1o_2s$.

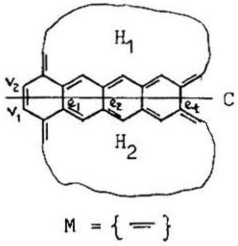

Fig.5

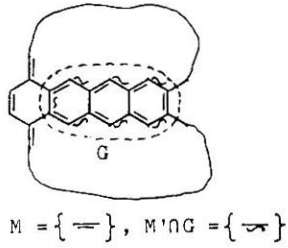

Fig.6

Subcase 2.2 $H-\{v_1,v_2\}$ is not a complete hexagonal system (see Fig. 7). Then by Lemma 1 let M be a Kekulé structure of H such that the boundary of H is an M-alternating cycle and $v_1v_2 \in M$. Then $v_5v_6 \notin M$(otherwise an odd cycle of H would be found which would contradicts to the fact that H is a bipartite graph). It is easy to see that $H=H_1 o_3 H_2$.

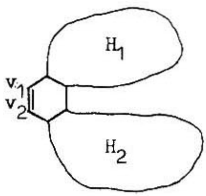

Fig.7

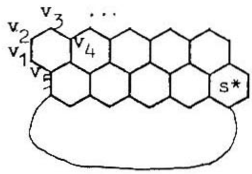

Fig.8

Case 3. There are five successive vertices v_5, v_1, v_2, v_3 and v_4 on the boundary of H, v_1, v_2 and v_3 having degree two, v_4 and v_5 having degree three. It is evident that $H'=H-\{v_1,v_2\}$ is not a complete hexagonal system. We delete the edge incident with an end vertex of degree one successively until it has no vertices with degree one. If the hexagon s* (see Fig.8) is not in H then we can not find a Kekulé structure of H such that the boundary of H is an M-alternating cycle. Therefore, this case can never happen. Thus $s^* \in H$.

For the remainder we need to consider the following (see Fig.9).

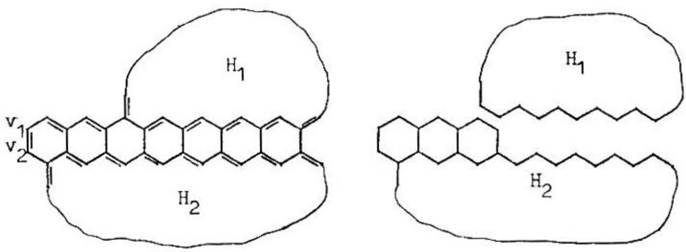

Fig.9

We take a Kekulé structure M of H such that the boundary of H is an M-alternating cycle and $v_1v_2 \in M$. If none of the edges of H intersected by the perpendicular bisector C of v_1v_2 belongs to M, it is easy to see that $H=H_1 o_1 H_2$. Otherwise there is at least one edge of H intersected by the line C belonging to M. Then as in case 2.1, there is an M-alternating cycle G such that $M'=M\Delta G$ is a Kekulé structure of H and the boundary of $H_1=H-\{v_1,v_2,\ldots,v_t\}$ is an M-alternating cycle. It is easy to see that $H=H_0 q H_1$. The theorem is thus proved.

The above theorem illustrates that any Kekuléan hexagonal system with every hexagon resonant can be constructed by four graph operations from smaller ones.
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This work was suported by NNSFC(No.1860559).

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