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P–V matrix and enumeration of Kekulé structures

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In this paper, a simple and intuitive proof of the theorem $K = |\det N(G)|$ [1, 2] is given.

Key words: HF graph — P–V matrix — Kekulé structure

1. Introduction

The enumeration of Kekulé structures of benzenoid hydrocarbons has fascinated many researchers [1–42]. It has been shown that very large benzenoid hydrocarbons can be examined by using theories that require only counts of Kekulé structures as input [43–47]. The considerable number of papers published [18–42] shows that the interest in this topic has increased substantially during the last few years.

In the present paper, we give a simple and intuitive proof of the recent result of John and Sachs [1, 2] ($K = |\det N(G)|$).

2. Definitions

HF graph [48, 49]. A finite planar connected graph in an infinite regular hexagonal lattice with vertical edges is called a honeycomb fragment graph (or simply, a HF graph).

KHF graph [48, 49]. If a HF graph is Kekuléan, it is called a KHF graph. For a HF graph $G(V, E)$, $V(G)$ is its vertex set and $E(G)$ is its edge set. Every edge of G has a length 1. Denote the number of elements in the two sets by $|V(G)|$ and $|E(G)|$, respectively. Colour the vertices of the hexagonal lattice black "•" and white "○" alternatively such that any two neighbouring vertices have different colour and every vertical edge has a black upper vertex and a white lower vertex. Thus, every vertex of a HF graph on the coloured hexagonal lattice is also coloured. For example, some HF graphs are shown in Fig. 1.

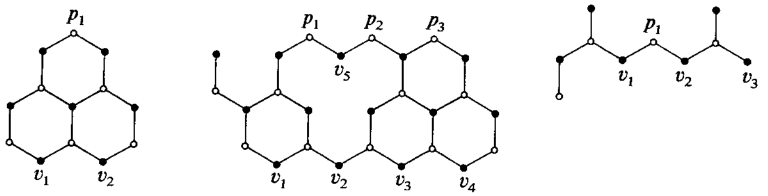


Fig. 1. HF graphs; peaks and valleys

Peaks and valleys [1, 2, 48, 50]. Consider a HF graph G. A peak is defined as a vertex lying above all its first neighbours, and a valley is a vertex lying below all its first neighbours (see Fig. 1). The peaks of G will be denoted by $p_1, p_2, \ldots, p_k$, and the valleys of G by $v_1, v_2, \ldots, v_h$.

P–V *path* [1, 2, 48, 50]. A P–V path in a HF graph is a path issuing from a peak, running monotonously down, and terminating in a valley.

Conjugated P–V *path* (*or perfect* P–V *path*) [1, 2, 48, 49]. In a given Kekulé structure of a KHF graph, if a P–V path with h vertices has $h/2$ conjugated double bond edges, then it is called a conjugated P–V path. In [50], Sachs established an one-to-one correspondence between Kekulé structures and perfect P–V path systems in hexagonal systems.

In [48], we proposed the P–V network flow method, which uses the maximum flow of the P–V network of a HF graph to determine whether a HF graph possesses Kekulé structures or not. We should note that a P–V path must have an odd path length, and so a path issuing from the peak p_i and terminating in the valley v_j has a path length $2I_{ij}-1$, where I_{ij} is the number of the diagonal edges in the P–V path.

If I_{ij} is an even number (i.e. $(-1)^{I_{ij}}=1$), then the P–V path is called an even P–V path, and if I_{ij} is an odd number (i.e. $(-1)^{I_{ij}}=-1$), then the P–V path is called an odd P–V path; $(-1)^{I_{ij}}$ is called the odd-even index of the P–V path. Obviously, all the possible P–V paths issuing from the peak p_i and terminating in the valley v_j have the same path length $2I_{ij}-1$ and the same odd-even index $(-1)^{I_{ij}}$.

P–V *matrix* $N(G)$ *of* G. Consider a HF graph G having peaks $p_1, p_2, \ldots, p_k$ and valleys $v_1, v_2, \ldots, v_h$. Its P–V matrix is a $k \times h$ matrix $N(G)$ with elements n_{ij} ($i=1,2,\ldots,k$; $j=1,2,\ldots,h$) equal to the number of the possible P–V paths issuing from p_i ($i=1,2,\ldots,k$) and terminating in v_j($j=1,2,\ldots,h$). For example, in Fig. 2, the P–V matrix $N(G)$ is

$$N(G)=\begin{bmatrix} 16 & 1 & 6 \\ 2 & 2 & 1 \\ 1 & 0 & 2 \end{bmatrix} \tag{1}$$

The value of n_{ij} can very easily be determined either by computer or by hands, with the following method (see Fig. 2). Let the valleys have the values

$$V_s=\begin{cases} 1 & (s=j) \\ 0 & (s\neq j) \end{cases} \tag{2}$$

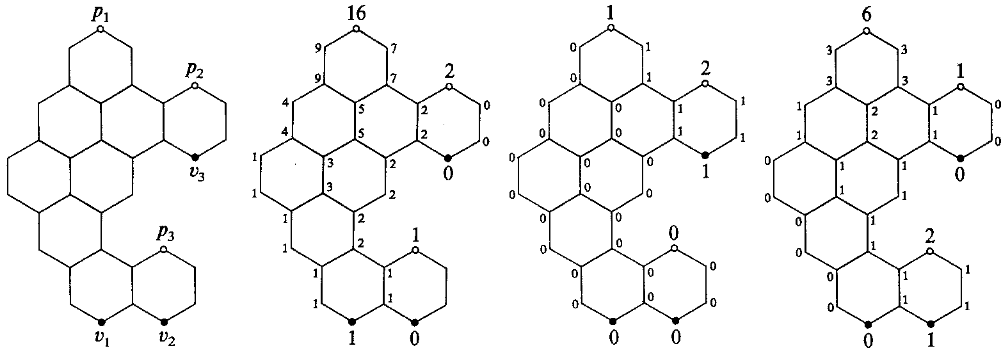


Fig. 2. Determination of n_{ij}

and every other vertex have a value equal to the sum of the values of the vertices which are below and adjacent to it. The obtained peak values are merely the values n_{ij} of the elements in the jth column of $N(G)$.

In the case of $h \neq k$, by entering additional rows (or columns) of zero elements, we can make the $k \times h$ P-V matric $N(G)$ become a $t \times t$ ($t = \max(k, h)$) square matrix. From now on, any P-V matrix will be considered as a square one.

Now, let us define another matrix $W(G)$ which has the elements

$$w_{ij} = (-1)^{I_{ij}} \times n_{ij}, \qquad (i = 1, 2, \ldots, t; j = 1, 2, \ldots, t), \tag{3}$$

where the n_{ij}s are the P-V matrix elements, and $(-1)^{I_{ij}}$ is the odd-even index of the P-V path issuing from p_i and terminating in v_j (in the case of $n_{ij} = 0$, I_{ij} is arbitrary).

3. Determinant of P-V matrix and the proof of John-Sachs theorem

Lemma. *For a* HF *graph,* $|\det N(G)| = |\det W(G)|$.

Proof. Suppose that all the elements n_{ij} in a P-V matrix are not equal to 0. Consider two P-V paths $p_i v_j$ and $p_{i'} v_j$ which have a common end v_j. The length difference of the two P-V paths doesn't depend on $j (j = 1, 2, \ldots, t)$. Neither does the value $I_{ij} - I_{i'j}$: the corresponding elements in any two rows (say the ith and the i'-th rows) of $W(G)$ have the same sign (if $(-1)^{I_{ij}}/(-1)^{I_{i'j}} = 1$) or the opposite sign (if $(-1)^{I_{ij}}/(-1)^{I_{i'j}} = -1$).

Although any zero elements ($n_{ij} = 0$) in the matrix $W(G)$ have arbitrary signs, by selecting suitable signs for them we can also make $(-1)^{I_{ij}}/(-1)^{I_{i'j}}$ in depend of j. So we have

$$(-1)^{I_{ij}}/(-1)^{I_{i'j}} = (-1)^{I_{i1} - I_{i'1}} \qquad (j = 1, 2, \ldots, t). \tag{4}$$

Let $I' = 1$. Equation (4) becomes

$$(-1)^{I_{ij}} = (-1)^{I_{11} + (I_{i1} - I_{11})} \qquad (i = 1, 2, \ldots, t; j = 1, 2, \ldots, t)$$

and thus,

$$\det W(G)=\begin{vmatrix} (-1)^{I_{11}}n_{11} & (-1)^{I_{12}}n_{12} & \cdots & (-1)^{I_{1t}}n_{1t} \\ (-1)^{I_{21}}n_{21} & (-1)^{I_{22}}n_{22} & \cdots & (-1)^{I_{2t}}n_{2t} \\ \cdots & \cdots & \cdots & \cdots \\ (-1)^{I_{21}}n_{t1} & (-1)^{I_{t2}}n_{t2} & \cdots & (-1)^{I_{tt}}n_{tt} \end{vmatrix}$$

$$=\begin{vmatrix} (-1)^{I_{11}+(I_{11}-I_{11})}n_{11} & (-1)^{I_{12}+(I_{11}-I_{11})}n_{12} & \cdots & (-1)^{I_{1t}+(I_{11}-I_{11})}n_{1t} \\ (-1)^{I_{11}+(I_{21}-I_{11})}n_{21} & (-1)^{I_{12}+(I_{21}-I_{11})}n_{22} & \cdots & (-1)^{I_{1t}+(I_{21}-I_{11})}n_{2t} \\ \cdots & \cdots & \cdots & \cdots \\ (-1)^{I_{11}+(I_{t1}-I_{11})}n_{t1} & (-1)^{I_{12}+(I_{t1}-I_{11})}n_{t2} & \cdots & (-1)^{I_{1t}+(I_{t1}-I_{11})}n_{tt} \end{vmatrix}$$

$$=(-1)^{(\sum_{i=1}^{t} I_{i1})-t^{I_{11}}}\times\begin{vmatrix} (-1)^{I_{11}}n_{11} & (-1)^{I_{12}}n_{12} & \cdots & (-1)^{I_{1t}}n_{1t} \\ (-1)^{I_{11}}n_{21} & (-1)^{I_{12}}n_{22} & \cdots & (-1)^{I_{1t}}n_{2t} \\ \cdots & \cdots & \cdots & \cdots \\ (-1)^{I_{11}}n_{t1} & (-1)^{12}n_{t2} & \cdots & (-1)^{I_{1t}}n_{tt} \end{vmatrix}$$

Hence

$$\det W(G)=A\times\begin{vmatrix} n_{11} & n_{12} & \cdots & n_{1t} \\ n_{21} & n_{22} & \cdots & n_{2t} \\ \cdots & \cdots & \cdots & \cdots \\ n_{t1} & \cdots & \cdots & n_{tt} \end{vmatrix}=A\times(\det N(G)),$$

where

$$A=(-1)^{(\sum_{i=1}^{t} I_{i1}+\sum_{j=1}^{t} I_{1j})-t^{I_{11}}}=(-1)^{\sum_{i=1}^{t} I_{ii}}.$$

John–Sachs theorem. *For a* HF *graph G,*

$$K(G)=|\det N(G)|, \tag{5}$$

where $K(G)$ is the number of kekulé structures of G.

Proof. If in the graph G, the number of the peaks is different from that of the valleys, we have $|\det N(G)|=0$; obviously, Eq. (5) holds [49, 50].

Now let us consider a HF graph G in which the number of the peaks is equal to the number of the valleys. From [49, 50], the number of the white vertices must be equal to the number of the black vertices. According to Ham's result [5] which was first proved by Cvetković DM, Gutman I and Trinajstić N (see [13]),

$$K(G)=|\det M(G)|, \tag{6}$$

where $M(G)$ is a $g\times g$ matrix with the elements:

$$m_{ij}=\begin{cases} 1 & (\text{if } w_i \text{ is adjacent to } b_j) \\ 0 & (\text{if } w_i \text{ is not adjacent to } b_j) \end{cases}$$

$$(i=1,2,\ldots,g;\ j=1,2,\ldots g;\ g=|V(G)|/2).$$

For convenience we will adopt the following conventions.

1. The peaks as well as valleys are labelled $1, 2, \ldots, t$, and the other white (black) vertices are labelled $t+1,\ t+2, \ldots, g\ (g=|V(G)|/2)$.

2. The labels $t+1, t+2, \ldots, g$ of the white vertices which are not peaks are given by sweeping from the left to the right and from top to bottom.

3. Every black vertex which is not a valley is given the same label as the white vertex immediately beneath it.

Thus, the $g \times g$ matrix $M(G)$ has the following properties.

1. As the degree of any vertex of G is less than or equal to 3, every row (column) has at most 3 nonzero elements. In particular, every row (column) of the first t rows (columns) has at most 2 nonzero elements.

2. The diagonal elements in the last $g-t$ rows (columns), m_{ii} equal 1 ($i \geq t+1$).

3. For the last $g-t$ columns ($j \geq t+1$), there are no nonzero elements below the diagonal elements.

Thus,

$$M(G)=\begin{bmatrix} m_{11} & m_{12} & \cdots & m_{1t} & m_{1,t+1} & m_{1,t+2} & m_{1,t+3} & \cdots & m_{1g} \\ m_{21} & m_{22} & \cdots & m_{2t} & m_{2,t+1} & m_{2,t+2} & m_{2,t+3} & \cdots & m_{2g} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \\ m_{t1} & m_{t2} & \cdots & m_{tt} & m_{t,t+1} & m_{t,t+2} & m_{t,t+3} & \cdots & m_{tg} \\ m_{t+1,1} & m_{t+1,2} & & m_{t+1,t} & 1 & m_{t+1,t+2} & m_{t+1,t+3} & \cdots & m_{t+1,g} \\ m_{t+2,1} & m_{t+2,2} & \cdots & m_{t+2,t} & & 1 & m_{t+2,t+3} & \cdots & m_{t+2,g} \\ \cdots & \cdots & \cdots & \cdots & & & 1 & \cdots & m_{t+3,g} \\ \cdots & \cdots & \cdots & \cdots & 0 & & & \cdots & \\ m_{g1} & m_{2g} & \cdots & m_{gt} & & & & & 1 \end{bmatrix}$$

Now let us transform the determinant det $M(G)$. To begin with consider the g-th column (supposing $g \geq t+1$). In this column, there are other nonzero elements than m_{gg}, say, m_{pg} and m_{qg} (i.e. $m_{pg}=m_{qg}=1$). This indicates that the black vertex b_g is adjacent to three white vertices w_g, w_p and w_q. By substracting the corresponding element values of the gth row from those of the pth row and from those of the qth row, we can make all the elements of the gth column, except the diagonal element m_{gg}, become zero. Using the same method, we can then make all the elements of the $(g-1)$th column except $m_{g-1,g-1}$ transform into zero. Continuing with such transformations will finally transform all the elements m_{ij} ($i=1,2,\ldots,g$; $j=t+1,\ t+2,\ldots,g$) except for m_{jj} ($j \geq t+1$) into zero.

Thus

$$\det M(G)=\begin{vmatrix} \acute{m}_{11} & \acute{m}_{12} & \cdots & \acute{m}_{1t} & 0 & 0 & \cdots & \cdots & 0 \\ \acute{m}_{21} & \acute{m}_{22} & \cdots & \acute{m}_{2t} & 0 & 0 & \cdots & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \acute{m}_{t1} & \acute{m}_{t2} & \cdots & \acute{m}_{tt} & 0 & 0 & \cdots & \cdots & 0 \\ \acute{m}_{t+1,1} & \acute{m}_{t+1,2} & \cdots & \acute{m}_{t+1,t} & 1 & & & 0 & \\ \acute{m}_{t+2,1} & \acute{m}_{t+2,2} & \cdots & \acute{m}_{t+2,t} & & 1 & & & \\ \cdots & \cdots & \cdots & \cdots & & & & & \\ \cdots & \cdots & \cdots & \cdots & & 0 & & & \\ \acute{m}_{g1} & \acute{m}_{g2} & \cdots & \acute{m}_{gt} & & & & & 1 \end{vmatrix}, \quad (8)$$

where the magnitude of $\acute{m}_{ij}$ $(i=1,2,\ldots,g; j=1,2,\ldots,t)$ is equal to the number of possible paths which run down monotonously from the white vertex w_i $(i=1,2,\ldots,g)$ to the valley v_j $(j=1,2,\ldots,t)$, and the sign of $\acute{m}_{ij}$ is equal to $(-1)^{I_{ij}}$, where I_{ij} is the number of the diagonal edges in each path w_iv_j; obviously

$$\acute{m}_{ij} = w_{ij} \quad (i=1,2,\ldots,t; j=1,2,\ldots,t) \tag{9}$$

Hence,

$$\det M(G) = \begin{vmatrix} \acute{m}_{11} & \acute{m}_{12} & \cdots & \acute{m}_{1t} \\ \acute{m}_{21} & \acute{m}_{22} & \cdots & \acute{m}_{2t} \\ & & \cdots & \\ \acute{m}_{t1} & \acute{m}_{t2} & \cdots & \acute{m}_{tt} \end{vmatrix} = \begin{vmatrix} w_{11} & w_{12} & \cdots & w_{1t} \\ w_{11} & w_{12} & \cdots & w_{1t} \\ & & \cdots & \\ w_{t1} & w_{t2} & \cdots & w_{tt} \end{vmatrix}, \tag{10}$$

and so

$$|\det M(G)| = |\det W(G)| = |\det N(G)|. \tag{11}$$

This completes the proof of the theorem.

4. Applications

1. For the graph G shown in Fig. 3 the vertices are as labelled, and the matrix $M(G)$ is as follows.

$$M(G) = \begin{bmatrix}
0&0&0&1&1&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&1&1&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&1\\
0&0&0&1&0&1&1&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&1&0&1&1&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&1&0&0&0&1&1&0&0&0&0&0&0\\
0&0&0&0&0&0&1&0&0&0&1&1&0&0&0&0&0\\
0&1&0&0&0&0&0&1&0&0&0&1&0&0&0&0&0\\
0&1&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&1&0&0&1&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&1&0&1&1&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&1&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&1&1&1&0\\
1&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0\\
1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&1&0\\
0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&1
\end{bmatrix}. \tag{12}$$

From Eq. (5), we immediately obtain

$$K(G) = |\det M(G)| = |\det N(G)| = \begin{vmatrix} 16 & 1 & 6 \\ 2 & 2 & 1 \\ 1 & 0 & 2 \end{vmatrix} = 49.$$

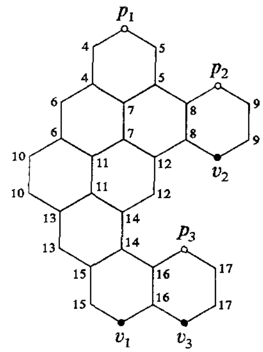


Fig. 3. Ordinal numbers of white and black vertices of a HF graph

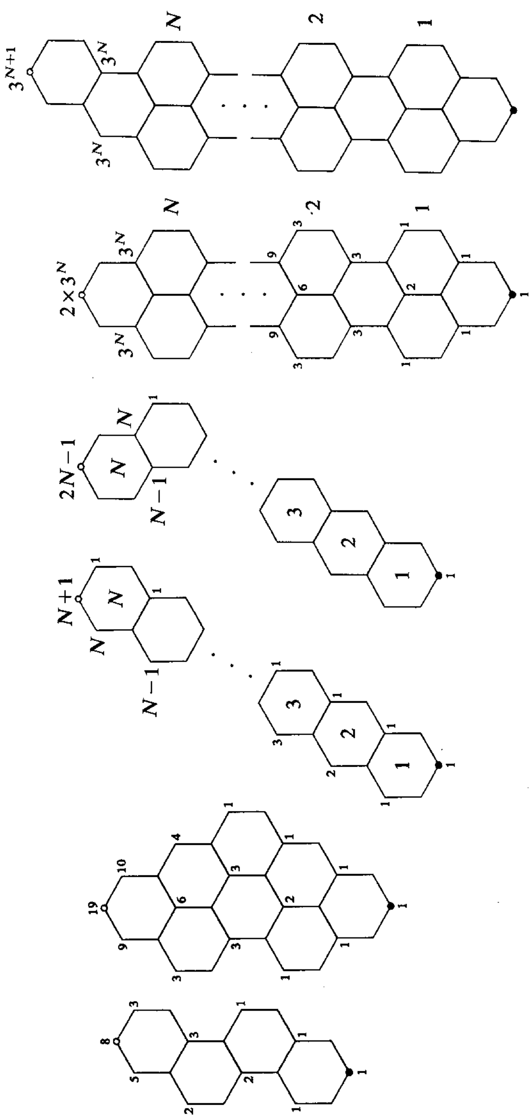
2. A KHF lattice is defined as a KHF graph in which there is a single dominant vertex (peak) and a single dominated vertex (valley). Examples of these are shown in Fig. 4, and the results are coincident with those given by Gordon and Davison [4], and Gutman [22].

3. For polymeric systems, such as the tetramer in Fig. 5a and the linear polymer made up of 5.6, 12.13-dibenzoperopyene monomeric units in Fig. 5b, we can easily obtain kekulé structure counts. For the former,

$$K_N(G)=\begin{vmatrix} 6 & 1 & & & & & & 0 & \\ 1 & 6 & 1 & & & & & & \\ & 1 & 6 & 1 & & & & & \\ & & \cdot & \cdot & \cdot & & & & \\ & & & \cdot & \cdot & \cdot & & & \\ & & & & \cdot & \cdot & \cdot & & \\ & & & & & 1 & 6 & 1 & \\ & 0 & & & & & 1 & 6 & 1 \\ & & & & & & & 1 & 6 \end{vmatrix} \tag{13}$$

while for the latter,

$$K_N(G)=\begin{vmatrix} 20 & 1 & & & & & & 0 \\ 1 & 20 & 1 & & & & & \\ & 1 & 20 & 1 & & & & \\ & & \cdot & \cdot & \cdot & & & \\ & & & \cdot & \cdot & \cdot & & \\ & & & & \cdot & \cdot & \cdot & \\ & 0 & & & & 1 & 20 & 1 \\ & & & & & & 1 & 20 \end{vmatrix}; \tag{14}$$


3^{N+1}
3^N
3^N
N
2
1
2×3^N
3^N
3^N
N
2
1
2N−1
N
N
N−1
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N+1
N
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N−1
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1
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10
9
8
5
3
2

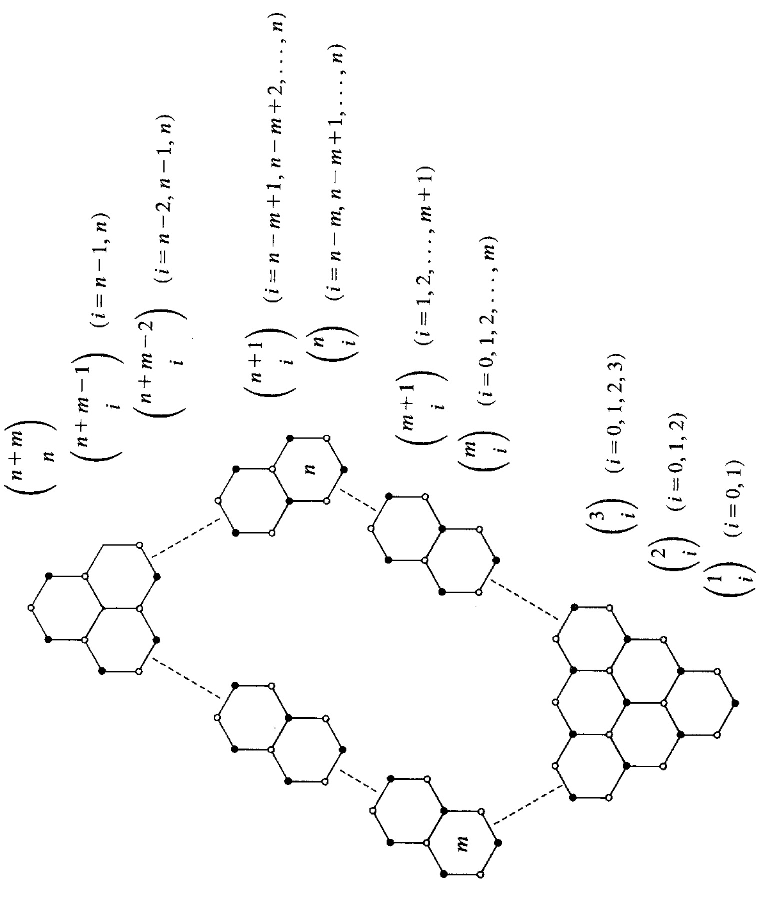

Fig. 4. Enumeration of Kekulé structures of KHF lattices

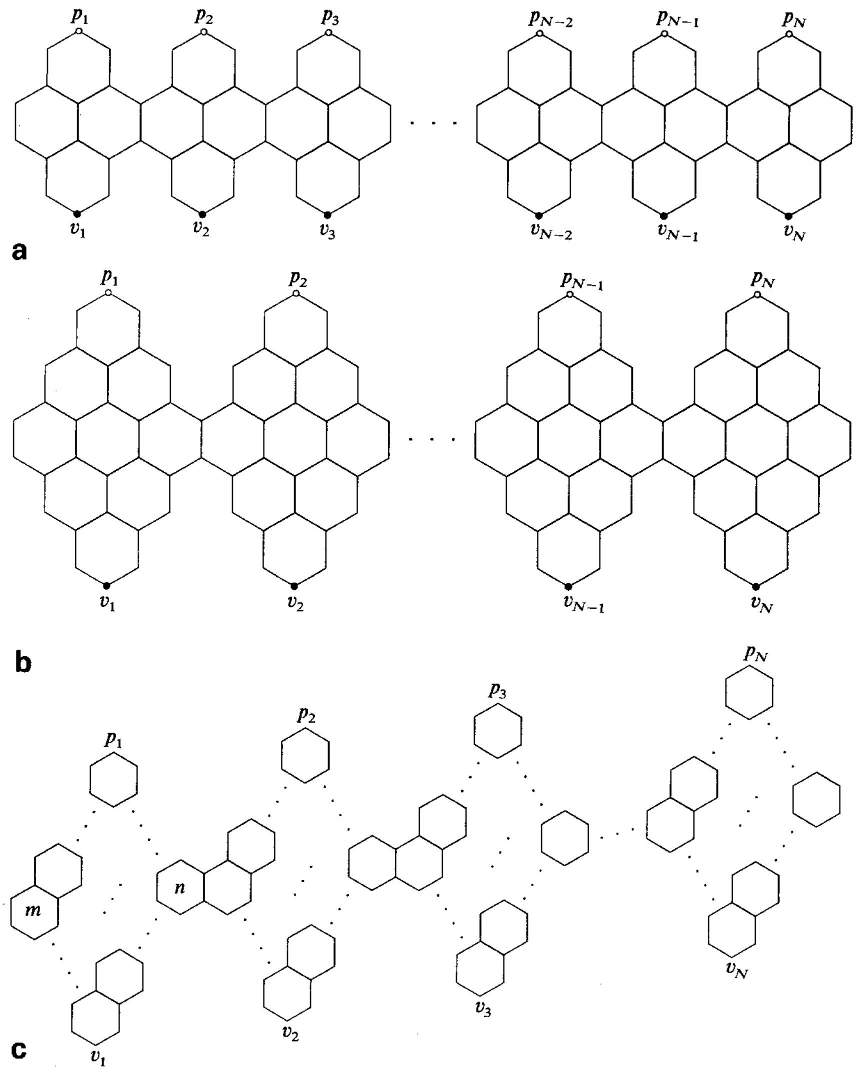

Fig. 5. Polymeric systems

the results are same as those in the literature [25, 33, 36, 40, 41]. From Eqs. (13) and (14) we can obtain the following recursion formulae [15, 34, 36]:

for Fig. 5a,

$$K_N(G) = 6K_{N-1}(G) - K_{N-2}(G) \qquad (N \geq 3), \tag{15}$$

and

$$K_1(G) = 6; \qquad K_2(G) = \begin{vmatrix} 6 & 1 \\ 1 & 6 \end{vmatrix} = 35,$$

while for Fig. 5b,

$$K_N(G) = 20K_{N-1}(G) - K_{N-2}(G) \qquad (N \geq 3), \tag{16}$$

and

$$K_1(G) = 20; \qquad K_2(G) = \begin{vmatrix} 20 & 1 \\ 1 & 20 \end{vmatrix} = 399.$$

In general, for the polymeric system shown in Fig. 5c

$$K_N(G) = \begin{vmatrix} \binom{n+m}{n} & 1 & & & & 0 \\ 1 & \binom{n+m}{n} & 1 & & & \\ & 1 & \binom{n+m}{n} & 1 & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & \cdot \\ & & & & \cdot & \cdot \quad \cdot \\ & 0 & & 1 & \binom{n+m}{n} & 1 \\ & & & & 1 & \binom{n+m}{n} \end{vmatrix}, \tag{17}$$

and

$$K_N(G) = \binom{n+m}{n} \times K_{N-1}(G) - K_{N-2}(G) \qquad (N \geq 3),$$

$$K_1(G) = \binom{n+m}{n}, \qquad K_2(G) = \begin{vmatrix} \binom{n+m}{n} & 1 \\ 1 & \binom{n+m}{n} \end{vmatrix} \tag{18}$$

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