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SOME TOPOLOGICAL PROPERTIES OF TWO TYPES OF S,T-ISOMERS

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ABSTRACT

Two types of S,T-isomers are considered. All of these which are called S_3, T_3, S_4, T_4-isomers are benzenoid systems formed from two identical subunits A and A'. It is proved that if the number of vertices of A is odd then the number of Kekulé structures of the $S_3(S_4)$-isomer is equal to zero. Furthermore, the $S_3(S_4)$-isomer does not have more aromatic π sextets than its corresponding $T_3(T_4)$-isomer. Analogous results for Kekulé structures are also obtained.

The concept of S,T-isomers was introduced in [1]. In [2], [3] and [4] some interesting topological properties of certain types of S,T-isomers were obtained. In this paper, two types of S,T-isomers are considered. Both of them are benzenoid systems. It is well known that any benzenoid system B is bipartite and its vertices can be colored by two colors, so that the vertices of the same color are never adjacent. Recall that a Clar formula is obtained by drawing circles in some of the hexagons of B. These circles represent the so called 'aromatic sextets'. The rules for constructing Clar formulas are the following:

(a) It is not allowed to draw circles in adjacent hexagons;

(b) Circles can be drawn in hexagons if the rest of the conjugated system has at least one Kekulé structure;

(c) A Clar formula contains the maximum number of circles, which can be drawn in accordance with the rules (a) and (b).

If only the rules (a) and (b) are obeyed, we have generalized Clar formulas. [5].

In [6], the three different models of topological related isomers S and T were given. Among those models, the model 2 is formed from three subunits: two terminal ones, A and B, and a central one, C. The terminal moieties are linked to the central one by l edges each, l = 2, 3, 4. The model 2(l = 4) is shown in Fig.1.

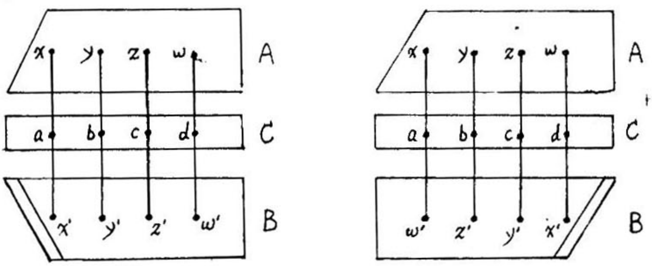


Fig.1.

Now we give the definition of the S_3,T_3 and the S_4,T_4-isomers. We restrict ourselves to the cases of benzenoid system.

Suppose that the two terminal subunits arising in the model 2(l = 4) are isomorphic, i.e.: A = B. For convenience, we shall always use the symbol A' instead of B. Let C be a central subunit consisting of four vertices a, b, c, d. Let x, y, z, w be four vertices of A and x', y', z', w' four vertices of A' corresponding to the x, y, z, w seperately. Conjugated system $S_3(T_3)$ is obtained from the S(T) by joining b to c. (See Fig.2.) These two conjugated systems are called S_3, T_3-isomers.

Furthermore, $S_4(T_4)$ isomer is obtained from the $S_3(T_3)$ by removing edge bc and joining a, c to b, d respectively. (See Fig.3.)

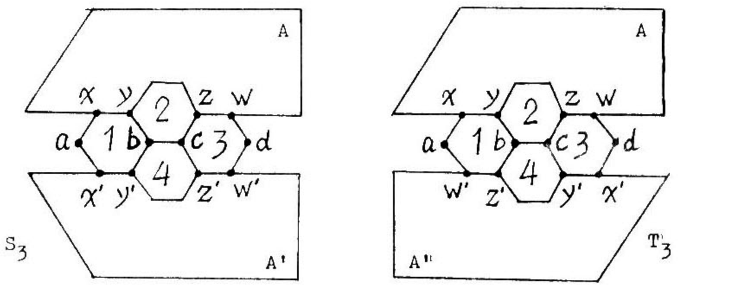


Fig.2.

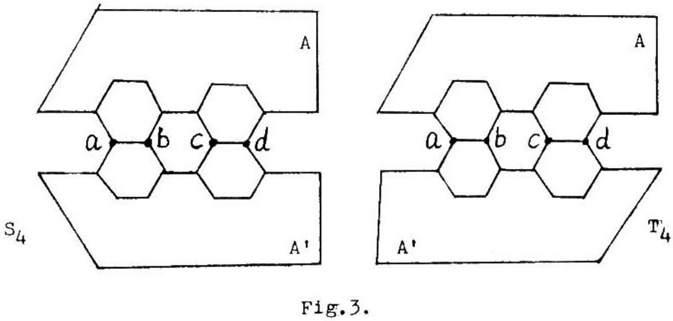


Fig.3.

It is not difficult to see that for the S,T-isomers of the model 2(l = 4) having two identical terminal subunits, if we restrict ourselves to the cases of benzenoid system, then only the S_3,T_3 and the S_4,T_4-isomers are possible.

For convenience, the hexagons of the $S_3(T_3)$ intersecting the vertices a, b, c, d are labelled by 1, 2, 3, 4.(See Fig.2) The subgraph of $S_3(T_3)$ consisting of these four hexagons will be denoted by H. Denote the number of Kekulé structures of S_3 (T_3) by $K(S_3)(K(T_3))$ and the number of aromatic π sextets(in a Clar formula) of $S_3(T_3)$ by $\sigma(S_3)(\sigma(T_3))$, respectively. Let P denote the set $\{a,b,c,d\}$ and $n(A)$ the number of vertices of A. The terminology not defined here is taken from [7]. Vertices removed from a graph will be denoted by an upper index; i.g.: the graph $A - \{x,y\}$ will be denoted by A^{xy}. If m is a matching of H that saturates the vertices of P, then the number of Kekulé structures of $S_3(T_3)$ in which the vertices of P are saturated by way of m will be denoted by $K_m(S_3)(K_m(T_3))$. Clearly, $K(S_3) = \sum K_m(S_3)$, $K(T_3) = \sum K_m(T_3)$, where the summation is over those matchings m which saturate the vertices of P.

<u>Theorem 1.</u> For any pair of S_3,T_3-isomers ,if $n(A)$ is even then

$$K(S_3) \leqslant K(T_3). \qquad (1)$$

<u>Proof.</u> If $n(A)$ is even, then the number of matchings of H which saturate the vertices of P is ten; we denote them by m_i(i = 1, 2,...,10) as shown in Fig.4. For convenience, we only draw the subgraph H of $S_3(T_3)$.

Clearly, $K_{m_1}(S_3) = K(A^{xw})\ K(A') = K(A^{xw})\cdot K(A) = K_{m_1}(T_3)$.

After some simple calculation, we have $K_{m_i}(S_3) = K_{m_i}(T_3)$,

$i = 1,\ 2,\ 3,\ 4,\ 5,\ 6.$

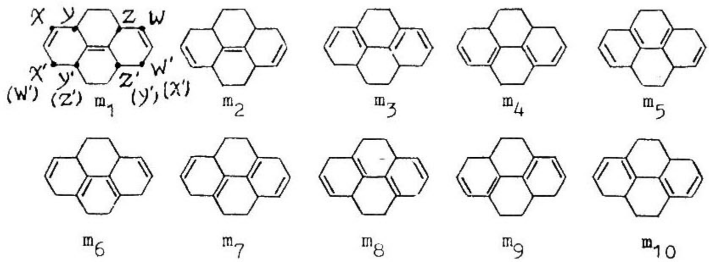


Fig.4.

A glance at Fig.2 and Fig.4 shows that

$$K_{m_7}(S_3) = K(A^{xz})\cdot K(A'^{y'w'}) = K(A^{xz})\cdot K(A^{yw});$$

$$K_{m_8}(S_3) = K(A^{yw})\cdot K(A'^{x'z'}) = K(A^{xz})\cdot K(A^{yw});$$

$$K_{m_9}(S_3) = K(A^{zw})\cdot K(A'^{x'y'}) = K(A^{zw})\cdot K(A^{xy});$$

$$K_{m_{10}}(S_3) = K(A^{xy})\cdot K(A'^{z'w'}) = K(A^{zw})\cdot K(A^{xy});$$

$$K_{m_7}(T_3) = K(A^{xz})\cdot K(A'^{x'z'}) = \left[K(A^{xz})\right]^2;$$

$$K_{m_8}(T_3) = K(A^{yw})\cdot K(A'^{y'w'}) = \left[K(A^{yw})\right]^2;$$

$$K_{m_9}(T_3) = K(A^{zw})\cdot K(A'^{z'w'}) = \left[K(A^{zw})\right]^2;$$

$$K_{m_{10}}(T_3) = K(A^{xy})\cdot K(A'^{x'y'}) = \left[K(A^{xy})\right]^2.$$

Therefore,

$$K(S_3) = \sum_{i=1}^{10} K_{m_i}(S_3) = \sum_{i=1}^{6} K_{m_i}(S_3) + 2K(A^{xz})\cdot K(A^{yw})$$
$$+ 2K(A^{zw})\cdot K(A^{xy});$$

$$K(T_3) = \sum_{i=1}^{10} K_{m_i}(T_3) = \sum_{i=1}^{6} K_{m_i}(S_3) + \left[K(A^{xz})\right]^2 +$$
$$+ \left[K(A^{yw})\right]^2 + \left[K(A^{zw})\right]^2 + \left[K(A^{xy})\right]^2.$$

From the expression of $K(S_3)$ and $K(T_3)$, it is easy to see that the inequality (1) holds.

Now we discuss the number of Clar formulas of S_3,T_3-isomers. Let $\sigma(A^{xy})$ be the maximum number of circles which can be drawn in A^{xy} with the rules (a) and (b). (Note that the A^{xy} need not be a benzenoid system.) Let m_i be a matching of H (see Fig. 4.), then the maximum number of circles which can be drawn in $S_3 - P(T_3 - P)$ with the rules (a) and (b) will be denoted by $\sigma_{m_i}(S_3)(\sigma_{m_i}(T_3))$ when the vertices of P are saturated by way of m_i.

Theorem 2. For any pair of S_3,T_3-isomers, if n(A) is even then

$$\sigma(S_3) \leqslant \sigma(T_3). \qquad (2)$$

Proof. The following three cases need to be considered.

Case 1. There exists a Clar formula of S_3 which has no sextets in H. Obviously, in this case, $\sigma(S_3) = \max_i \sigma_{m_i}(S_3)$. If $\sigma(S_3) = \sigma_{m_1}(S_3)$, namely $\sigma(S_3) = \sigma(A^{xw}) + \sigma(A)$, then, since $\sigma_{m_1}(T_3) = \sigma(A^{xw}) + \sigma(A) = \sigma_{m_1}(S_3)$, we have $\sigma(T_3) \geqslant \sigma_{m_1}(T_3) = \sigma_{m_1}(S_3) = \sigma(S_3)$. The inequality (2) holds.

It is easy to check that $\sigma_{m_i}(S_3) = \sigma_{m_i}(T_3)$, i = 1, 2, 3, 4, 5, 6, therefore, if $\sigma(S_3) = \sigma_{m_i}(S_3)$, i = 1, 2, 3, 4, 5, 6, then $\sigma(S_3) \leqslant \sigma(T_3)$.

Suppose that $\sigma(S_3) = \sigma_{m_7}(S_3)$, namely, $\sigma(S_3) = \sigma(A^{xz}) + \sigma(A^{yw})$. If $\sigma(A^{xz}) \geqslant \sigma(A^{yw})$ then $\sigma(T_3) \geqslant \sigma_{m_7}(T_3) = \sigma(A^{xz}) +$

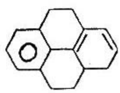
$+ \sigma(A'^{x'z'}) = 2\sigma(A^{xz}) \geqslant \sigma(A^{xz}) + \sigma(A^{yw}) = \sigma(S_3)$; if $\sigma(A^{xz}) <$ $< \sigma(A^{yw})$ then $\sigma(T_3) \geqslant \sigma_{m_8}(T_3) = \sigma(A^{yw}) + \sigma(A''^{y'w'}) = 2\sigma(A^{yw}) \geqslant$ $\geqslant \sigma(A^{yw}) + \sigma(A^{xz}) = \sigma(S_3)$. Thus, when $\sigma(S_3) = \sigma_{m_7}(S_3)$, the inequality (2) holds.

If $\sigma(S_3) = \sigma_{m_j}(S_3)$, $j = 8, 9, 10$, then in the same way as for the case $\sigma(S_3) = \sigma_{m_7}(S_3)$, one can get the inequality (2).

Case 2. There is a Clar formula of S_3 which has only one sextet in H. We consider four subcases as follows:

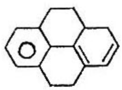
1) The sextet is in hexagon 1. There are two ways to saturate the rest vertices of P, as shown in the following graphs:

(i)



From Fig.2, we have $\sigma(S_3) = \sigma(A^{xyzw}) + \sigma(A^{xy}) + 1$. Obviously, T_3 has a Clar formula in which the number of sextets is $\sigma(A^{xyzw}) + \sigma(A^{xy}) + 1$, thus, $\sigma(S_3) \lesssim \sigma(T_3)$.

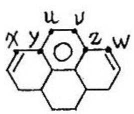
(ii)



In this case, one can get the result in the same way as shown in (i).

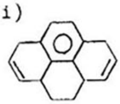
2) The sextet is in hexagon 2. It has two ways to saturate the rest vertices of P, as drawn in the following graphs:

(i)



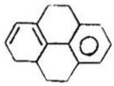
We have $\sigma(S_3) = \sigma(A^{xyzwuv}) + \sigma(A) + 1$. From Fig.2, it is clear that there is a Clar formula of T_3 in which the number of sextets is $\sigma(A^{xyzwuv}) + \sigma(A) + 1$, thus, the inequality (2) holds.

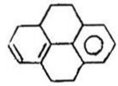
(ii)



In the same way as the proof of (i), one can get the inequality (2).

3) The sextet is in hexagon 3. It has two ways to saturate the rest vertices of P as follows:

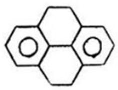




In a fully analogous manner as for subcase 1), one can get the result (2).

4) The sextet is in hexagon 4. This subcase is fully equivalent to subcase 2).

Case 3. There is a Clar formulas which has two sextets in



H. In this case, it is clear that $\sigma(S_3) = \sigma(T_3) = 2\sigma(A^{xyzw}) + 2$. Hence, the inequality (2) holds.

The proof is thus completed.

Now we discuss the case when $n(A)$ is odd. Let S_3 be given, $n(A)$ is odd. Suppose that we put S_3 in such a position that the edge xy is horizontal. Following [8], we call the 2-degree vertices those of the form $\cdot\!<$ ($>\!\cdot$) the peaks(valleys) of S_3 and denote the number of peaks(valleys) of S_3 by $P(S_3)(V(S_3))$.

<u>Theorem 3.</u> For any S_3-isomer, if $n(A)$ is odd then $K(S_3) = 0$.

<u>Proof.</u> Denote the number of peaks and valleys of a benzenoid system B by $P(B)$ and $V(B)$, respectively. For any two-coloring of B, $P(B) - V(B)$ is equal to the difference of the number of

differently colored vertices. Hence, if $n(A)$ is odd, then $P(A) - V(A) = 2k+1$, where k is an integer. Bearing in mind the construction of S_3, it follows that $P(S_3) - V(S_3) = 4k+2$. Consequently, $P(S_3) \neq V(S_3)$, which immediately implies(see [8]) the nonexistence of Kekulé structures of S_3.

The proof is completed.

Remark: when $n(A)$ is odd, $K(T_3) > 0$ may hold, see Fig.5.

S_3 T_3

Fig.5

Summarizing the above theorems, we have

Theorem 4. For any pair of S_3,T_3-isomers, $\sigma(S_3) \leqslant \sigma(T_3)$, $K(S_3) \leqslant K(T_3)$.

Lastly, we give the following

Theorem 5. For any pair of S_4,T_4-isomers, we have the following results:

1) $\sigma(S_4) \leqslant \sigma(T_4)$, $K(S_4) \leqslant K(T_4)$;

2) if $n(A)$ is odd, then $K(S_4) = 0$.

The proof is analogous to those of the theorems 1-4.

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