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B U L L E T I N

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Dedicated to the memory of
Professor Leszek Wojtczak

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MATHEMATICS BEHIND TWO RELATED NOBEL PRIZES 2016: IN PHYSICS - TOPOLOGY GOVERNING PHYSICS OF PHASE TRANSITIONS, IN CHEMISTRY GEOMETRY OF MOLECULAR NANOENGINES

Summary

Pentacene and other polymers are discussed form the point of view of theoretical discoveries of topological phase transitions and phases of matter (Nobel Prize in Physics 2016) and for the design and synthesis of molecular nanoengines (Nobel Prize in Chemistry 2016), in particular, the changes of senary to quinary structures and vice versa.

Keywords and phrases: topological phase transition of matter, topological phase of matter, molecular nanoengine, pentacene, polymer, pentagonal (quinary) structure, hexagonal (senary) structure

Contents

Introduction and aim of the paper

We are dealing with mathematical aspects of two recent Nobel prizes 2016 in physics and chemistry, respectively. The Nobel Prize in Physics 2016 was awarded to D. J. Thouless, F. D. N. Haldane, and J. N. Costerlitz [37] for theoretical discoveries of topological phase transitions and topological phases of matter. The Nobel Prize in Chemistry 2016 was awarded to J.-P. Sauvage, Sir J. Frazer Stoddart, and Bernard L. Pheringa [32] for the design and synthesis of molecular machines.

We study mathematical aspects of these properties in some pentagonal (quinary) and hexagonal (senary) structures, in pentacene and some other polymer structures, in particular the rapid changes of hexagonal (senary) structures to pentagonal (quinary) structures and vice versa. We discuss also the leaves foliation structure of the objects in question on a silicone background and a slightly wave solitary behaviour of the leaves.

1. Choosing suitable algebras and controlling non-commutativity

Our basic tools for choosing as an algebra suitable for a Dirac-like particle motion equation are:

1) the Cayley-Dickson process

$$\mathbb{C} = \mathbb{R} \oplus \mathbb{R}i \ \ \mathbb{H} = \mathbb{H} \oplus \mathbb{H}j, \ \ \mathbb{O} = \mathbb{H} \oplus \mathbb{H}\ell, \ \ \mathbb{S} = \mathbb{O} \oplus \mathbb{O}p, \ \ etc.,$$

where they i, j, ℓ, p are proper units,

2) passing form the complex algebra to a binary and then to a ternary Clifford algebra [17, 36],

3) passing from the cubic algebra to 3×3-matrix, quaternion-like algebra and then to 3×3-matrix octonion-like algebra [35, 31, 11, 20],

4) passing form the 3×3-matrix quaternion-like algebra to the nonion algebra, and then, to the duodevicenion algebra [24, 26, 27, 28].

The first two procedures are closely related to an idea of M. Planck (1900) of controlled noncommutativity: if Q is the operator of positon, and P operator of momentum, then already for quaternions, where we are loosing commutativity, it is natural to demand that

$$PQ - QP = nhI_n, \ \ n \in \mathbb{Z}, \tag{1}$$

and I_n being the $n \times n$ unit matrix and n being a positive small constant. In the physical reality it is indispensable to take $h \approx 6.626 \cdot 10^{-34} J \cdot s$.

The second two procedures are closely related to the idea of Sylvester

$$PQ - \lambda QP = 0, \quad \lambda \in \mathbb{C} \tag{2}$$

instead of (1).

2. The binary ternary quaternary structure correspondences

As far as the correspondence of binary and ternary structures is concerned, the main idea is explained in [23](cf. Fig. 5): 18 triangles of the basic region in the fractal representation may be groupped as two collections of three equivalent triangles or, equivalently, by three collections of two equivalent triangles [21, 22].

Now passing from the complex to quaternion algebra is connected with taking $\lambda^2 = 1$ in (2), yet taking $\lambda^3 = 1$, $\lambda \neq 1$ we arrive at the construction of the cubic algebra, nonion algebra, and duodevicenion algebra (18 generators), cf. Fig. 10 in [20], where $\mathbf{j}^3 = 1$, $j \neq 1$. The passage

$$\text{cubic algebra} \leftrightarrow \text{nonion algebra} \leftrightarrow \text{duodevicenion algebra}$$

corresponds to the passage [24]

$$\text{binary structures} \leftrightarrow \text{ternary structures} \leftrightarrow \text{quaternary structures.}$$

It is important to notice that, mathematically, the passages of (3×3)-matrices algebras:

$$\text{quaternion-like algrebras} \to \text{octonion-like algebras}$$

and

$$\text{nonion algebra} \to \text{duodevicenion algebra}$$

are related with $1/2\pi$ turn around the origin transformation

$$a^{\alpha\beta} = a^{\beta,4-\alpha}, \quad \alpha, \beta = 1, 2, 3,$$

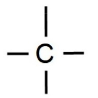
$\alpha, \beta = 1, 2, 3$, which in an elegant way may be visualized on the four sheeted or two-sheeted Riemann surface models [20], Figs 8 and 9.

3. Passing from a hexagonal (senary) structure to a pentagonal (quinary) structure in a molecular nanoengine

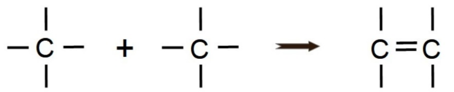
In contrast to a ternary structure, where the passage to a binary structure might be a purely mathematical construction, in case of pentacene Fig. 3 in [6], Fig. 2 in [33] and some other polymers this might be connected with drastic passage of hexagonal to pentagonal structure in a high energy in the molecular nanoengine. There are several possibilities for a new pentagonal structure [6] which arises with some probability [8] and the opposite change from a pentagonal to hexagonal structure if possible as well because the absorbance representing the total energy has two closely related nearby sharp maxima, Fig. 2 in [6], Fig. 4 in [33].

The same situation is connected with the infrared activity (Fig. 5 in [33] and Raman activity Fig. 6 in [33]). For polymers (which of course include pentacene) we have a general problem of evolution of binary and ternary systems, namely, de Gennes developed the theory on polymers [1]. The main idea is the scaling assumption on the distribution of polymers. The heart of the theory is the application of the self-avoiding random walk.

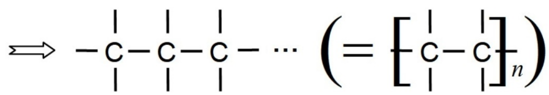
In this connection let us first notice the electronic structure of carbon:



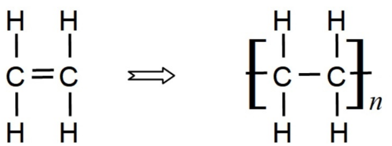
Considering binary bonds of carbon:



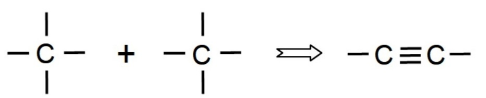
In this way we obtain a polymer



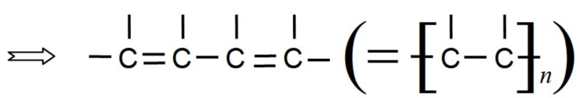
and below we have an example



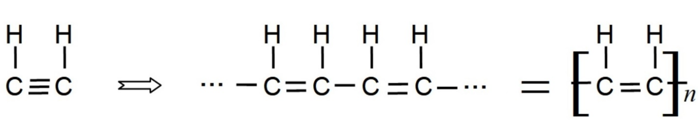
Considering ternary bonds of carbon:



In this way we obtain a polymer



and below we have an example



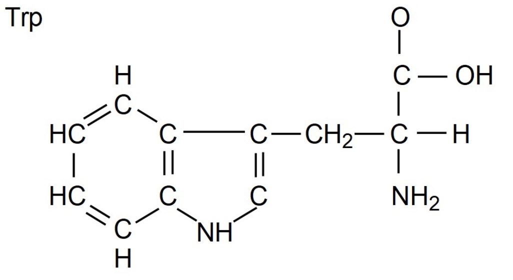


Fig. 1. Tryptophane amino acid having both pentagonal and hexagonal subsystems.

We have

Theorem 1. *In polymers we have either binary or ternary bonds. (koniec 9-3) The binary and ternary extension type leading to polymer are shown in Figs 7 and 8, respectively, in* [33].

In such a way a quinary subsystem in a polymer can easily be decomposed into binary systems and a senary subsystem can be easily decomposed into ternary systems. The situation becomes more complicated in some proteins, where we have both a pentagonal and hexagonal subsystems. Then the problem of decomposition becomes more complicated and requires further investigation.

4. Zigzags, meanders, and solitary leaves of the polymer foliation

Within the structure of polymer and its leaves often starting with a silicone background (e.g. SiO_2 [33]) one may observe the sine-like or cosine-like soliton behaviour which affects the whole foliation.

It is interesting to notice the foliations with left-twisted and right-twisted leaves. Fig 2 and cf. Figs 11 and 13 of [33].

Solitary equations of the mentioned leaf borders will be developed in a future research.

Perspectives for further research

It seems important to analyze for a given polymer with a hexagonal structure a possibility of the corresponding pentagonal structures. The other important direction is to find within pentagonal and hexagonal structures those that can be reduced to the binary structures only or to ternary structures only.

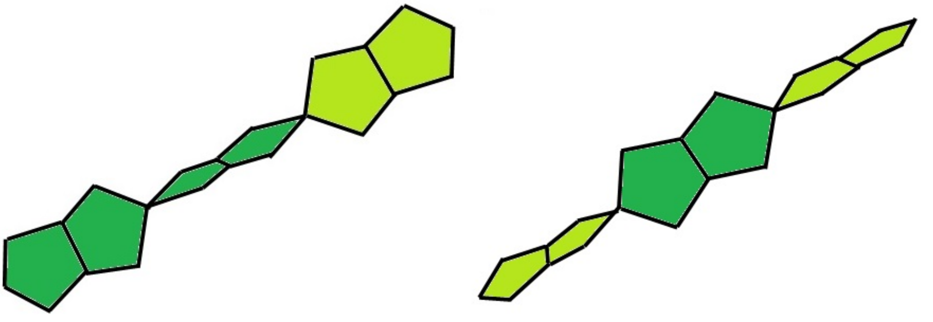


Fig. 2. Left and right twisted foliation pentacene leaves.

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MATEMATYCZNE ZAPLECZE DWÓCH POWIĄZANYCH ZE SOBĄ NAGRÓD NOBLA Z ROKU 2016: Z FIZYKI TOPOLOGIA STANOWIĄCA PODSTAWĘ FIZYKI PRZEJŚĆ FAZOWYCH; Z CHEMII - GEOMETRIA MOLEKULARNYCH NANOSILNIKÓW

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

Praca omawia pentacen i inne polimery z punktu widzenia topologii stanowiącej podstawę fizyki przejść fazowych i stanów materii (nagroda Nobla z fizyki w 2016r.) oraz ukształtowania i syntezy silników molekularnych (nagroda Nobla z chemii w 2016r.), a w szczególności, zmiany struktur senarnych w kwinarne i odwrotnie.

Słowa kluczowe: topologiczne przejścia fazowe materii, fazy topologiczne materii, molekularne nanosilniki, pentacen, polimer, struktura pięciokątna (pentagonalna), struktura sześciokątna (hexagonalna)