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DIRECTED TREE STRUCTURE OF THE SET OF KEKULÉ STRUCTURES OF ESSENTIALLY DISCONNECTED BENZENOIDS

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Abstract: The directed tree structure of the set of Kekulé structures of essentially disconnected benzenoids is studied. We define an operation $\otimes$ on directed trees T_1, T_2, ..., and T_n. It is reported that the directed tree of the set of Kekulé structures of an essentially disconnected benzenoid can be obtained by operating on the directed trees of the sets of Kekulé structures of the effective units of the essentially disconnected benzenoid.

In this paper we consider the set of Kekulé structures of an essentially disconnected benzenoid. In order to simplify the discussion, a benzenoid is to be placed on the plane so that two edges of each hexagon are parallel to the vertical line. The sets of three circularly arranged double bonds in a hexagon of a given Kekulé structure (see Fig. 1) are called proper and improper sextets, respectively.

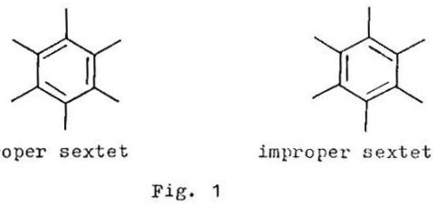

Fig. 1

The sextet rotation R is defined as a simultaneous rotation of all the proper sextets in a given Kekulé structure K into the improper sextets to give another Kekulé structure $K'=R(K)$(see Fig. 2)

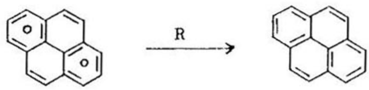

Fig. 2

Let B be a benzenoid and represent every Kekulé structure K of B by a vertex (point) $v=v(K)$; draw an arc from $v(K')$ to $v(K'')$ if and only if $K''=R(K')$. It is known that the resulting graph is a directed rooted tree $T=T(B)$, where the "root" v_o of T (which has outdegree zero) corresponds to the unique Kekulé structure (the root Kekulé structure K_o) of B which does not have any proper sextet [1,2] (cf. Fig. 2).

An essentially disconnected benzenoid is a Kekuléan with some fixed bonds. It consists of two kinds of parts: effective units and junctions [3]. The effective units are normal benzenoids i.e. benzenoids without fixed bonds. In the following we study the relationship between the directed tree of an essentially disconnected benzenoid and the directed trees of its effective units.

Let T_1 and T_2 be two directed trees. V_i and A_i denote the point set and the arc set of the tree T_i $(i=1,2)$, respectively. We say that T is obtained from T_1 and T_2 by an operation $\otimes$ if

$$V(T)=\{(v_1,v_2)\mid v_1\in V \text{ and } v_2\in V_2\}$$

and there is an arc from point (v_1', v_2') to point (v_1'', v_2'') if and only if

(1) there is an arc from v_1' to v_1'' in T_1 and there is an arc from v_2' to v_2'' in T_2; or

(2) $v_1'=v_1''$ is the root of the tree T_1 and there is an arc from v_2' to v_2'' in the tree T_2; or

(3) $v_2' = v_2''$ is the root of the tree T_2 and there is an arc from v_1' to v_1'' in the tree T_1.

An example is shown in Fig. 3.

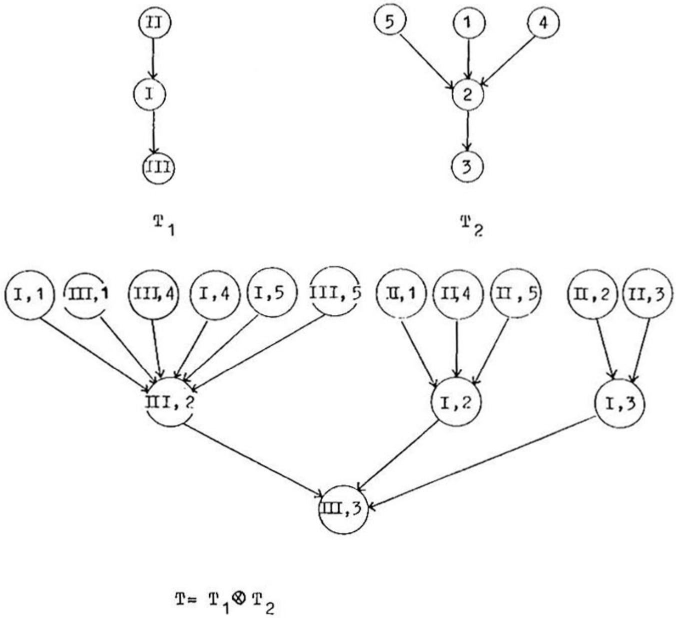

Fig. 3

Let B be an essentially disconnected benzenoid. In the following we use $B_1, B_2, \ldots, B_n$ to denote the effective units of B.

<u>Theorem 1</u> Let B be an essentially disconnected benzenoid with

two effective units B_1 and B_2. Then we have $T(B)=T(B_1)\otimes T(B_2)$.

Proof. Since B is essentially disconnected and B_1 and B_2 are effective units of B, each Kekulé structure K of B corresponds to a pair of Kekulé structures K_1 and K_2, where K_i is a Kekulé structure of B_i for i=1,2. Suppose that v_i corresponds to K_i (i=1,2). It is reasonable to use the pair (v_1,v_2) to denote the point of T(B) corresponding to the Kekulé structure K of B. This means that the point set of T(B) is as follows:

$$V(T) = \{ (v_1,v_2) \mid v_1 \in V(T_1) \text{ and } v_2 \in V(T_2)\}$$

Assume that (v_1',v_2') and (v_1'',v_2'') are two points of T(B), where $v_i'(v_i'')$ corresponds to the Kekulé structure K_i' (K_i'') of B_i (i= 1,2). It is not difficult to see that there is an arc in T(B) from (v_1',v_2') to (v_1'',v_2'') if and only if

(1) $R(K_1') = K_1''$ and $R(K_2') = K_2''$; or

(2) $K_1' = K_1''$ is the root Kekulé structure of B_1, and $R(K_2') = K_2''$; or

(3) $K_2' = K_2''$ is the root Kekulé structure of B_2, and $R(K_1') = K_1''$.

These statements are equivalent to the following:

(1) There is an arc from v_1' to v_1'' in $T(B_1)$ and there is an arc from v_2' to v_2'' in $T(B_2)$; or

(2) $v_1' = v_1''$ is the root of $T(B_1)$, and there is an arc from v_2' to v_2'' in $T(B_2)$; or

(3) $v_2' = v_2''$ is the root of $T(B_2)$, and there is an arc from v_1' to v_1'' in $T(B_1)$.

Therefore, by the definition of $T(B_1)\otimes T(B_2)$, we have

$$T(B) = T(B_1)\otimes T(B_2) .$$

The proof is thus completed.

In the following we give an example. The two effective units B_1 and B_2 are shown in Fig. 4. We assign to each Kekulé structure a number for B_1 and B_2, and a pair of numbers for B, as shown in Fig. 4. It is easy to see that $T(B_1)$, $T(B_2)$ and $T(B)$ are just T_1, T_2 and T in Fig. 3, respectively.

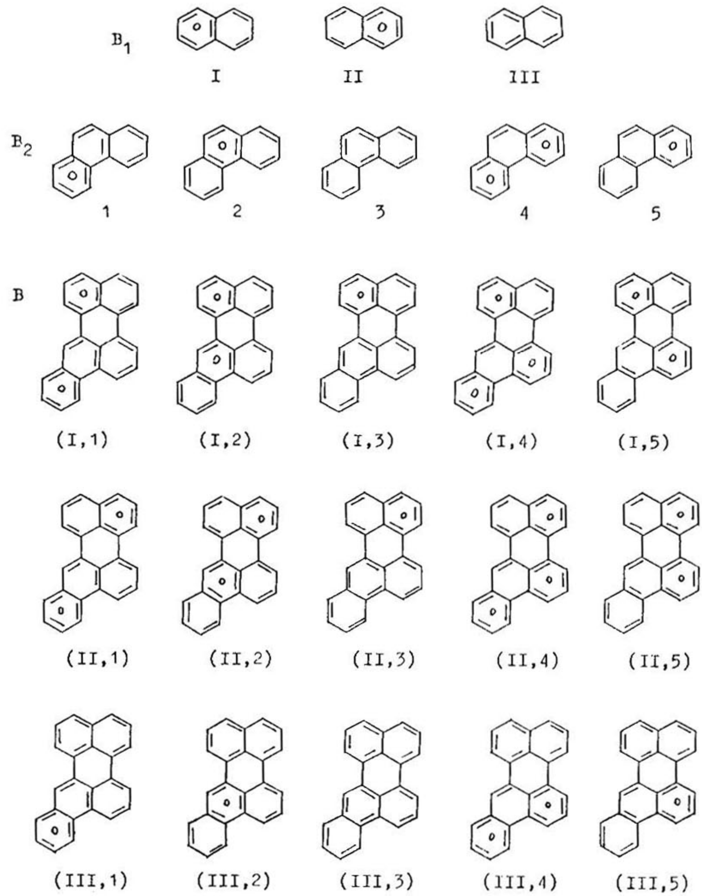

Fig. 4

In general, an essentially disconnected benzenoid may have more than two effective units. Therefore, we define an operation on directed rooted trees T_1, T_2, ..., T_n ($n \geq 2$). $T(V,A)$ is said to be obtained from $T_1(V_1,A_1)$, $T_2(V_2,A_2)$, ..., $T_n(V_n,A_n)$ by operation $\otimes$ if

$$V = \{(v_1,v_2,\ldots,v_n) \mid v_i \in V_i,\ i=1,2,\ldots,n\}$$

and there is an arc from point $(v_1',v_2',\ldots,v_n')$ to point $(v_1'',v_2'',\ldots,v_n'')$ if and only if the set $\{1,2,\ldots,n\}$ decomposes into disjoint sets I, J (i.e., $I \cup J = \{1,2,\ldots,n\}$, $I \cap J = \emptyset$) where $I \neq \emptyset$ such that for each $i \in I$, there is an arc from v_i' to v_i'' in T_i, and for each $j \in J$, $v_j' = v_j''$ is the root of T_j. With the above operation $\otimes$, we have the following theorem generalizing Theorem 1.

<u>Theorem 2</u> Let B be an essentially disconnected benzenoid with effective unites B_1, B_2, ..., B_n. Then we have

$$T(B)=T(B_1)\otimes T(B_2)\otimes \cdots \otimes T(B_n).$$

<u>Proof.</u> Since B is an essentially disconnected benzenoid with effective units B_1, B_2, ..., B_n, each Kekulé structure K of B corresponds to a set of Kekulé structures K_1, K_2, ..., K_n, where K_i is a Kekulé structure of B_i for $i=1,2,\ldots,n$. Hence we denote the Kekulé structure of B by $K=(K_1, K_2, \ldots, K_n)$. Let $T(B_i)=T_i(V_i,A_i)$ be the directed tree corresponding to B_i for $i=1,2,\ldots,n$. Assume that K_i corresponds to $v_i \in V_i$ ($i=1,2,\ldots,n$). It is resonable to denote the point of $T(B)$ corresponding to Kekulé structure $K=(K_1, K_2,\ldots, K_n)$ by $(v_1, v_2, \ldots, v_n)$. By the definition of $T(B)$ there is an arc in $T(B)$ from point $(v_1', v_2', \ldots, v_n')$ to point $(v_1'', v_2'', \ldots, v_n'')$ if and only if $(K_1'', K_2'', \ldots, K_n'') = R(K_1', K_2', \ldots, K_n')$. The above equation implies that $K_i'' = R(K_i')$ for $i=1,2,\ldots, n$. It is not difficult to see that $K_i'' = R(K_i') = K_i'$ if and only if K_i' is the root Kekulé structure of B_i, or equally, $v_i' = v_j''$ is the root of $T(B_i)$. Similarly, $K_i'' = R(K_i') \neq K_i'$ if and only if there is an arc from v_j' to v_i'' in $T(B_i)$. Let I denote the set of such i's

satisfying $K''_i = R(K'_i) \neq K'_i$, and J the set of such j's satisfying $K''_j = R(K'_j) = K'_j$. Evidently, $I \neq \emptyset$, $I \cap J = \emptyset$ and $I \cup J = \{1,2,\ldots,n\}$. Then for each $i \in I$ there is an arc from v'_i to v''_i in $T(B_i)$, and for each $j \in J$, $v'_j = v''_j$ is the root of $T(B_j)$. Now by the definition of operation $\otimes$, we have

$$T(B) = T(B_1) \otimes T(B_2) \otimes \ldots \otimes T(B_n).$$

Now we give an example. Let B be the benzenoid depicted in Fig. 5. It is an essentially disconnected benzenoid with three isomorphic effective units B_1, B_2 and B_3. It is easy to get the directed rooted tree $T(B_i)$ $(i=1,2,3)$. By Theorem 2 T(B) is just $T(B_1) \otimes T(B_2) \otimes T(B_3)$ (Fig. 5).

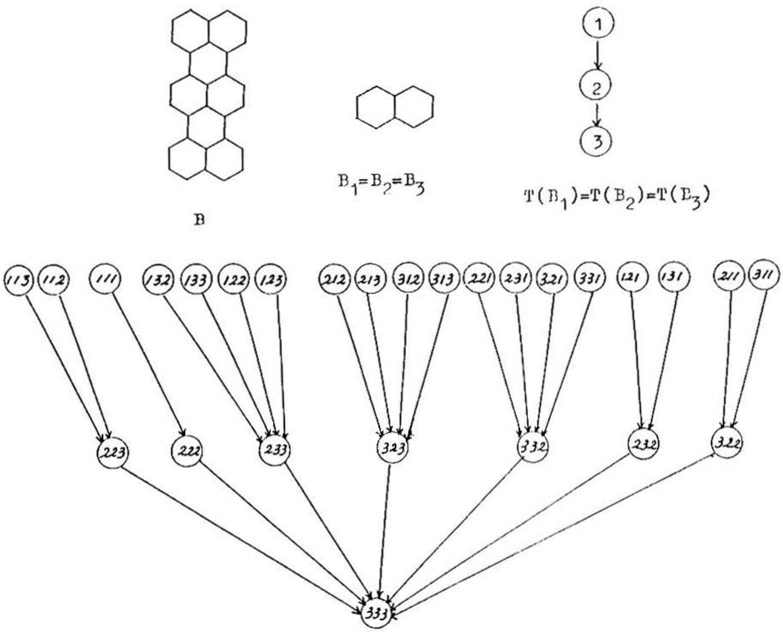

Fig. 5 $T(B)=T(B_1) \otimes T(B_2) \otimes T(B_3)$

We denote the length of a longest directed path in a directed tree T by L(T). Note that L(T(B)) is the maximum number of successive rotations needed to reach the root Kekulé structure of B. The following theorem describes the relationship between L(T(B)) and the $L(T(B_i))$.

Theorem 3 Let B be an essentially disconnected benzenoid with effective units $B_1, B_2, \ldots, B_n$. Then we have

$$L(T(B)) = \max_{i=1,2,\ldots,n} \{ L(T(B_i)) \}$$

The proof is left to the reader.

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