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

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Abstract

Two types of radical S,T-isomers are introduced. They are developed from the structure of perinaphenyl radical which was recently found in various flint samples. Some of their topological properties are established.

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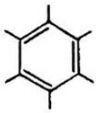
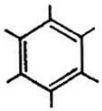
A variety of research [2,3,5-10] has been devoted to the study of topological properties of benzenoid S,T-isomers and their generalizations since the concept of S,T-isomers was introduced in 1982[8]. In the present paper, we shall consider two types of new isomers, called radical S_1,T_1-isomers and radical S_2,T_2-isomers. These isomers are developed from the structure(Fig. 1) of perinaphenyl radical which was recently found in various flint samples(see[1]).

Fig. 1 The structure of perinaphenyl radical

The symbolism and terminology used in the present work is the same as in [8] and the review [4]. Note that a Kekulé pattern is a chemical notion which coincides with what is known in graph theory under the name "perfect matching". The number of Kekulé patterns of a graph G is denoted as K(G). In order to simplify the discussion, we always place a benzenoid graph G on a plane so that two edges of each hexagon are parallel to the vertical line. Then $\sigma(G)$, the number of aromatic π-sextets (in a Clar formula) of G, is equal to the maximum integer σ for which σ proper sextets(see Fig.2) are contained in a Kekulé pattern of G.



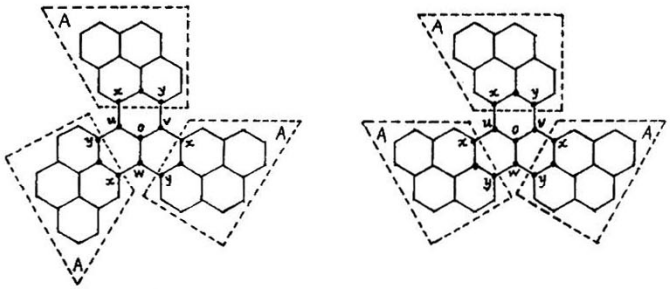
proper sextet



improper sextet

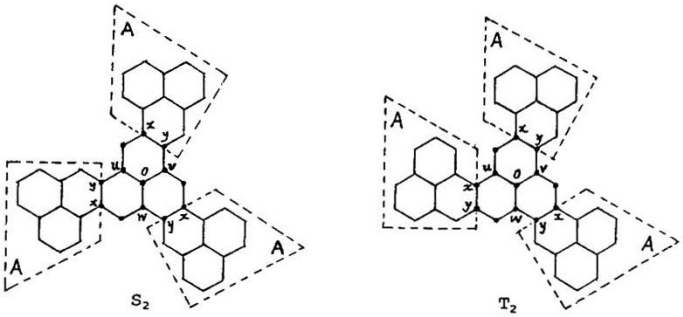
Fig. 2

The radical S_1,T_1-isomers and radical S_2,T_2-isomers are obtained by attaching three isomorphic fragments(planar graphs) to the perinaphenyl radical in distinct ways. Their structures are depicted in Fig. 3 and Fig. 4. For convenience, sometimes we may simply call them as S_1,T_1-isomers and S_2,T_2-isomers . When the attached fragments are benzenoid, these isomers are called benzenoid radical S_i,T_i-isomers (i=1,2). The S_i,T_i-isomers with non-benzenoid fragments are called non-benzenoid radical S_i,T_i-isomers.



S_1 T_1

Fig. 3 The radical S_1,T_1-isomers



S_2 T_2

Fig. 4 The radical S_2,T_2-isomers

It is evident that S_1 and S_2 have rotational symmetry which T_1 and T_2 do not have (unless in the trivial cases $T_1=S_1$ and $T_2=S_2$).

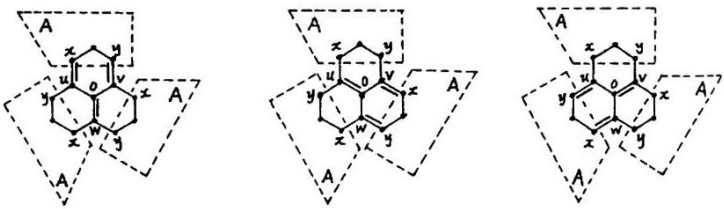
As in [9], we let A^x denote the subgraph obtained from A by deleting its vertex x, and $A^{x,y}$ denote the subgraph obtained from A by deleting its vertices x and y; etc.

For notational simplicity, we also use A, A^x and $A^{x,y}$, etc., to denote the numbers of Kekulé patterns of the corresponding graphs A, A^x and $A^{x,y}$, etc.,in case no confusion will occur.

<u>Theorem 1.</u> For any pair of radical S_1,T_1-isomers, $K(S_1) = K(T_1) = 3(A^{x,y})(A)^2$.

<u>Proof.</u> It is trivial if $|V(A)|$ is odd since both S_1 and T_1 also have an odd number of vertices so that no perfect matchings exist. So we may assume that $|V(A)|$ is even.

According to the situation of the vertices o,u,v and w in a perfect matching of S_1, we may divide the KeKulé patterns of S_1 into the following three cases(note that in Fig.5, u and v must both match vertices of the top fragment A or both match no vertices of this fragment. There are similar claims for v and w, and for w and u.):



Case 1 Case 2 Case 3

Fig. 5 Three cases of Kekulé patterns of S_1

Let K_1, K_2 and K_3 denote the numbers of Kekulé patterns in the three cases, respectively. Then it is easily seen that

$$K_1=K_2=K_3=(A^{x,y})(A)(A).$$

So, $K(S_1)=K_1+K_2+K_3=3(A^{x,y})(A)^2$.

Note that T_1 is obtained from S_1 by turning over one of the three fragments so that the vertices x and y in that fragment interchange their attachment to the radical part. Then we also have $K(T_1)=K(S_1)=3(A^{x,y})(A)^2$.

It completes the proof of Theorem 1.

<u>Corollary 1.</u> For any pair of benzenoid radical S_1,T_1-isomers, $K(S_1) = K(T_1) = \sigma(S_1) = \sigma(T_1) = 0$.

<u>Proof.</u> It is well known that any benzenoid graph is 2-colorable. In any 2-coloring of the S_1(or T_1)-isomer, the vertices x and y in a fragment A must have same color. So, either A or $A^{x,y}$ must have different number of vertices in distinct colors. Thus, A and $A^{x,y}$ can not both have Kekulé patterns. Corollary 1 then immediately follows from Theorem 1.

It should be pointed out that for non-benzenoid radical S_1,T_1-isomers we may have $K(S_1) = K(T_1) > 0$, which can be seen from the two examples as shown in Fig. 6.

A_1 A_2

Fig.6 Examples(A_1 and A_2) of fragment A in S_1,T_1-isomers with $A_i > 0$ and $(A_i)^{x,y} > 0$ (i=1,2).

Now we come to consider the radical S_2,T_2-isomers. The results are quite different from the radical S_1,T_1-isomers.

It is clear that we only need to consider S_2,T_2-isomers with an even number of vertices, i.e., $|V(A)|$ is odd. (Otherwise, we have $K(S_2)=K(T_2)=\sigma(S_2)=\sigma(T_2)=0$ since no perfect matchings exist.)

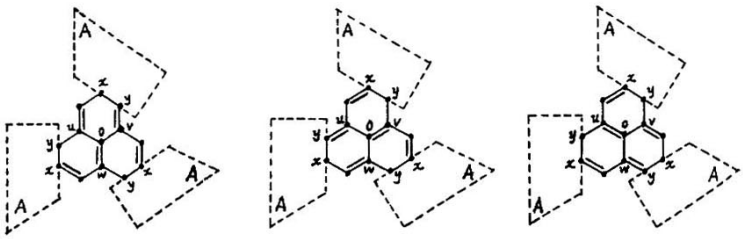
<u>Theorem 2.</u> For any pair of radical S_2,T_2-isomers with $|V(A)|$ odd,

$K(S_2) > K(T_2)$ if and only if $A^J < A^X < 2A^J$;

$K(S_2) < K(T_2)$ if and only if $0 < A^X < A^J$ or $A^X > 2A^J$;

$K(S_2) = K(T_2)$ if and only if $A^X = A^J$, $2A^J$ or 0.

<u>Proof.</u> According to the situation of the vertices o,u,v and w in a perfect matching of S_2, we may divide the KeKulé patterns of S_2 into the three cases described in Fig. 7 (note that since $|V(A)|$ is odd, exactly one of x and y in each fragment A must match a vertex not belonging to A.):



Case 1 Case 2 Case 3

Fig. 7 Three cases of Kekulé patterns of S_2

Let K_1, K_2 and K_3 denote the numbers of Kekulé patterns in

the three cases, respectively. Then it is easily seen that

$K_1=K_2=K_3=(A^X)^2(A^Y)$.

So, $K(S_2)=K_1+K_2+K_3=3(A^X)^2(A^Y)$ .....(1)

Note that T_1 is obtained from S_1 by turning over one of the three fragments so that the vertices x and y in that fragment interchange their attachment to the radical part. Then we have

$K(T_2)=(A^X)^3+2(A^X)(A^Y)^2$ .....(2)

So, $K(S_2)-K(T_2)=3(A^X)^2(A^Y)-[(A^X)^3+2(A^X)(A^Y)^2]$

$= (A^X)[\ 3(A^X)(A^Y)-(A^X)^2-2(A^Y)^2\ ]$

$= (A^X)(A^X-A^Y)(2A^Y-A^X)$.

Then, the conclusions of Theorem 2 follow immediately.

<u>Corollary 2.</u> For any pair of benzenoid radical S_2,T_2-isomers , $K(S_2)=\sigma(S_2)=0$, $K(T_2)=(A^X)^3$ and $\sigma(T_2)=3\sigma(A^X)$.

<u>Proof.</u> It is trivial when $|V(A)|$is even since no Kekulé patterns exist in A^X, S_2 and T_2. So we may assume $|V(A)|$is odd. From (1) and (2) in the proof of Theorem 2, we have $K(S_2)=3(A^X)^2(A^Y)$ and $K(T_2)=(A^X)^3+2(A^X)(A^Y)^2$.

Note that in any 2-coloring of the S_2(or T_2)-isomer, the vertices x and y of a fragment A must have distinct colors. So, either A^X or A^Y must have different number of vertices in distinct colors. Thus, A^X and A^Y can not both have KeKulé patterns. Therefore, we have $K(S_2)=\sigma(S_2)=0$ and $K(T_2)=(A^X)^3$.

To prove $\sigma(T_2)=3\sigma(A^X)$, we only need to consider the case $A^X > 0$(and so $A^Y = 0$). Then the equality is easily seen by considering the three cases given in the proof of Theorem 2 (refer to Fig. 7 and Fig.4).

From Corollary 2, we see that for any pair of benzenoid radical S_2,T_2-isomers, $K(S_2) \le K(T_2)$ and $\sigma(S_2) \le \sigma(T_2)$. However, for non-benzenoid radical S_2,T_2-isomers, all the three cases

indicated in Theorem 2 do exist, which can be seen from the following examples given in Fig.8.

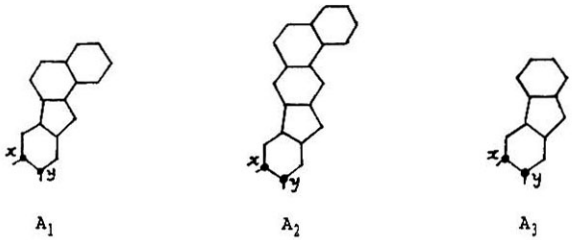


Fig. 8 Examples of fragment A for the three cases in Theorem 2.

It is easy to see that $(A_1)^X = 3$, $(A_1)^Y = 2$, $(A_2)^X = 5$, $(A_2)^Y = 2$, $(A_3)^X = 2$, and $(A_3)^Y = 1$ so that $(A_1)^Y < (A_1)^X < 2(A_1)^Y$, $(A_2)^X > 2(A_2)^Y$ and $(A_3)^X = 2(A_3)^Y$.

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