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THE CLAR COVERING POLYNOMIALS OF S,T–ISOMERS

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ABSTRACT

The difference of the Clar covering polynomials for a type of S,T–isomers of benzenoid hydrocarbons is obtained. From this difference polynomial the previous results on topological properties of the S,T–isomers can be deduced directly. It is also used to deduce new results. Analogous conclusions about some other types of S,T–isomers are also derived.

1. INTRODUCTION

The concept of S,T–isomers was introduced in [1]. Henceforth a variety of types of S,T–isomers of benzenoid systems were introduced and their topological properties extensively studied [2–5]. In [6] the author of the present paper and Prof. Zhang Fuji gave the concept of Clar covering polynomials of benzenoid systems and obtained many of its important properties. It is easily seen that the Clar covering polynomial of a benzenoid system is a special type of circuit polynomials [7] with appropriately chosen weights. In this paper we mainly obtain the difference of the Clar covering polynomials for a pair of so–called generalized S,T–isomers introduced in [3]. Then we deduce in a convenient way some results on its topological properties. Analogous results for other pairs of S,T–isomers are also listed in this paper.

2. PRELIMINARY

A benzenoid system is a finite 2–connected plane graph in which every interior region is a regular hexagon of side length 1. Recall that a Kekulé structure of a benzenoid system coincides with what in graph theory is known under the name "perfect matching". The number of Kekulé structures of a benzenoid system B will be denoted by K(B). A spanning subgraph C of a benzenoid system B is called a Clar cover of B if each component of it is either a hexagon or an edge. We denote by h(C) the number of hexagons of C. Now we define the Clar covering polynomial of B as [6]:

$$P(B,w) = \sum_{C} w^{h(C)} ,$$

where the summation goes over all Clar covers C of B. For the sake of convenience, we make two conventions: if B has not a Kekulé structure, P(B,w) = 0; if B is an empty graph (without vertices), P(B,w) = 1. It is easy to see that a Clar cover with maximum number of hexagons corresponds to a Clar formula, which is well known [3]. Denote by $\sigma(B)$ the cardinality of a Clar formula of B. Thus the Clar covering polynomial of a benzenoid system B can be expressed as:

$$P(B) = P(B,w) = \sum_{i=0}^{\sigma(B)} \sigma(B,i)\, w^{i} ,$$

where $\sigma(B,i)$ denotes the number of Clar covers having i hexagons.

In [6] we have shown that there exists a bijection between the set of Clar covers with $\sigma(B)$ hexagons and the set of Clar formulas for B. Now we sum up some results.

Lemma 1 [6]. For any benzenoid system B, when adopting the above notations, we have

(a) $\sigma(B,0) = K(B)$,

(b) $\sigma(B)$ is equal to the degree of P(B,w),

(c) $\sigma(B,\sigma(B))$ = the number of Clar formulas of B,

(d) $\sigma(B,1) = h_1(B)$ (say the first Herndon number, see [8]).

It is obvious that the definition of the Clar covering polynomial for a benzenoid system may be extended to generalized benzenoid systems, a subgraph of a benzenoid system (simply benzenoid graph), by the same means. The properties (a), (b) and (d) of Lemma 1 are also valid for a benzenoid graph.

In the following we introduce some elementary properties for the Clar covering polynomial of benzenoid graphs.

Lemma 2 [6]. Let B be a benzenoid graph whose components are B_1, B_2, ..., B_k. Then

$$P(B,w) = \prod_{i=1}^{k} P(B_i,w) \ .$$

Lemma 3 [6]. Let B be a benzenoid graph and $e = xy$ an edge of B. Let s_1 and s_2 be hexagons containing e (if they exist). Then

$$P(B,w) = w \sum_{i=1}^{2} P(B - s_i) + P(B{-}xy,w) + P(B{-}x{-}y,w) \ ,$$

where $B - s_i$ denotes a subgraph obtained from B by deleting all vertices of s_i together with their incident edges.

For further details the reader is referred to [6].

3. MAIN RESULTS

We first give the definition of a type of S,T–isomers [3]. Let A and A' be two isomorphic subunits of a benzenoid graph without holes. Furthermore, let a_i (a_i') be vertices of A (A') with the same color class, where $1 \leq i \leq p$. There exists an isomorphic mapping from A onto A' such that a_i' is an image of a_i for all $0 \leq i \leq p$. The benzenoid system S (T) is formed from the subunits A and A' which are linked by the edges a_ia_i' (a_ia_{p-i}') for $0 \leq i \leq p$, as is illustrated in Fig. 1.

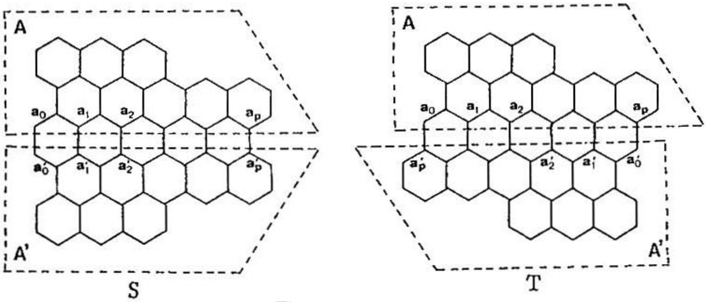


Fig. 1. S,T–isomer

The hexagons formed by joining the subunits A and A' will be called the central ring chain (of S or T) and denoted by R. P denotes the set of all vertical edges of R as shown in Fig. 1. A restriction of a Clar cover for S (or T) in R is its subgraph consisting of the components of the Clar cover containing edges in P.

A subgraph C of R is called a partial Clar cover of R if each of its components is either a hexagon or a vertical edge. One can see that a restriction of each Clar cover for S or T in R is a partial Clar cover of R. We reverse a partial Clar cover C of R and obtain another partial Clar cover which is called the reversion (write C') of C (see Fig. 2).

Fig. 2. A partial Clar cover C of R and its reversion C'

Theorem 1. The difference polynomial of the Clar covering polynomial of the generalized S,T–isomers is

$$\Delta(w) = P(S)-P(T) = \frac{1}{2}\sum_{C} w^{h(C)}\{P(A-V(C) \cap V(A)) - P(A-V(C') \cap V(A))\}^2 ,$$

where the summation runs over all partial Clar covers C of R.

Proof. We take a partial Clar cover C of R. It is easy to see that C contributes $w^{h(C)}P(S-V(C)-P) = w^{h(C)}P(A-V(C) \cap V(A))\, P(A'-V(C) \cap V(A')) = w^{h(C)}[P(A-V(C) \cap V(A))]^2$ to P(S) and contributes $w^{h(C)}P(T-V(C)-P) = w^{h(C)}P(A-V(C) \cap V(A))P(A'-V(C) \cap V(A')) = w^{h(C)}P(A-V(C) \cap V(A))P(A-V(C') \cap V(A))$ (because $A'-V(C) \cap V(A') \cong A-V(C') \cap V(A)$ for T) to P(T) by Lemma 2. If C is not a restriction of some Clar cover for S, then it contributes $w^{h(C)}P(S-V(C)-P) = 0$ to P(S) (because S–V(C)–P has no Kekulé structure). The same applies to T. Therefore the above statements are valid for any partial Clar cover of R.

If C = C', i.e. C is symmetric, then it contributes the same polynomial $w^{h(C)}P^2(A-V(C) \cap V(A))$ to both P(S) and P(T). In other words, C contributes 0 to their difference polynomial. Therefore we restrict the treatment to non–symmetric partial Clar cover of R in the following.

Let C be a partial Clar cover of R and C' be its reversion ($C \neq C'$). Then C and C' contribute to P(S)

$$\begin{aligned} & w^{h(C)}P^2(A-V(C) \cap V(A)) + w^{h(C')}P^2(A-V(C') \cap V(A)) \\ & = w^{h(C)}[P^2(A-V(C) \cap V(A)) + P^2(A-V(C') \cap V(A))] , \end{aligned}$$

and to P(T)

$$\begin{aligned} & w^{h(C)}P(A-V(C) \cap V(A))P(A-V(C') \cap V(A)) \\ & + w^{h(C')}P(A-V(C') \cap V(A))P(A-V((C')') \cap V(A)) \\ & = 2\, w^{h(C)}P(A-V(C) \cap V(A))P(A-V(C') \cap V(A)) \qquad (C = (C')') \end{aligned}$$

Hence C and C' contribute to P(S)–P(T)

$$w^{h(C)}\{P(A-V(C)\cap V(A))-P(A-V(C')\cap V(A))\}^2 \ .$$

Since the summation runs over all partial covers C of R, and each pair C and C' need to be taken twice, the proof is completed.

Now we immediately obtain the following results.

Theorem 2. For S and T isomers of benzenoid systems, we have

(a) $K(S) \geq K(T)$; furthermore, if $K(S) = K(T)$, then $h_1(S) \geq h_1(T)$.

(b) $\sigma(S) \geq \sigma(T)$; furthermore, if $\sigma(S) = \sigma(T) = m$, then $\sigma(S,m) \geq \sigma(T,m)$, i.e. the number of Clar formulas of T does not exceed that of S.

Proof. From Theorem 1 we have $\Delta(w) = P(s,w) - P(T,w) \geq 0$ for any non–negative real number w. Obviously, $\Delta(0) \geq 0$ implies that $K(S) \geq K(T)$. If $K(S) = K(T)$, we can derive that $h_1(S) \geq h_1(T)$ by choosing a sufficiently small positive number w. The second part of the theorem follows by choosing a sufficiently large number w.

Some additional types of S,T–isomers of benzenoid systems, such as S_i,T_i–isomers for all $1 \leq i \leq 4$, are indicated in Figures 3–6. For their precise definitions the readers are referred to [4,5]. In the following we only list their main results.

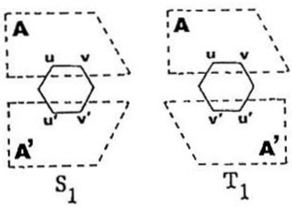


Fig. 3. S_1,T_1–isomer

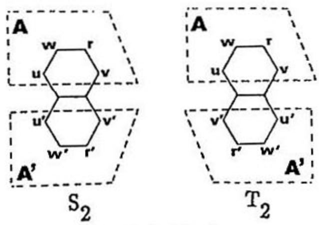
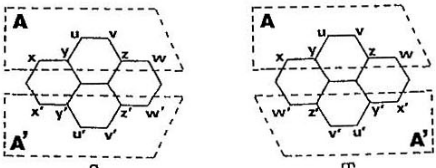
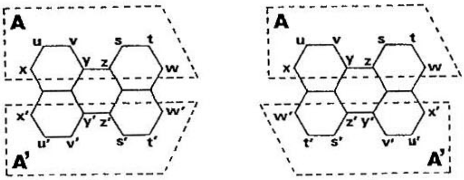


Fig. 4. S_2,T_2–isomer



S_3 T_3

Fig. 5. S_3,T_3–isomer



S_4 T_4

Fig. 6. S_4,T_4–isomer

For convenience of the following statements, we introduce some additional notations. Denote by $A^{xy\cdots v}$ a subgraph obtained from A by deleting the vertices x, y, ..., v together with their incident edges, and let $n(A)$ be the number of vertices of the subunit A. We assume that f is a permutation $\binom{x\ y\ z\ w}{w\ z\ y\ x}$ on the subset $\{x,y,z,w\} \subseteq V(A)$ (see Fig. 5 or 6). If $\{i,j\} \subseteq \{x,y,z,w\}$ is a 2–element subset, then $\overline{ij}$ will denote its complement.

Theorem 3. For $S_1(S_2),T_1(T_2)$–isomer, we have

$$\Delta(w) = P(T_i) - P(S_i) = [P(A^u) - P(A^v)]^2$$

for $i = 1, 2$.

Corollary 1. If $n(A)$ is odd, then $P(S_i) = 0$. Otherwise $P(S_i) = P(T_i)$, thus $\sigma(T_i,j) = \sigma(S_i,j)$ for all $j \geq 0$, where $i = 1, 2$.

Theorem 4. For $S_3(S_4),T_3(T_4)$–isomer, if $n(A)$ is odd, then $P(S_i) = 0$ $(i = 3, 4)$. Otherwise, we have

$$P(T_3) - P(S_3) = \sum_{\{i,j\}} [P(A^{ij}) - P(A^{\bar{i}\bar{j}})]^2 ,$$

where the summation goes over 2–element subsets $\{i,j\} \subseteq \{x,y,z,w\}$ such that $f(i) \neq j$, and

$$P(T_4) - P(S_4) = \{[P(A^{xy})-P(A^{zw})] + w[P(A^{xuvy})-P(A^{zstw})]\}^2 + \sum_{\{i,j\}\neq\{x,y\}} [P(A^{ij})-P(A^{\bar{i}\bar{j}})]^2 ,$$

where the summation of the last term goes over 2–element subsets $\{i,j\} \subseteq \{x,y,z,w\}$ such that $f(i) \neq j$ and $\{i,j\} \neq \{x,y\}$.

Corollary 2. Assume that $n(A)$ is even. For $i = 3, 4$ we have

(a) $K(T_i) \geq K(S_i)$; furthermore, if $K(S_i) = K(T_i)$, then $h_1(T_i) \geq h_1(S_i)$.

(b) $\sigma(T_i) \geq \sigma(S_i)$; furthermore, if $\sigma(T_i) = \sigma(S_i) = m$, then $\sigma(T_i,m) \geq \sigma(S_i,m)$, i.e. the number of Clar formulas of S_i does not exceed that of S_i.

(c) if $\sigma(T_i)$ is odd, then $\sigma(T_i) = \sigma(S_i)$.

4. CONCLUSIONS

The Clar covering polynomial of a benzenoid system unifies some of its topological indices. From the context we can find that it is very convenient to use this polynomial in discussing some topological properties of S,T–isomers. In some sense the Clar covering polynomial of benzenoid systems plays an important role in the topological theory of chemistry. Recently the author of [9] studied some topological properties of a new type of S,T–isomers by using the polynomial, thus demonstrating its usefulness further. It is intended to pursue the studies along these lines to obtain additional significant results.

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REFERENCES

1 O. E. Polansky and M. Zander, J. Mol. Struct. 84, 361(1982)

2 I. Gutman, O. E. Polansky and M. Zander, Match 15, 145(1984)

3 Zhang Fuji, Chen Zhibo and I. Gutman, Match 18, 101(1985)

4 Zhang Fuji and Chen Zhibo, Match 21, 187(1986)

5 Elkin Vumar, Match 23, 153(1988)

6 Zhang Heping and Zhang Fuji, The Clar covering polynomial of a benzenoid system (I), submitted to J. Math. Chem.

7 E. J. Farrell, J. Comb. Theory B, 26, 111(1979)

8 I. Gutman and S. El–Basil, Chem. Phys. Letters 115, 416(1985)

9 Li Xueliang, Topological properties of some novel S,T–isomers (II), submitted to Match.