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THE NUMBER OF KEKULÉ STRUCTURES OF UNBRANCHED CATACONDENSED BENZENOID SYSTEMS AND PRIMITIVE CORONOID SYSTEMS

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ABSTRACT

A simplification of Tošič and Bodroža's formula[1] is given for the number of Kekulé structures of unbranched catacondensed benzenoid systems. Further, an explicit formula is derived for the number of Kekulé structures of primitive coronoid systems (i.e. unbranched catacondensed coronoid systems).

1. INTRODUCTION

The enumeration of Kekulé structures (1-factors) of conjugated hydrocarbons has tremendously accelerated in the past few years, particularly for benzenoid hydrocarbons. Numerous results have been obtained for benzenoid systems.[1-4] But much less work for this topic has been done for coronoid systems. Several combinatorial K formulas are available for special classes of primitive coronoid systems.[5-11] However, a general formula for primitive coronoid systems has never been given before. In the present paper, we put forward a simplication of Tošič and Bodroža's formula[1] for unbranched catacondensed benzenoid systems, and arrive at a polynomial expression for the number of Kekulé structures of an arbitrary primitive coronoid system.

2. A SIMPLIFICATION OF TOŠIĆ AND BODROŽA'S K FORMULA FOR UNBRANCHED CATACONDENSED BENZENOID SYSTEMS

An unbranched catacondensed bezenoid system contains n linear segments, say $L_1, L_2, \ldots, L_n$, satisfying that two terminal segments L_1 and L_n contain one kink respectively, and L_i $(2 \leqslant i \leqslant n-1)$ contains two kinks(Fig.1). This benzenoid system is denoted by $L_n(x_1, x_2, \ldots, x_n)$ if L_i possesses x_i hexagons, $i=1,2,\ldots,n$. Fig.2 shows $L_5(2,3,2,2,3)$.

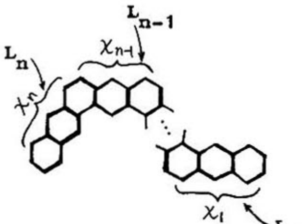


Fig.1

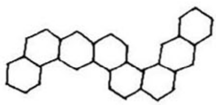


Fig.2

In their recent paper,[1] Tošić and Bodroža adopted the following notation:

$$[x_1, x_2, \ldots, x_n] = L_n(x_1+1, x_2+1, \ldots, x_{n-1}+1, x_n). \tag{1}$$

The number of Kekulé structures of $[x_1, x_2, \ldots, x_n]$ is denoted by $K_n[x_1, x_2, \ldots, x_n]$. They got the following recurrence relation:

$$K_n[x_1, x_2, \ldots, x_n] = x_n K_{n-1}[x_1, \ldots, x_{n-1}] + K_{n-2}[x_1, \ldots, x_{n-2}],$$

while $K_0=1$, $K_1[x] = 1+x$. (2)

From (2) they deduced the following formula.

$$K_n[x_1,\dots,x_n] = 1 + \sum_{\substack{1 \leqslant l_1 < l_2 < \dots < l_k \leqslant n,\\ l_k \equiv n \pmod 2,\\ l_{j+1}-l_j \equiv 1 \pmod 2\\ \text{for } j=1,2,\dots,k-1.}} x_{l_1}x_{l_2}\cdots x_{l_k}, \tag{3}$$

where $x_1,x_2,\dots,x_n$ are positive integers.

It is easy to see that $K_n[0,x_2,\dots,x_n]=K_{n-1}[x_2,\dots,x_n]$, and that formula (3) also applies to the case of $x_1=0$. Thus, from (1) and (3), we can derive the following result.

THEOREM 1. For positive integers $x_1,x_2,\dots,x_n$,

$$K\{L_n(x_1,x_2+1,x_3+1,\dots,x_{n-1}+1,x_n)\} = K_n[x_1-1,x_2,x_3,\dots,x_n]$$

$$= 1 + \sum_{\substack{1 \leqslant l_1 < l_2 < \dots < l_k \leqslant n,\\ k \equiv l_k \equiv n \pmod 2,\\ l_{j+1}-l_j \equiv 1 \pmod 2\\ \text{for } j=1,2,\dots,k-1.}} x_{l_1}x_{l_2}\cdots x_{l_k}. \tag{4}$$

It was shown[1] that the polynomial (3) has F_{n+2} terms, where F_i is the ith member of Fibonacci sequence $F_0=0$, $F_1=1$; $F_i=F_{i-1}+F_{i-2}$, for $i \geqslant 2$. Obviously, the number of terms in polynomial (3) is equal to

$$K_n[1,1,\dots,1] = F_{n+2}. \tag{5}$$

Therefore, the number of terms in polynomial (4) is

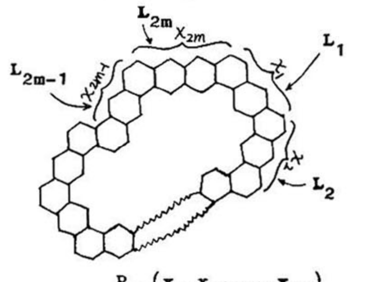
$$K\{L_n(1,2,2,\dots 2,1)\} = K_n[0,1,1,\dots,1]$$

$$= K_{n-1}[1,1,\dots,1] = F_{n+1}.$$

The difference between the numbers of terms in (3) and (4) is $F_{n+2}-F_{n+1}=F_n$. Hence, (4) is simpler than (3).

3. A K FORMULA FOR PRIMITIVE CORONOID SYSTEMS

A primitive coronoid system consists of a circular single chain of hexagons, and its inner perimeter is not a hexagon. A primitive coronoid system contains 2m ($m \geqslant 3$) linear segments, say $L_1, L_2, \ldots, L_{2m}$, satisfying that L_1 and L_{2m} share a kink, while L_i and L_{i+1} share a kink for $i=1,2,\ldots,2m-1$ (Fig.3). This coronoid system is denoted by $P_{2m}(x_1, x_2, \ldots, x_{2m})$ if L_i possesses x_i hexagons, $i=1,2,\ldots,2m$. Fig.4 depicts $P_8(5,2,4,4,2,2,2,2)$.



$P_{2m}(x_1, x_2, \ldots, x_{2m})$

Fig.3

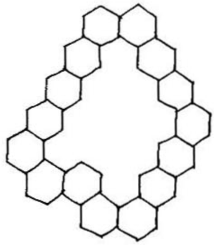
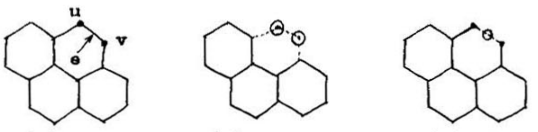


Fig.4

Let u and v be two adjacent vertices of a graph G, and $e=\{u,v\}$ (Fig.5a). G-u-v denotes the remaining part obtained by deleting u and v from G (Fig.5b), and G-e



(a) G (b) G-u-v (c) G-e

Fig.5

designates the remaining part obtained by deleting e from G (Fig.5c). It is well known that

$$K\{G\} = K\{G-u-v\} + K\{G-e\}. \tag{6}$$

Let $R=P_{2m}(x_1+1,x_2+1,\ldots,x_{2m}+1)$. (7)

R contains 2m linear segments $L_1,L_2,\ldots,L_{2m}$. Consider the kink hexagon L_1 shares with L_{2m}(Fig.6I). a,b,c and d are vertices belonging to the kink hexagon, $e_1=\{a,b\}$, $e_2=\{c,d\}$, and it is satisfied that e_1 is parallel to e_2 and both a and b are of degree two.

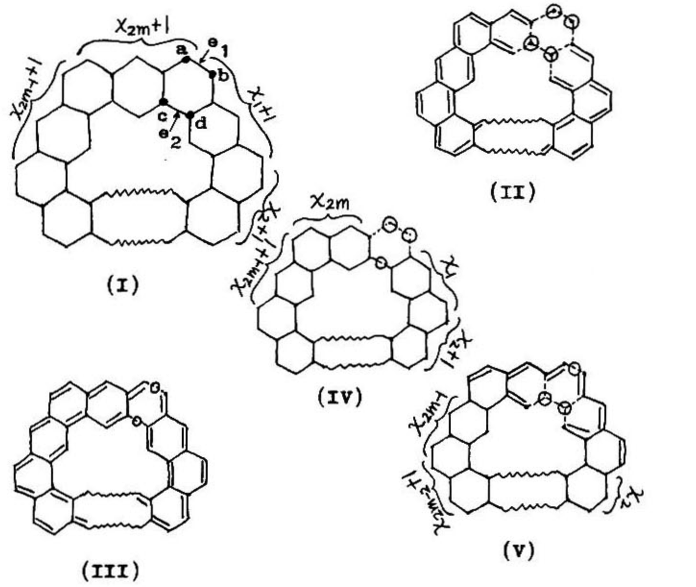


Fig.6

We obtain

$$K\{R-a-b-c-d\} = 1 \text{ (Fig.6II)}, \tag{8}$$

$$K\{R-e_1-e_2\} = 1 \text{ (Fig.6III)}, \tag{9}$$

$$K\{R-a-b-e_2\} = K\{L_{2m}(x_1, x_2+1, x_3+1, \ldots, x_{2m-1}+1, x_{2m})\} \text{ (Fig.6IV)}, \tag{10}$$

$$K\{R-e_1-c-d\} = K\{L_{2m-2}(x_2, x_3+1, x_4+1, \ldots, x_{2m-2}+1, x_{2m-1})\} \text{ (Fig.6V)}. \tag{11}$$

From (6)-(11), we get

$$K\{P_{2m}(x_1+1, x_2+1, \ldots, x_n+1)\} = K\{R\}$$
$$= K\{R-a-b\} + K\{R-e_1\}$$
$$= K\{R-a-b-c-d\} + K\{R-a-b-e_2\} + K\{R-e_1-c-d\} + K\{R-e_1-e_2\}$$
$$= 2 + K\{L_{2m}(x_1, x_2+1, x_3+1, \ldots, x_{2m-1}+1, x_{2m})\}$$
$$+ K\{L_{2m-2}(x_2, x_3+1, x_4+1, \ldots, x_{2m-2}+1, x_{2m-1})\}. \tag{12}$$

By (4) and (12), we can derive the following theorem.

THEOREM 2. For positive integers $x_1, x_2, \ldots, x_{2m}$,

$$K\{P_{2m}(x_1+1, x_2+1, \ldots, x_{2m}+1)\}$$
$$= 4 + \sum_{\substack{1 \leqslant l_1 < l_2 < \ldots < l_{2k} \leqslant 2m, \\ l_{j+1} - l_j \equiv 1 \pmod 2 \\ \text{for } j=1,2,\ldots,2k-1.}} x_{l_1} x_{l_2} \cdots x_{l_{2k}}.$$

The number of terms in the above polynomial is

$$K\{P_{2m}(2,2,\ldots,2)\} - 3$$
$$= K\{L_{2m}(1,2,2,\ldots,2,1)\} + K\{L_{2m-2}(1,2,2,\ldots,2,1)\} - 1$$
$$= F_{2m+1} + F_{2m-1} - 1.$$

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