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## THE ROLE OF BINARY AND TERNARY SYSTEMS IN PROTEIN STUDIES

### Summary

Various aspects of binary, ternary, quaternary, quinary, and senary structures for alloys, polymers and, in particular, proteins are studied. We refer to quinary and senary structures in some polymers indicating the role of total energy maxima in the infrared and Raman activity energy spectra. Decomposition of quinary structures to ternary structures is discussed. A complex analytical method of binary and ternary Galois extension is proposed as well as its realization in terms of Riemann surfaces. Slightly wavy behaviour of the system of hexagons in a polymer leaf is investigated.

*Keywords and phrases:* binary physical structure, ternary physical structure, quaternary physical structure, quinary physical structure, senary physical structure, alloy, pentacene, polymer, protein, peptide, amino acid, Galois extension, Riemann surface

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## Introduction and aim of the paper

We are studying various aspects of binary, ternary, quaternary, quinary, and senary structures for alloys, polymers and proteins. In particular, we refer to quinary and senary structures in some polymers indicating the role of total energy maxima in the infrared and Raman activity energy spectra [6, 18]. Decomposition of quinary structures to ternary structures is discussed.

Next we apply complex analytical method of binary and ternary Galois extension. Then we realize the Galois extensions in terms of Riemann surfaces. Slightly wavy behaviour of the system of hexagons in a polymer leaf is investigated.

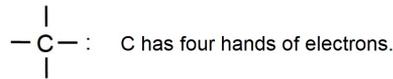
## 1. Basic facts about polymers

We recall the basic facts about polymers which supply bases of our observations:

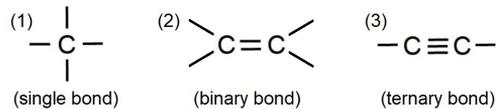
- (i) the binary and ternary bond structure of atoms of carbon, C;
- (ii) classification of polymers.

- (i) The binary and ternary bond structure of atoms of carbon

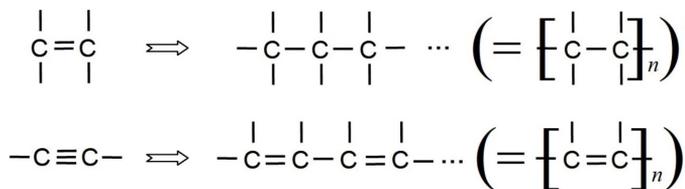
At first we notice the electronic structure of carbon:



We have the following three types of monomers of carbon:



We have the following polymers

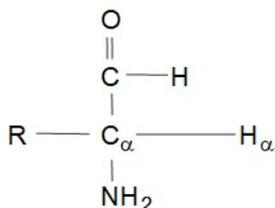


- (ii) Classification of polymers

We may classify polymers in the following manner:

- (1) Polymers of linear type





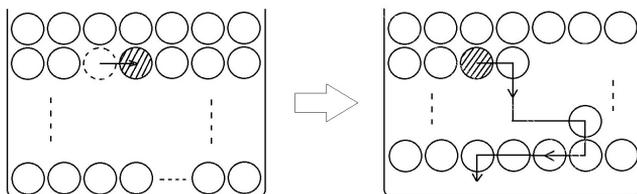
We have two basic structures of amino acids: linear and cylindrical. The cylindrical contain pentagonal, hexagonal or both pentagonal and cylindrical ring of carbons or carbon and nitrogen. The linear ones do not contain any "rings". The examples of amino acids are shown in Fig. 1.

## 2. de Genne theory on polymers

The most important part of de Genne theory on polymer physics can give the distribution with of power law in polymer physics. In the traditional physics and statistic the distribution of exponential type appears commonly, for example simple random walk, Brownian motion, and Maxwell distribution in statistic mechanics. de Genne has introduced the concept of self-avoiding random walk (= s.a. random walk) [2] and obtained the distribution of power law type for polymers.

Here we state his idea briefly.

Let us consider a large box filled with balls of the same size without free space.



(i) We choose a reference ball  and move it to the right. Then the left space of the ball is filled with another ball. Hence we can move it to the right. The move to other directions can be performed in the same manner.

(ii) Repeating the process, the ball  can make a random walk in the lattice.

Next let us consider a polymer composed of several (long) monomers with two hands, for simplicity sake:



Here we assume the polymer is easily bent. Then it makes a similar move to that of monomers but it cannot make self-interactions. Hence it makes a self-avoiding random walks.

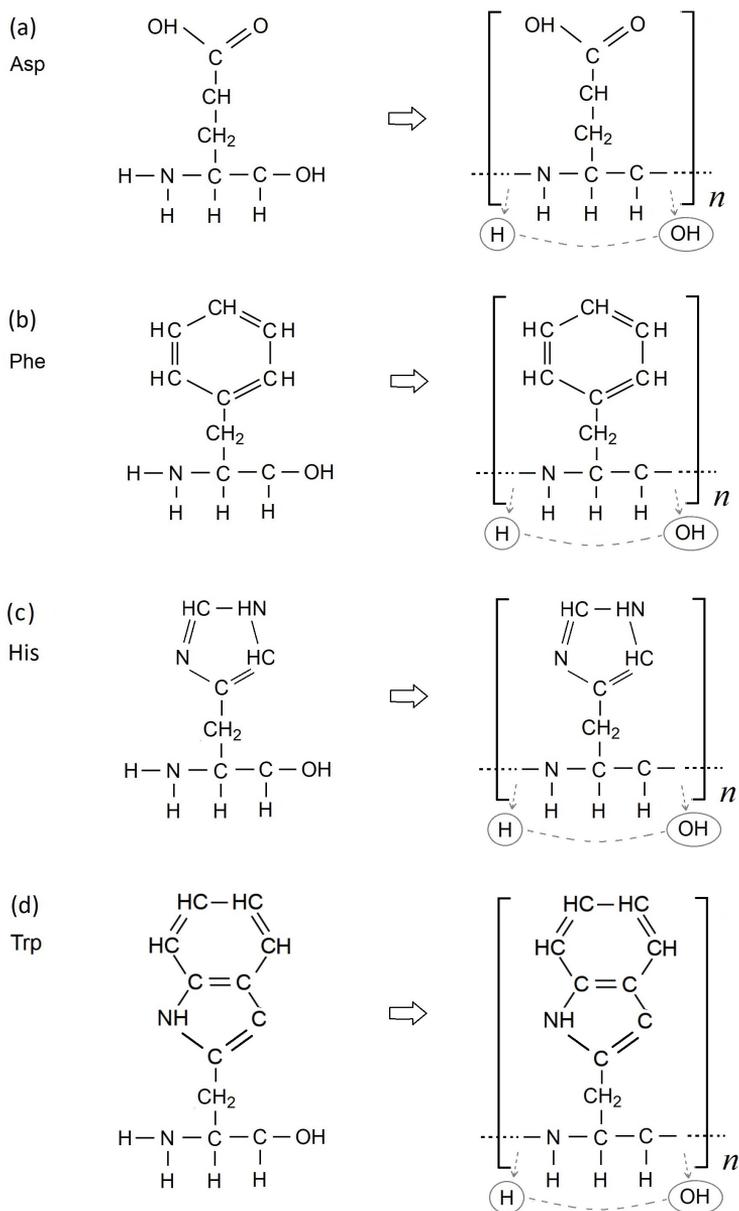


Fig. 1. Examples of aminoacids (on the left) and their polymerization (on the right) (a) linear, (b) cylindrical with hexagonal ring, (c) cylindrical with pentagonal ring, (d) cylindrical with both pentagonal and hexagonal ring. During the process of polymerization  $H_2O$  is produced.

### 3. Total energy maxima; infrared and Raman energy activity maxima their structural role in the molecular motors

Total energy calculations for polymers as well as infrared and Raman energy activity already have been discussed in our previous papers [6, 4]. We have to take into account the economizing of energy caused by zigzags, meanders and wavy soliton-like structures. A good account on the role of these aspects of total energy calculations can be found in [1].

An important element of the corresponding comparison of the procedure of the quoted energy is their rescaling connected with fixing each of the main two maxima at the same point (Fig. 2).

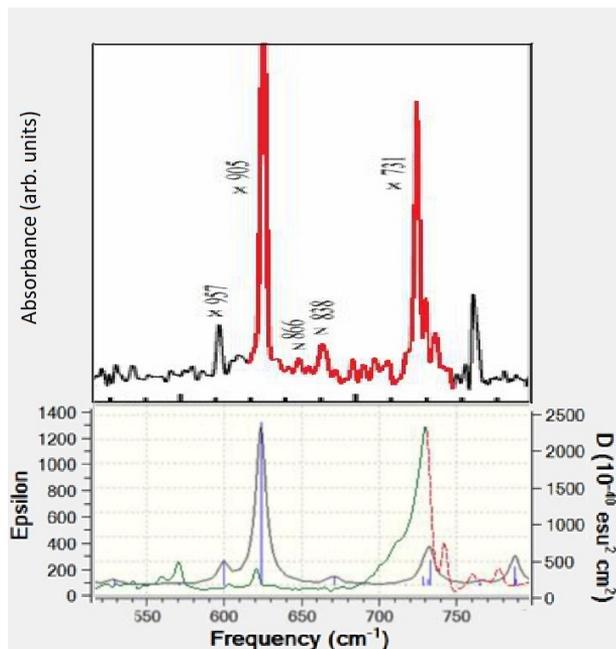


Fig. 2. Total energy (absorbance) vs infrared activity of pentacene molecule thin film after rescaling according to the sharp maxima points, cf. [18], Figs. 4, 5, 6.

### 4. Complex analytical method for polymers

We propose a complex analytical method for polymers and determine polymers of planar type. The basic idea can be stated as follows:

- (1) First we realize the binary and ternary bonds of carbon C on a ramified covering

over  $\mathbb{P}^1$ .

- (2) Next we shall realize the process from monomers to polymers by use of the universal covering of the Riemann surface in (1).
- (3) Analyzing the process (2) we can determine the polymers.

We shall describe each step in the successive subsections separately.

#### 4.1. The realization of binary and ternary bonds by Galois extensions as Riemann surface

We begin with recalling basic Riemann surfaces and try to associate the binary and ternary bonds of monomers to Riemann surfaces.

By binary (ternary) non-commutative Galois extension  $\mathcal{A}(z)$  of the algebra  $\mathcal{A}$  we mean the following

$$\mathcal{A} \implies \mathcal{A}(z), \quad z \notin \mathcal{A},$$

where  $z^2 \in \mathcal{A}$  ( $z^3 \in \mathcal{A}$ , resp.), and where the algebra  $\mathcal{A}$  need not be commutative [7, 8, 9]. We can observe the correspondence between Galois extensions of algebras and chemical structures of both polymers and proteins (c.f. [4]). We can construct polymers from the Galois extension in the following way. The classical Galois extension can be described in terms of the root of polynomials:

$$f(x) = 0.$$

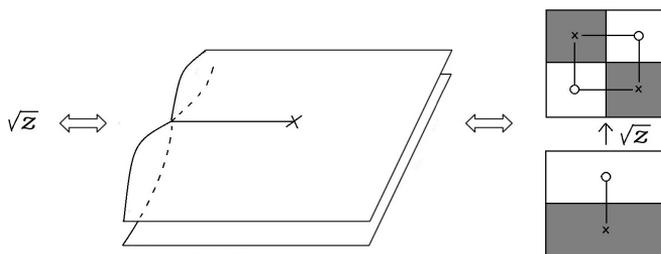
We can realize the roots by a Riemann surface defined by

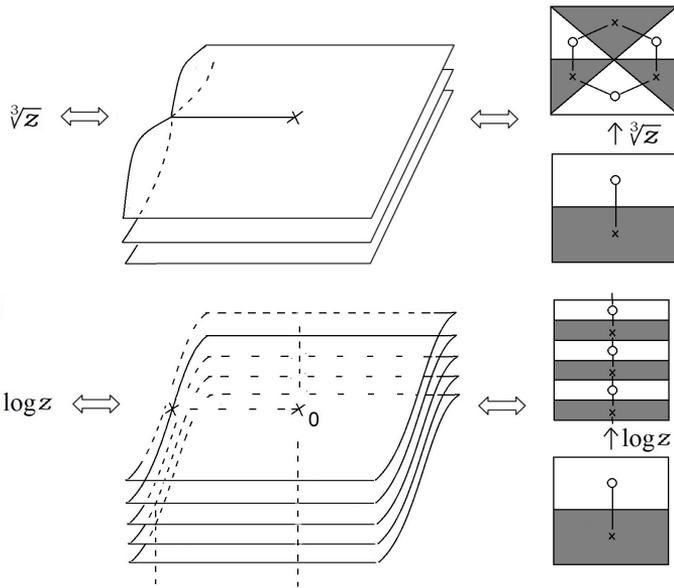
$$y = f(z).$$

In order to realize the solvable group we see that the Riemann surface can be generated by the binary and ternary covering surface:

$$\sqrt{z-a}, \quad \sqrt[3]{z-b}.$$

We can realize Galois extensions in the form of Riemann surfaces as can be shown in the diagrams below:



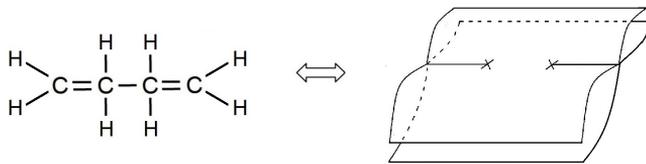


Here we will try to associate the binary and ternary bonds of monomers to these coverings:



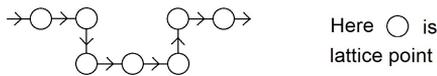
We may expect to associate more general monomers to more general Riemann surfaces.

**Example (Butaine)**

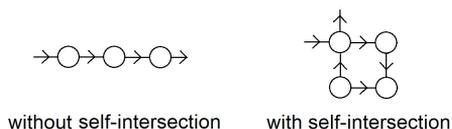


**4.2. Construction of a self-avoiding path in the universal covering**

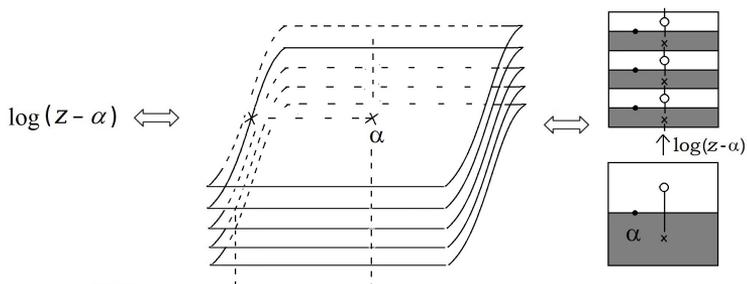
We have observed that a self-avoiding path can be identified with a path of the form:



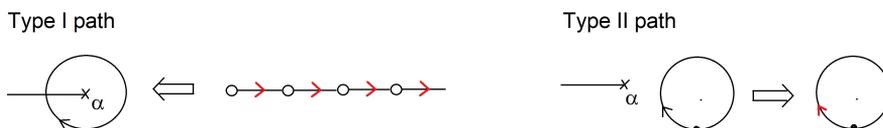
The path is connected with indefinite number of line segments. On the other hand we have an arbitrary path which includes a closed path as a subpath, for example



We can make a difference between these two kinds of paths in the universal covering Riemann surface. For this we choose a point  $\alpha \in \mathbb{C}$  and make the infinite covering of the form:  $w = \log(z - \alpha)$ :

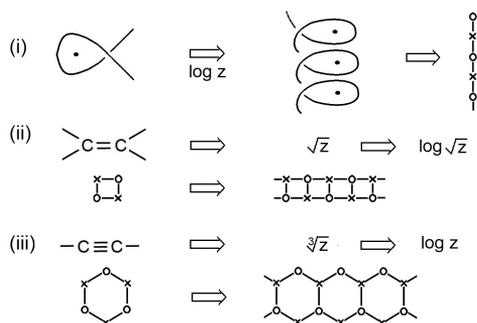


We classify the paths into two types depending on whether it surrounds  $\alpha$  or not, which shall be called Type I or Type II, respectively. In the case of Type I path we can make a polymerization, and remain unchanged for Type II path.



Hence we can associate a self-avoiding path to Type I and that of general type to Type II.

We can realize self-avoiding paths or polymerisation in the universal covering in the following manner:



**Remark.** We may expect to realize the polymerizations of planar type by the Schwartz-Christoffel mapping:

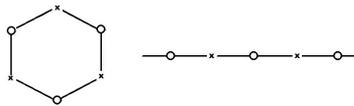
$$\begin{array}{ccc}
 \begin{array}{|c|c|} \hline \alpha_4 & \alpha_3 \\ \hline \alpha_1 & \alpha_2 \\ \hline \end{array} & \Rightarrow & \int^z \frac{dz}{(z-\alpha_1)(z-\alpha_2)(z-\alpha_3)(z-\alpha_4)} \Rightarrow \begin{array}{|c|c|c|c|} \hline \times & \times & \times & \times \\ \hline \times & \times & \times & \times \\ \hline \times & \times & \times & \times \\ \hline \times & \times & \times & \times \\ \hline \end{array}
 \end{array}$$

### 4.3 The determination of polymers of planar type

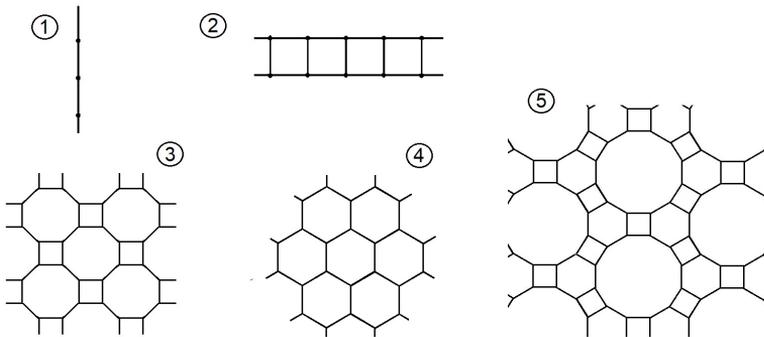
Using the observations given in Section 4.2 we can list up the polymers of planar type with binary and ternary bonds by the use of the following

**Theorem.** For finite or infinite coverings with  $q$ -branch points we have the following diagram which is defined by the deck-transformation in the case of  $q=2$  or  $q=3$ : (Let us pay our attention to the appearance of the binary and ternary structures [10])

(1)  $q = 2$



(2)  $q = 3$



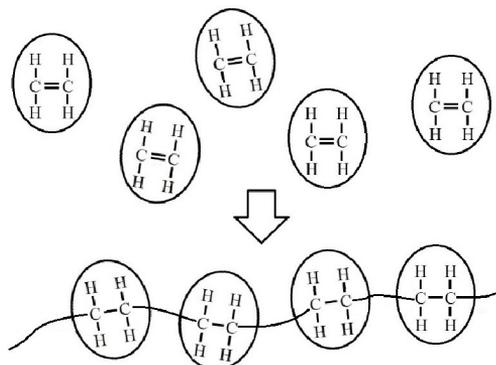
① Polyacetylene ② Magnetic body ③ Zeolite ④ Graphite ⑤ Zeolite?

## 5. The generation and decomposition problems of complex systems of polymers and alloys

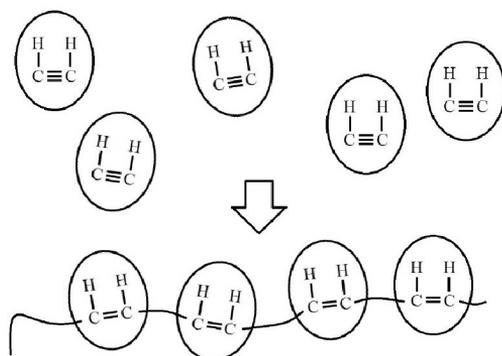
In this section we shall consider the complex systems which are generated by monomers and discuss the basic problems:

- (1) The generation problems
- (2) The decomposition problem

I. Binary extension type



II. Ternary extension type



III. Binary / ternary mixed type

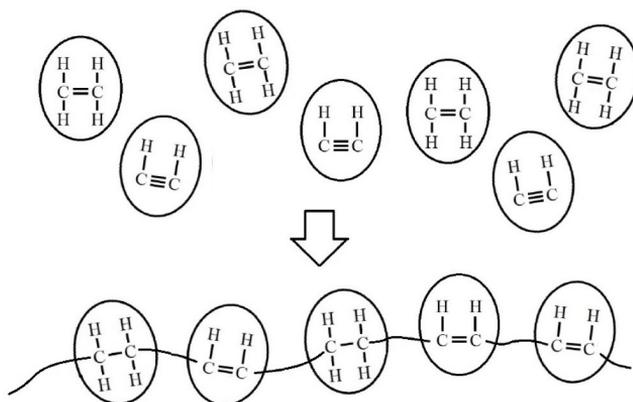
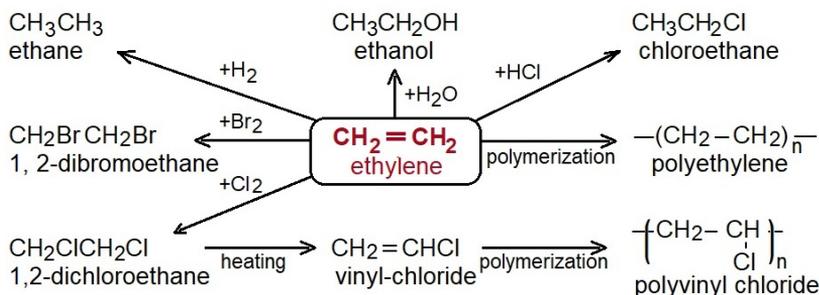


Fig. 3. Polymer structures involving binary, ternary, and both binary and ternary elements together (cf. [18]).

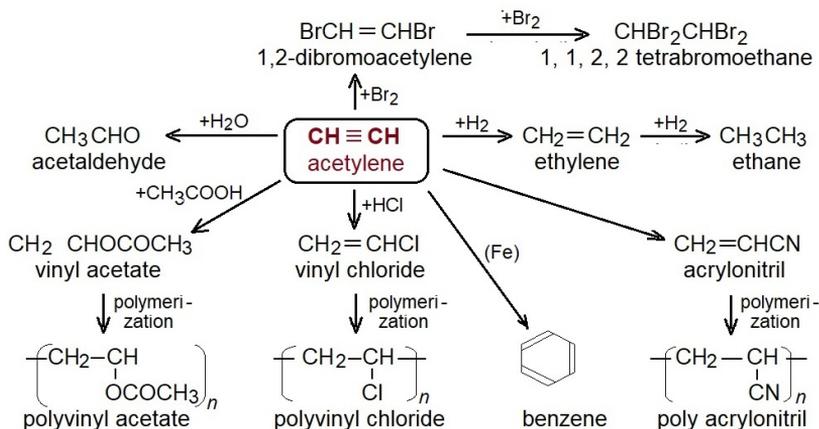
## 5.1 Generation problems

Here we will describe the generation of hydrocarbon polymers of linear type in terms of binary extensions. We begin with examples of binary, ternary generation of polymers as seen in Fig. 3. Next we proceed to the generations of monomers and polymers. We give two generation families:

### Examples of ethylene family



### Examples of acetylene family



Then we can propose the following problems:

**Problem 1.** How can we generate hydrocarbon polymers of general type from (1) methane, or (2) ethylene, or (3) acetylene?

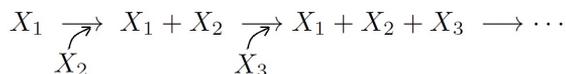
**Problem 2.** How can we generate polymers of general type by polymerizations of monomers in the answers of problem 1?

We will treat this problem by the use of binary and ternary and their successive non-commutative Galois extensions. For example, we may check the BTBB-structure of the structure. Namely, we may check whether there exists or not a sequence of the following extensions:

$$B_1 \rightarrow T_1 \rightarrow B_2 \rightarrow B_3,$$

where  $B_i$  ( $T_1$ ) denote the binary (ternary, respectively) extension,  $i = 1, 2, 3$ .

We notice that we can describe the polymerization by successive binary extensions. We choose a sequence of monomers:  $X_1, X_2, \dots, X_n, \dots$  and make a polymer by the successive binary extensions:

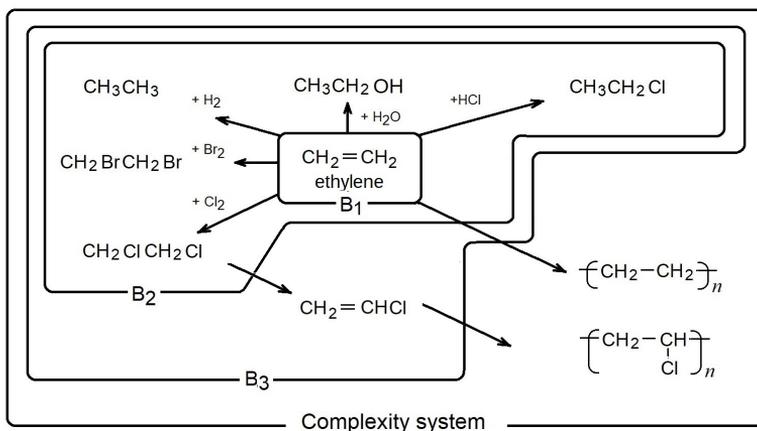


Here we will construct the BTBB-structure for the hydro-carbon polymers/monomers. We follow the scheme of evolutions in [16].

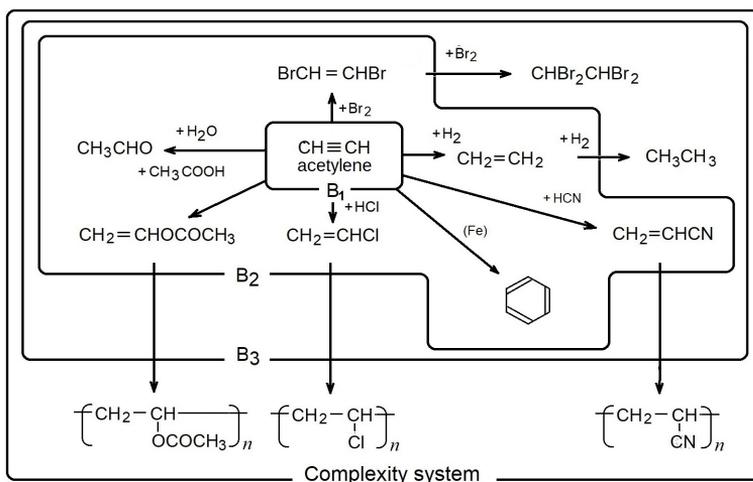
(0) We choose  $\{C, H\}$  as the seeds. (1) We choose the binary extension  $B_1$  as the ethylene. (2) We choose the ternary extension  $T_1$  as the acetylene. (3) We choose the successive binary extensions  $B_2, B_3$  as the generations on the ethylene and acetylene family. This might be the construction of the BTBB structure. (4) We may associate the complexity structure to the polymers.

Then we can find partial answers to the problems posed on the base of the given families:

### The BTBB and its complexity system of ethylene



### The BTBB and its complexity system of acetylene



**Remark.** The polymers which appear in biology are completely different from the hydro carbon type polymers. Also polymers including Si (including C of diamonds) may be of another type. Hence we can propose the problem:

**Problem 3.** Classify polymers.

## 5.2 The decomposition problem for quinary and senary structures of polymers and proteins

Here we discuss the decomposition problem which is converse of the generation problem.

In connection with the reduction procedure of quinary and senary structures to binary and ternary structures resp. we may consider polymer structures involving quinary and senary structures together and decompose them to structures involving binary and ternary elements together (Fig. 3). In case of proteins we have four different atoms: carbon C, hydrogen H, nitrogen N, oxygen O and sometimes sulfur S. It seems impossible to reduce proteins to binary and ternary structures but rather to ternary and quaternary structures. Nonion and duodevicienion algebras are of help to describe this situation [11, 12, 13].

## 6. An outlook of complex systems/foliations determined by polymers and alloys

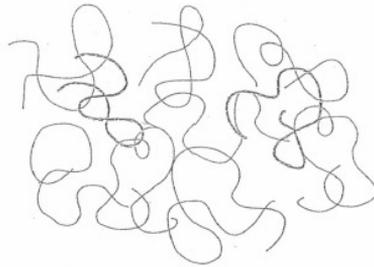
Here we discuss the complex systems of polymers and alloys.

- (1) The basic structure of the distribution of polymers.

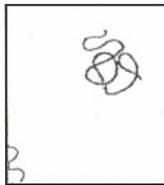
- (2) The complex analytical description of the distributions.
- (3) The foliations determined by polymers and alloys.

### 6.1 The basic structure of the distribution of polymers

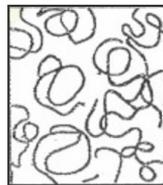
(1) de Genne theory tells that the polymers make self-avoiding random walks and their distribution is given by power law



(2) The entropy of the states of polymers plays essential roles in the description of the states.



(a) dilute solution



(b) critical solution



(c) concentrated solution



random coil molecule

(3) Polymers constitute knots/braid structures

$\alpha$  - spiral structure



$\beta$  - structure



collagen 3-line spiral



Here we notice that we may expect to describe the structure in terms knots/braid structure. In fact, we know the binary and ternary structures in the generation of knots/braides by Reidemeister moves. Comparing the structures in proteins and those of knos/braids, we may find binary and ternary structures in the complex structures of proteins.

Binary and ternary structures

Reidemeister I move	?	$\alpha$ -spiral structure
Reidemeister II move	$\iff$	$\beta$ -structure
Reidemeister III move		collagen 3-line spirals

**6.2 The complex analytic description of the distribution**

Finally we will give explicit descriptions of the distributions in terms of complex analysis. We can show that the distribution gives the solutions of differential equation of Fuchsian type. The solution gives regular singularities which may give the critical exponents of the original distributions [15].

We give several examples:

$$\begin{array}{l}
 \circ - \circ - \circ - \circ - \circ \iff \int^z \frac{dw}{w} \\
 \begin{array}{c} \circ - \circ - \circ - \circ - \circ \\ \circ - \circ - \circ - \circ - \circ \end{array} \iff \int^z \frac{dw}{\sqrt{1-w^2}} \\
 \begin{array}{c} \circ - \circ - \circ - \circ - \circ \\ \circ - \circ - \circ - \circ - \circ \\ \circ - \circ - \circ - \circ - \circ \end{array} \iff \int^z \frac{dw}{\sqrt{1-w^4}}
 \end{array}$$

We may expect that the integral function  $\int^z f(w)dw$  gives the distribution of the paths of self-avoiding random walks. We notice that  $z$  gives the parameter of the paths.

This will be discussed in detail in another paper.

**6.3 Foliations determined by polymers and alloys**

In analogy to Section 3 we may consider left and right twisted leaves in one foliation characterizing more complex situation in the polymer or protein concerned (see Fig. 4).

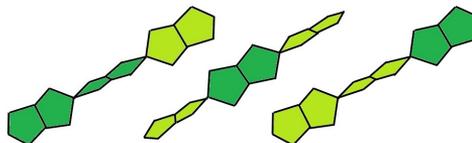


Fig. 4. Left and right twisted leaves in a polymer structure foliation.

## Perspectives for further research

The perspectives for further research in the context of this paper are going in the direction of generalizing, similarly to [4] in the direction of replacing binary and ternary components by quaternary and quaternary ones involving, besides of C and H, also N, O and S. The mathematical part of the pattern requires separation theorems concerning ternary and quaternary structures in terms of composition formulae developed in [11, 12, 13].

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## **ROLA SYSTEMÓW BINARNYCH I TERNARNYCH W BADANIU BIAŁEK**

### **S t r e s z c z e n i e**

Rozważamy rozmaite aspekty struktur binarnych, ternarnych, kwaternarnych i senarnych dla stopów, polimerów i protein. W szczególności odnosimy się do struktur kwinarnych i senarnych w niektórych polimerach wskazując na rolę maksimów energii w spektrach podczerwieni i aktywności Ramana. Dyskutujemy rozkład struktur kwinarnych do ternarnych. Proponujemy zespoloną metodę analityczną dla binarnych i ternarnych rozszerzeń Galois, jak również ich realizację na powierzchniach Riemanna. Omawiamy lekko falujące zachowanie układu sześciokątów w liściu polimeru.

*Słowa kluczowe:* binarna struktura fizyczna, ternarna struktura fizyczna, kwaternarna struktura fizyczna, kwinarna struktura fizyczna, senarna struktura fizyczna, stop, pentacen, polimer, białko, peptyd, aminokwas, rozszerzenie Galois, powierzchnia Riemanna