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LINEAR RECURSION RELATIONS AND THE ENUMERATION OF KEKULÉ STRUCTURES OF BENZENOID HYDROCARBONS

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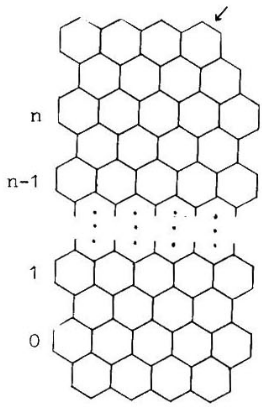
Abstract. By using the theory of linear recursion relations,explicit analytical formulas for the number of Kekulé structures of some homologous series of benzenoid hydrocarbons are deduced.This is a further development of a previous work by Gutman.

Our interest in the problem of the enumeration of Kekulé structures of benzenoid molecules was prompted by the work of Gutman(1) .Instead of studying one single homologous series,Gutman first developed an approach which enables the simultaneous consideration of a group of mutually related homologous series.Our work will further illustrate the power and ability of the approach .

In the present paper we offer some formulas which enable the direct evaluation of the number of Kekulé structures of benzenoid hydrocarbons. In particular, we shall deal with the eighteen homologous series— $(H_i)_n$, i=1,2,.. ..,18.



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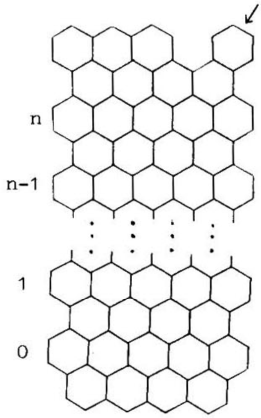

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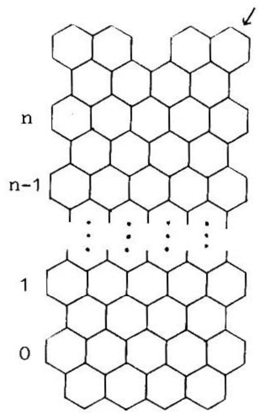

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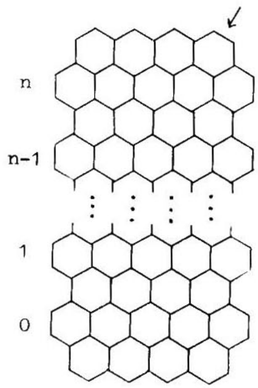

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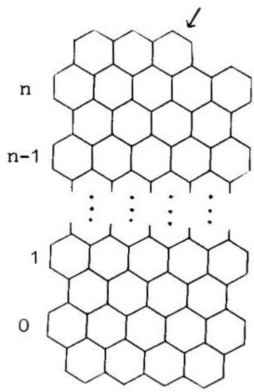
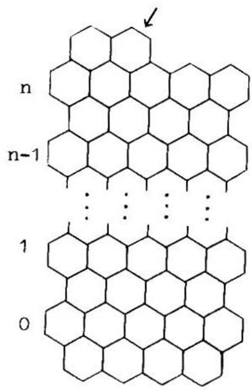


H_5



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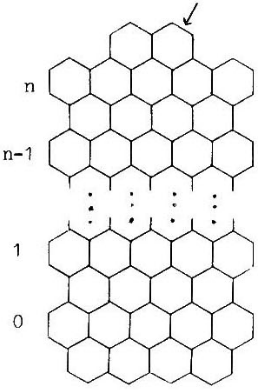

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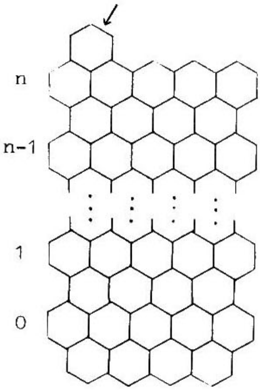
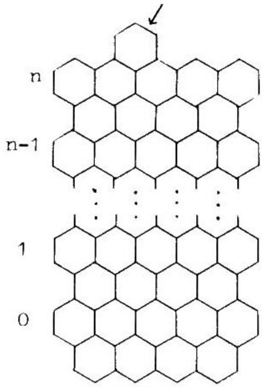


H_8



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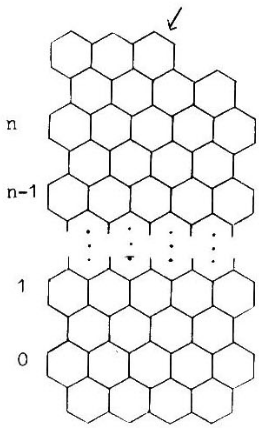
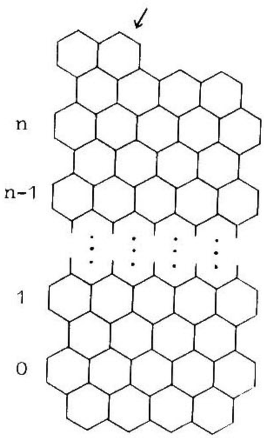
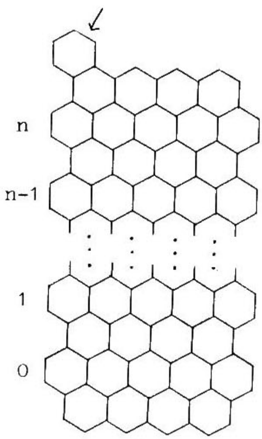


H_{10}



H_{11}



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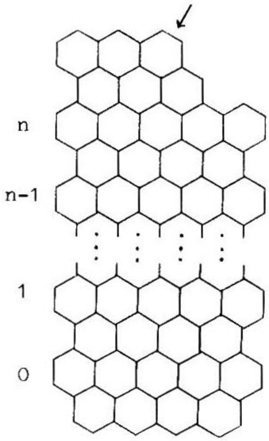

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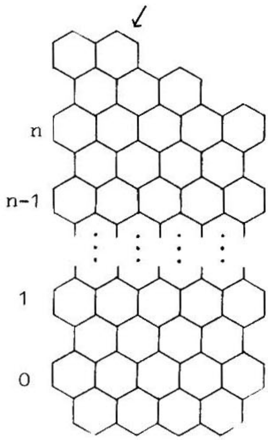
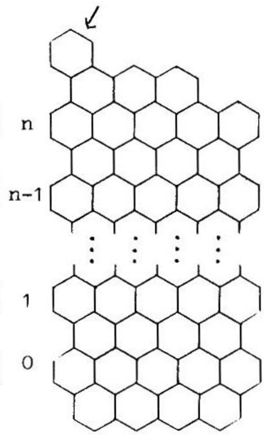
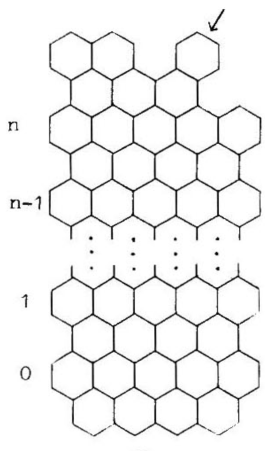


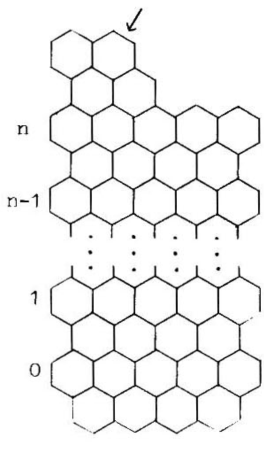
H_{14}



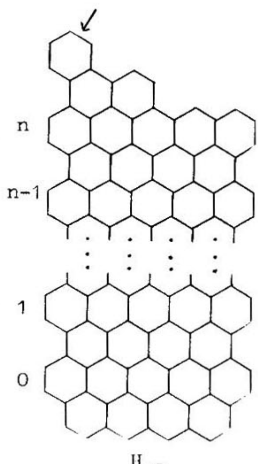
H_{15}



H_{16}



H_{17}



H_{18}

Denote by $K(H_i)_n$ the number of Kekulé structures of a conjugated system whose molecular graph is $(H_i)_n$, $i=1,2,\ldots,18$. Evidently, the numbers $K(H_i)_n$, $n=0,1,2,\ldots$, form a sequence of number $(K(H_i)_n)_{n\geq 0}$. Thus finding the explicit analytical formulas for the number $K(H_i)_n$ is equivalent to seeking for the expression of the general term of the sequence $(K(H_i)_n)_{n\geq 0}$. For the expression of the general term of a sequence of number satisfying linear recursion relations we have the following.

<u>Lemma 1</u> (2). Let $(u_n)_{n\geq 0}$ be a sequence of number satisfying the linear recursion relations

$$u_{n+m}=c_1u_{n+m-1}+c_2u_{n+m-2}+\ldots+c_{m-1}u_{n+1}+c_mu_n \quad (n\geq 0),$$

where $c_1,\ldots,c_m$ are constants. Let $\dfrac{h(x)}{f(x)} = \displaystyle\sum_{1\leq i\leq s}\sum_{1\leq l\leq e_i}\frac{\beta_{il}}{(1-\alpha_i x)^l}$, where

$$h(x)=(u_0+u_1x+\ldots+u_nx^n+\ldots)(1-c_1x-c_2x^2-\ldots-c_mx^m),$$
$$f(x)=1-c_1x-c_2x^2-\ldots-c_mx^m=(1-\alpha_1x)^{e_1}(1-\alpha_2x)^{e_2}\ldots(1-\alpha_sx)^{e_s},$$

where $\alpha_i\neq\alpha_j$ for $i\neq j$; $e_1+e_2+\ldots+e_s=m$. Then we have

$$u_n=\sum_{1\leq i\leq s}\sum_{1\leq l\leq e_i}\beta_{il}\binom{n+l-1}{l-1}\alpha_i^n \quad \text{for } n\geq 0,$$

where $\displaystyle\binom{n+i-1}{l-1}=\frac{(n+l-1)(n+l-2)\ldots(n+1)}{1.2.\ldots.(l-1)}$

In particular, if $s=m$, $e_1=e_2=\ldots=e_m=1$, then $u_n=\displaystyle\sum_{i=1}^{m}p_i\alpha_i^n$,

where p_i, $i=1,2,\ldots,m$, are determined by the system of linear equations:

$$\begin{cases} p_1 + p_2 + \dots + p_m = u_o \\ \alpha_1 p_1 + \alpha_2 p_2 + \dots + \alpha_m p_m = u_1 \\ \vdots \\ \alpha_1^{m-1} p_1 + \alpha_2^{m-1} p_2 + \dots + \alpha_m^{m-1} p_m = u_{m-1} \end{cases}$$

In the case when there is a group of mutually related sequences of numbers, we may obtain the linear recursion relation for each single sequence of numbers by using the following lemma.

Lemma 2. Let $(u_n^{(1)})_{n \geqslant o}, \dots, (u_n^{(m)})_{n \geqslant o}$ be m sequences of numbers satisfying

$$u_{n+1}^{(i)} = a_{i1} u_n^{(1)} + a_{i2} u_n^{(2)} + \dots + a_{im} u_n^{(m)} \qquad (n \geqslant 0)$$

for each $i, 1 \leqslant i \leqslant m$, where $a_{ij}, 1 \leqslant i,j \leqslant m$ are constants. Let A be the $m \times m$ square matrix whose entry in position (i,j) is a_{ij}, and the characteristic polynomial of A be $\lambda^m - c_1 \lambda^{m-1} - \dots - c_{m-1}\lambda - c_m$. Then for each $i, 1 \leqslant i \leqslant m$, we have

$$u_{n+m}^{(i)} = c_1 u_{n+m-1}^{(i)} + c_2 u_{n+m-2}^{(i)} + \dots + c_{m-1} u_{n+1}^{(i)} + c_m u_n^{(i)} .$$

Proof. It is not difficult to deduce the conclusion by using Hamilton-Cayley theorem in matrix theory. We omit the details.

We are now in a position to find the number $K(H_i)_n$.

Let H be a graph, e be an (arbitrary) edge of H connecting the vertices v_r and v_t of H. It is well-known [3] that

$$K(H)=K(H-e)+K(H-v_r-v_t) \quad (1)$$

In particular, if one of v_r and v_t has degree one, then

$$K(H)=K(H-v_r-v_t) \quad (2)$$

Applying (1) to the edges of H_i, i=1,...,18, which are indicated by arrows, and by a repeated use of (2), we arrive to

$$K(H_1)_n = K(H_{10})_n + K(H_1)_{n-1}$$

$$K(H_2)_n = K(H_{10})_n + K(H_{13})_n$$

$$K(H_3)_n = K(H_{11})_n + K(H_{16})_n$$

$$K(H_4)_n = K(H_1)_{n-1} + K(H_5)_n$$

$$K(H_5)_n = K(H_2)_{n-1} + K(H_6)_n$$

$$K(H_6)_n = K(H_3)_{n-1} + K(H_8)_n$$

$$K(H_7)_n = K(H_2)_{n-1} + K(H_9)_n$$

$$K(H_8)_n = K(H_1)_{n-1} + K(H_2)_{n-1}$$

$$K(H_9)_n = K(H_2)_{n-1} + K(H_3)_{n-1}$$

$$K(H_{10})_n = K(H_8)_n + K(H_{11})_n$$

$$K(H_{11})_n = K(H_6)_n + K(H_{12})_n$$

$$K(H_{12})_n = K(H_4)_n + K(H_5)_n$$

$$K(H_{13})_n = K(H_2)_{n-1} + K(H_{14})_n$$

$K(H_{14})_n = K(H_9)_n + K(H_{15})_n$

$K(H_{15})_n = K(H_5)_n + K(H_7)_n$

$K(H_{16})_n = K(H_{14})_n + K(H_{17})_n$

$K(H_{17})_n = K(H_3)_{n-1} + K(H_{18})_n$

$K(H_{18})_n = K(H_6)_n + K(H_9)_n$

A simple caculation will lead to the following.

$K(H_1)_n = 6\ K(H_1)_{n-1} + 6K(H_2)_{n-1} + 3\ K(H_3)_{n-1}$

$K(H_2)_n = 6\ K(H_1)_{n-1} + 12\ K(H_2)_{n-1} + 6\ K(H_3)_{n-1}$

$K(H_3)_n = 6\ K(H_1)_{n-1} + 12\ K(H_2)_{n-1} + 9\ K(H_3)_{n-1}$

$K(H_4)_n = 2\ K(H_1)_{n-1} + 2\ K(H_2)_{n-1} + K(H_3)_{n-1}$

$K(H_5)_n = K(H_1)_{n-1} + 2\ K(H_2)_{n-1} + K(H_3)_{n-1}$

$K(H_6)_n = K(H_1)_{n-1} + K(H_2)_{n-1} + K(H_3)_{n-1}$

$K(H_7)_n = 2\ K(H_2)_{n-1} + K(H_3)_{n-1}$

$K(H_8)_n = K(H_1)_{n-1} + K(H_2)_{n-1}$

$K(H_9)_n = K(H_2)_{n-1} + K(H_3)_{n-1}$

$K(H_{10})_n = 5\ K(H_1)_{n-1} + 6\ K(H_2)_{n-1} + 3\ K(H_3)_{n-1}$

$K(H_{11})_n = 4\ K(H_1)_{n-1} + 5\ K(H_2)_{n-1} + 3\ K(H_3)_{n-1}$

$K(H_{12})_n = 3\ K(H_1)_{n-1} + 4\ K(H_2)_{n-1} + 2\ K(H_3)_{n-1}$

$K(H_{13})_n = K(H_1)_{n-1} + 6\ K(H_2)_{n-1} + 3\ K(H_3)_{n-1}$

$$K(H_{14})_n = K(H_1)_{n-1} + 5\,K(H_2)_{n-1} + 3\,K(H_3)_{n-1}$$

$$K(H_{15})_n = K(H_1)_{n-1} + 4\,K(H_2)_{n-1} + 2\,K(H_3)_{n-1}$$

$$K(H_{16})_n = 2\,K(H_1)_{n-1} + 7\,K(H_2)_{n-1} + 6\,K(H_3)_{n-1}$$

$$K(H_{17})_n = K(H_1)_{n-1} + 2\,K(H_2)_{n-1} + 3\,K(H_3)_{n-1}$$

$$K(H_{18})_n = K(H_1)_{n-1} + 2\,K(H_2)_{n-1} + 2\,K(H_3)_{n-1}$$

We now apply Lemma 2 to the sequences of numbers $(K(H_1)_n)_{n \geqslant 0}$, $(K(H_2)_n)_{n \geqslant 0}$ and $(K(H_3)_n)_{n \geqslant 0}$ .Let

$$A = \begin{pmatrix} 6 & 6 & 3 \\ 6 & 12 & 6 \\ 6 & 12 & 9 \end{pmatrix}$$

Thus the characteristic polynomial of A is

$$\lambda^3 - 27\lambda^2 + 108\lambda - 108 \; .$$

Therefore, we have

$$K(H_i)_{n+3} = 27K(H_i)_{n+2} - 108\,K(H_i)_{n+1} + 108\,K(H_i)_n \quad (n \geqslant 0) \quad (3)$$

for $i=1,2,3$.

Furthermore, the linear recursion relations (3) hold for $j=4,5,\ldots,18$. In fact, $K(H_j)_{n+3}$, $j=4,5,\ldots,18$, can be expressed as follows.

$$K(H_j)_{n+3} = b_{j1}\,K(H_1)_{n+2} + b_{j2}\,K(H_2)_{n+2} + b_{j3}\,K(H_3)_{n+2} \quad (4)$$

Substitution of the linear recursion relations for $(K(H_1)_n)_{n \geqslant 0}$ $(K(H_2)_n)_{n \geqslant 0}$ and $(K(H_3)_n)_{n \geqslant 0}$ into (4) gives

$$K(H_j)_{n+3} = 27(b_{j1}K(H_1)_{n+1} + b_{j2}K(H_2)_{n+1} + b_{j3}K(H_3)_{n+1})$$
$$-108(b_{j1}K(H_1)_n + b_{j2}K(H_2)_n + b_{j3}K(H_3)_n)$$
$$+108(b_{j1}K(H_1)_{n-1} + b_{j2}K(H_2)_{n-1} + b_{j3}K(H_3)_{n-1})$$
$$= 27K(H_j)_{n+2} - 108K(H_j)_{n+1} + 108K(H_j)_n$$

Since we have the following decomposition

$$1-27x+108x^2-108x^3=(1-3x)(1-6(2+\sqrt{3})x)(1-6(2-\sqrt{3})x),$$

we can use the particular case of Lemma 2. The initial conditions $K(H_i)_o, K(H_i)_1$ and $K(H_i)_2$ can be obtained by direct calculation by a repeated use of the formulas (1) and (2). We omit the details. Our main results are as follows.

$$K(H_1)_n=3^{n+1}+6^{n+1}(26+15\sqrt{3})(2+\sqrt{3})^n+6^{n+1}(26-15\sqrt{3})(2-\sqrt{3})^n$$
$$K(H_2)_n= 6^{n+1}(168+97\sqrt{3})(2+\sqrt{3})^{n-1} +6^{n+1}(168-97\sqrt{3})(2-\sqrt{3})^{n-1}$$
$$K(H_3)_n=-3^{n+1}+6^{n+1}(194+112\sqrt{3})(2+\sqrt{3})^{n-1}+6^{n+1}(194-112\sqrt{3})(2-\sqrt{3})^{n-1}$$
$$K(H_4)_n=3^n+2\ 6^n(26+15\sqrt{3})(2+\sqrt{3})^n+2\ 6^n(26-15\sqrt{3})(2-\sqrt{3})^n$$
$$K(H_5)_n=6^n(168+97\sqrt{3})(2+\sqrt{3})^{n-1}+6^n(168-97\sqrt{3})(2-\sqrt{3})^{n-1}$$
$$K(H_6)_n=6^n(459+265\sqrt{3})(2+\sqrt{3})^{n-2} +6^n(459-265\sqrt{3})(2-\sqrt{3})^{n-2}$$
$$K(H_7)_n=-3^n+6^n(530+306\sqrt{3})(2+\sqrt{3})^{n-2}+6^n(530-306\sqrt{3})(2-\sqrt{3})^{n-2}$$
$$K(H_8)_n=3^n+6^n(265+153\sqrt{3})(2+\sqrt{3})^{n-2}+6^n(265-153\sqrt{3})(2-\sqrt{3})^{n-2}$$
$$K(H_9)_n=-3^n+6^n(362+209\sqrt{3})(2+\sqrt{3})^{n-2}+6^n(362-209\sqrt{3})(2-\sqrt{3})^{n-2}$$

$$K(H_{10})_n=2\cdot 3^n+6^n(2075+1198\sqrt{3})(2+\sqrt{3})^{n-2}+6^n(2075-1198\sqrt{3})(2-\sqrt{3})^{n-2}$$

$$K(H_{11})_n=3^n+6^n(1810+1045\sqrt{3})(2+\sqrt{3})^{n-2}+6^n(1810-1045\sqrt{3})(2-\sqrt{3})^{n-2}$$

$$K(H_{12})_n=3^n+6^n(362+209\sqrt{3})(2+\sqrt{3})^{n-1}+6^n(362-209\sqrt{3})(2-\sqrt{3})^{n-2}$$

$$K(H_{13})_n=-2\cdot 3^n+6^n(1687+974\sqrt{3})(2+\sqrt{3})^{n-2}+6^n(1687-974\sqrt{3})(2-\sqrt{3})^{n-2}$$

$$K(H_{14})_n=-2\cdot 3^n+6^n(1519+877\sqrt{3})(2+\sqrt{3})^{n-2}+6^n(1519+877\sqrt{3})(2-\sqrt{3})^{n-2}$$

$$K(H_{15})_n=-3^n+6^n(1157+688\sqrt{3})(2+\sqrt{3})^{n-2}+6^n(1157-688\sqrt{3})(2-\sqrt{3})^{n-2}$$

$$K(H_{16})_n=-4\cdot 3^n+6^n(2534+1463\sqrt{3})(2+\sqrt{3})^{n-2}+6^n(2534-1463\sqrt{3})(2-\sqrt{3})^{n-2}$$

$$K(H_{17})_n=-2\cdot 3^n+6^n(1015+586\sqrt{3})(2+\sqrt{3})^{n-2}+6^n(1015-586\sqrt{3})(2-\sqrt{3})^{n-2}$$

$$K(H_{18})_n=-3^n+6^n(821+474\sqrt{3})(2+\sqrt{3})^{n-2}+6^n(821-474\sqrt{3})(2-\sqrt{3})^{n-2}$$

Concluding this paper we would like to point out the importance of Lemma 2. Although our method for finding the number of Kekulé structures of homologous series is based on the simultaneous consideration of a group of mutually related homologous series, Lemma 2 enables us to obtain easily the linear recursion relations for each single homologous series. The solution of the linear recursions will lead to the general formulas for the number of Kekulé structures.

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