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Dedicated to the memory of
Professor Yurii B. Zelinskii

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SOME GEOMETRICAL ASPECTS OF BINARY, TERNARY, QUATERNARY, QUINARY AND SENARY STRUCTURES IN PHYSICS

Summary

It is observed that quinary and senary structures like in pentacene and several other polymers may be composed from binary and ternary structures in the sense of differential-equational and geometrical description. In the case of pentacene its leaves are attached to the silicon background and have the form of five connected carbon-hydrogen hexagons; in total they do not form the precisely planar structure but a slightly wavy structure which minimizes total energy. In the case of a quinary structure the leaves form solitary, nearly periodical zigzags and meanders.

Keywords and phrases: finite-dimensional algebras, associative rings and algebras, binary physical structure, ternary physical structure, quinary physical structure, senary physical structure, pentacene, polymer

Contents and introduction

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6. Zigzag or meander soliton behaviour of a twisted structure of pentagons in a pentacene leaf. The sine-like case
7. An analogue of a pentacene structure in the cosine-like case
8. Pentacene as a foliated manifold with a soliton behaviour of leaves

This paper in some sense is a continuation of the paper [3] by E. Z. Frątczak, J. Ławrynowicz, M. Nowak-Kępczyk, H. Polatoglou, L. Wojtczak and [7] by J. Ławrynowicz, M. Nowak-Kępczyk, and O. Suzuki.

1. Quinary and senary structures in pentacene and several other polymers

When looking at formulae for chromophore P in the elongated form (A, B) and the cyclic form (C, D): A,C – Pr, B,D–Pfr, where Pr and Pfr are red-absorbing (infra-red-absorbing) forms of phytochrome, respectively (Fig. 1, cf. [1, 2, 6, 10]) we can see a quinary structure together with a senary structure.

In the case of pentacene in the usual form $C_{22}H_{14}$ (Fig. 2) where C stands for the carbon atom, H for hydrogen atom, a thin film of pentacene forms almost co-planar leaves consisting of five pentagons with each pair having one side of the vertices of hexagons in common, attached as the whole structure to the silicone SiO_2 substrate. An example of a quinary structure in principle possible for pentacene is shown in Fig. 3. There are two basic forms of position of pentacene leaves with respect to substrate, as shown in the figure.

2. The role of total energy maxima for the infrared and Raman activity energy spectra

When changing the wave number we meet two sharp energy maxima (Fig. 4) which may serve for the corresponding nanomolecule as the nanomotor where the original energy structure is changed to a quinary structure (cf. J. -P. Sauvage, Sir J. Fraser Stoddart, and B. L. Feringa [11]), more precisely, for a structure of leaves corresponding to Fig. 3.

Looking more carefully, when changing the wave number in both infrared and Raman activity energy spectra (Figs 5 and 6) we meet again two sharp maxima which may serve for the corresponding nanomolecule as nanomotors where the original senary structure has changed into a quinary structure according to the formulae [3]:

$$xC_{22}H_{14} + zH_2 \leftrightarrow yC_\xi H_\eta, \tag{1}$$

where x, y, ξ, η are positive integers and z is an integer.

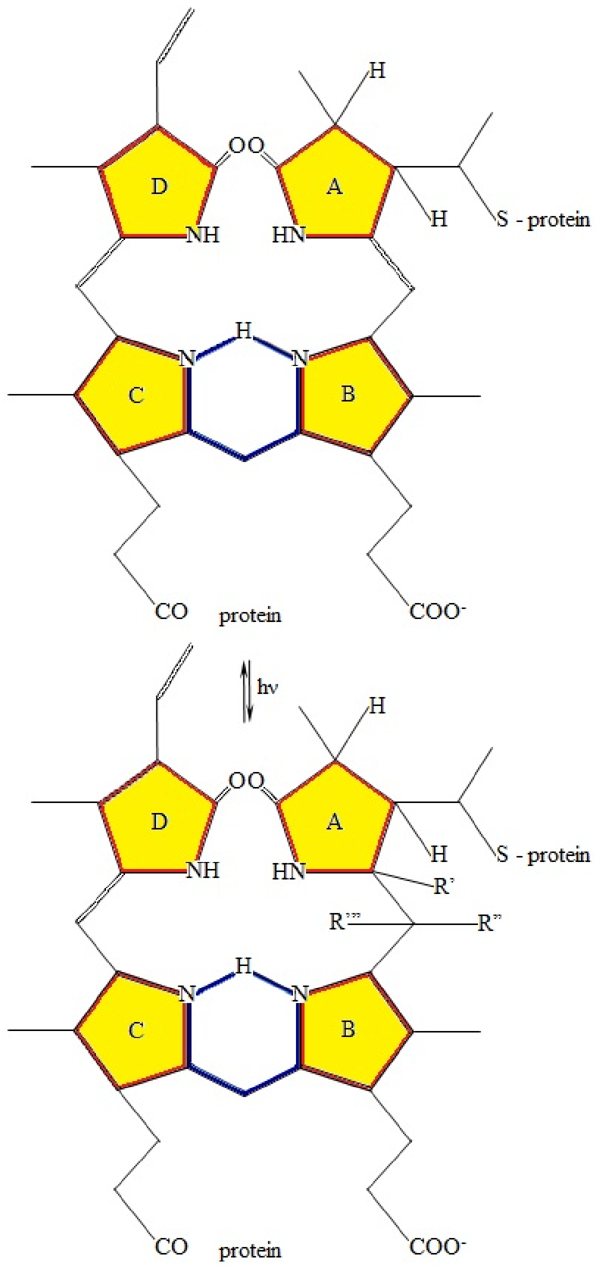

Fig. 1. Structural formula for chromophore P.

More precisely, in the case of leaves consisting of six pentagons, with help of the urn model of Gaveau and Schulmann [5] (cf. also [4]) it is possible to calculate the probability of the occurence of the transformation (1) for definite (ξ, η). For our calculations we take $\xi = 22$, $\eta = 16$,

$$c \equiv 11\frac{\eta}{\xi} - 7 = 0. \tag{2}$$

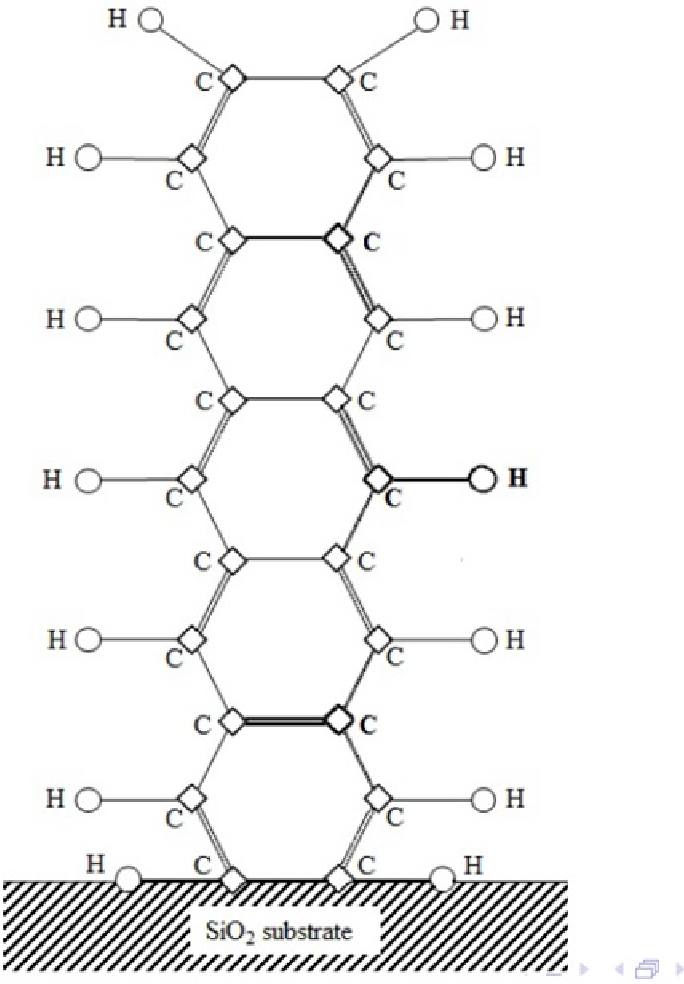

Fig. 2. The pentacene molecule $C_{22}H_{14}$ in the usual form.

3. Decomposition of a quinary structure to binary structures

The carbon atom C has four 3-hands of electrons whereas the hydrogen atom H has one hand. Therefore the corresponding binary extension leading to a polymer may be proposed as shown in Fig. 7 (cf. [13]).

4. Decomposition of a senary structure to ternary structures

In analogy to the previous Section the corresponding ternary extension leading to a polymer may be proposed as shown in Fig. 8.

It is possible (cf. Section 1) to have polymer involving both pentagons and hexagons, for instance five pentagons and one hexagon with carbon atoms in the edges. At the moment we are leaving aside the question of composing it from the binaries only or the ternaries only (cf. [8, 9]).

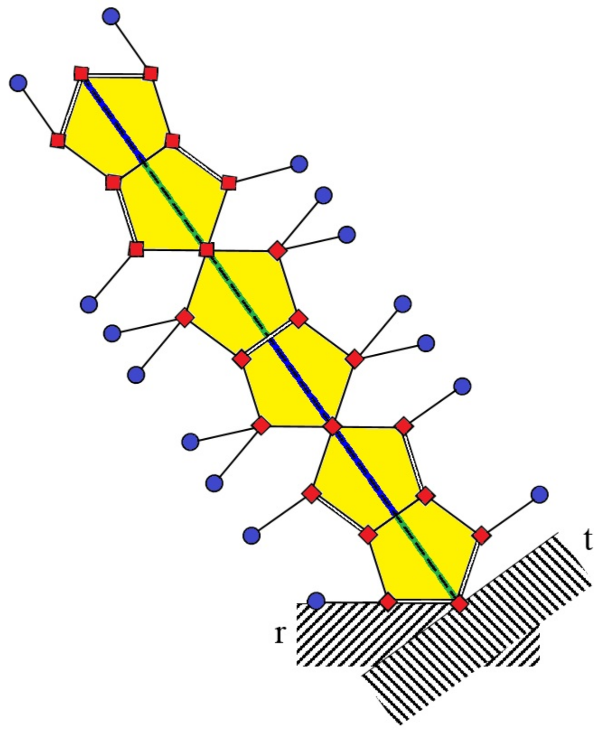

Fig. 3. A candidate for the pentacene molecule $C_{22}H_{16}$ in the form of six pentagons (c.f. the next Section).

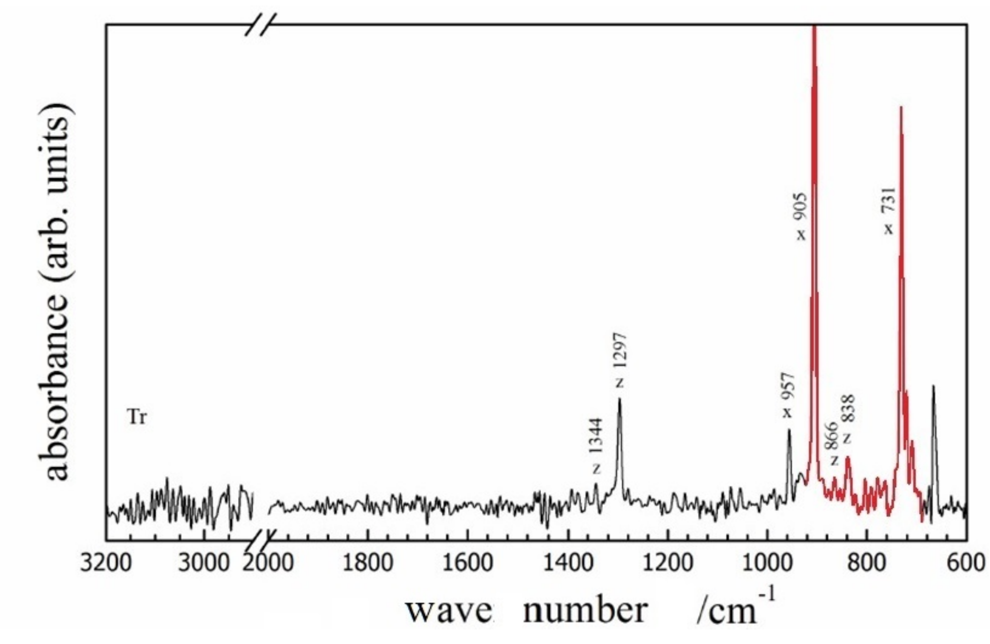

Fig. 4. The total energy (absorbance) maxima.

5. Slightly wavy behaviour of the system of hexagons in a pentacene leaf

The distance between the usual pentacene $C_{22}H_{14}$ leaves (having five carbon-atomic hexagons) amount ca. at $d \approx 1.6$ nm. It appears that the leaves of pentacene are not

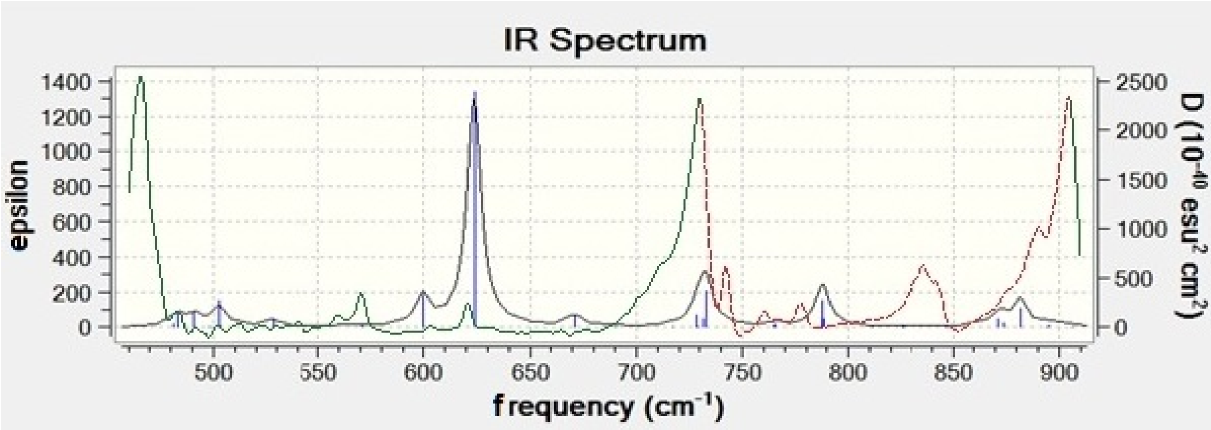

Fig. 5. Infrared activity spectrum.

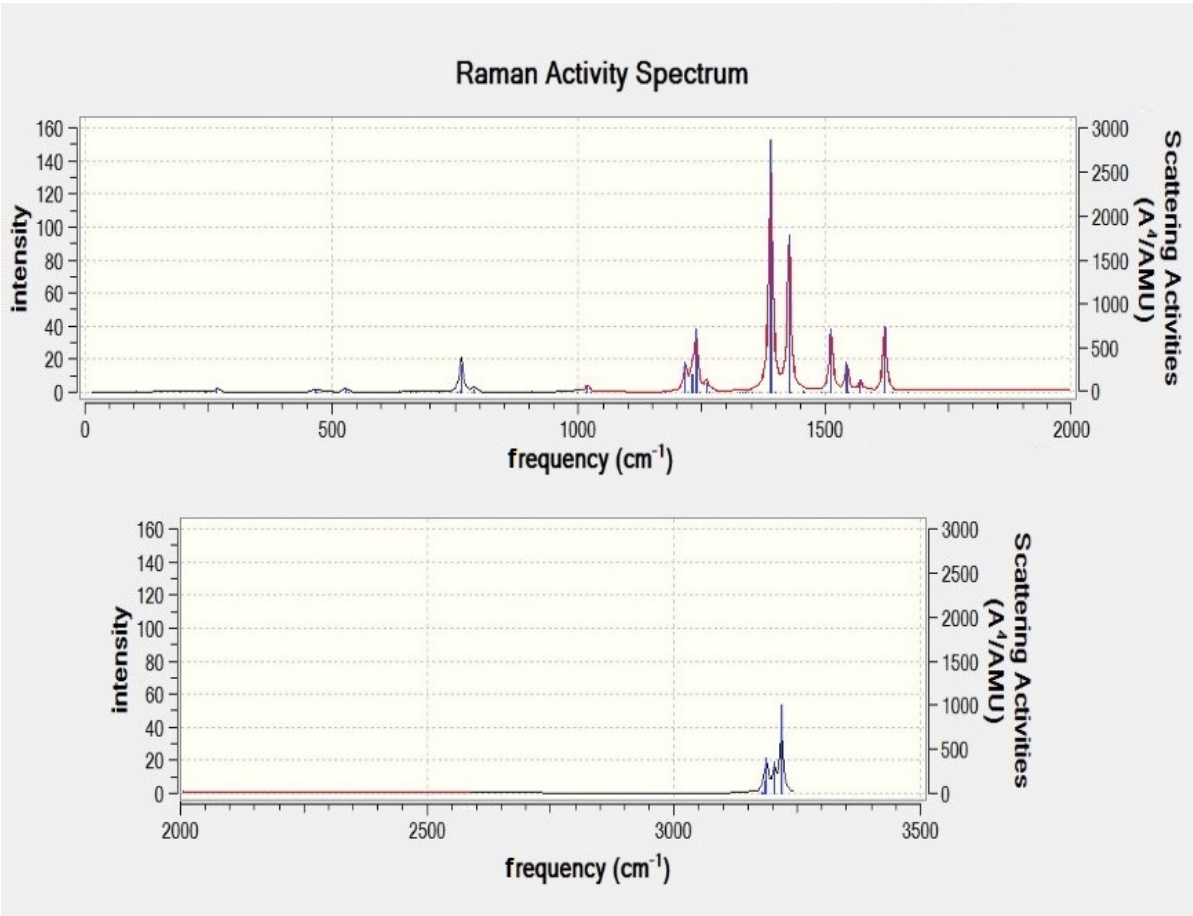

Fig. 6. Raman activity spectrum.

precisely co-planar; they meet optimal global energetic conditions when they have a slightly wavy behaviour:

Theorem 1. *A section of the pentacene* $C_{22}H_{14}$ *orthogonal to the silicone* SiO_2

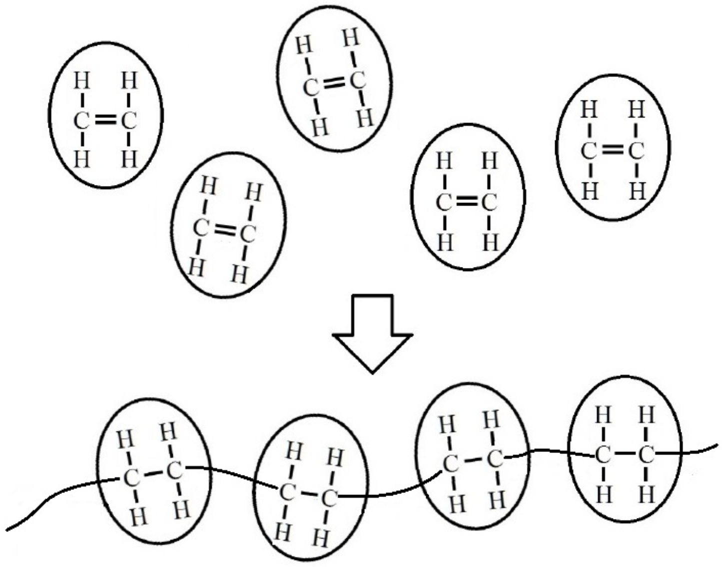

Fig. 7. The binary extension type leading to a polymer related to C and H.

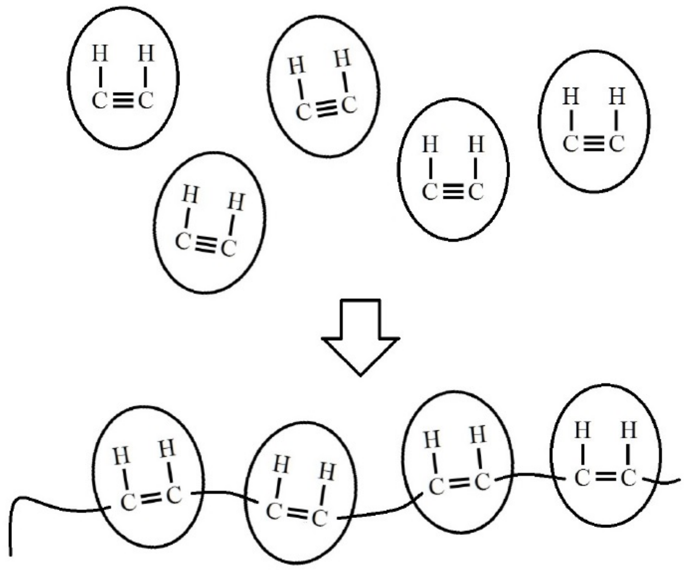

Fig. 8. The ternary extension type leading to a polymer related to C and H.

substrate is a sine-like soliton curve with maxima at $\delta \in (0.013\,\mathrm{nm}; 0.014\,\mathrm{nm})$ (cf. Figs 2, 8, 9).

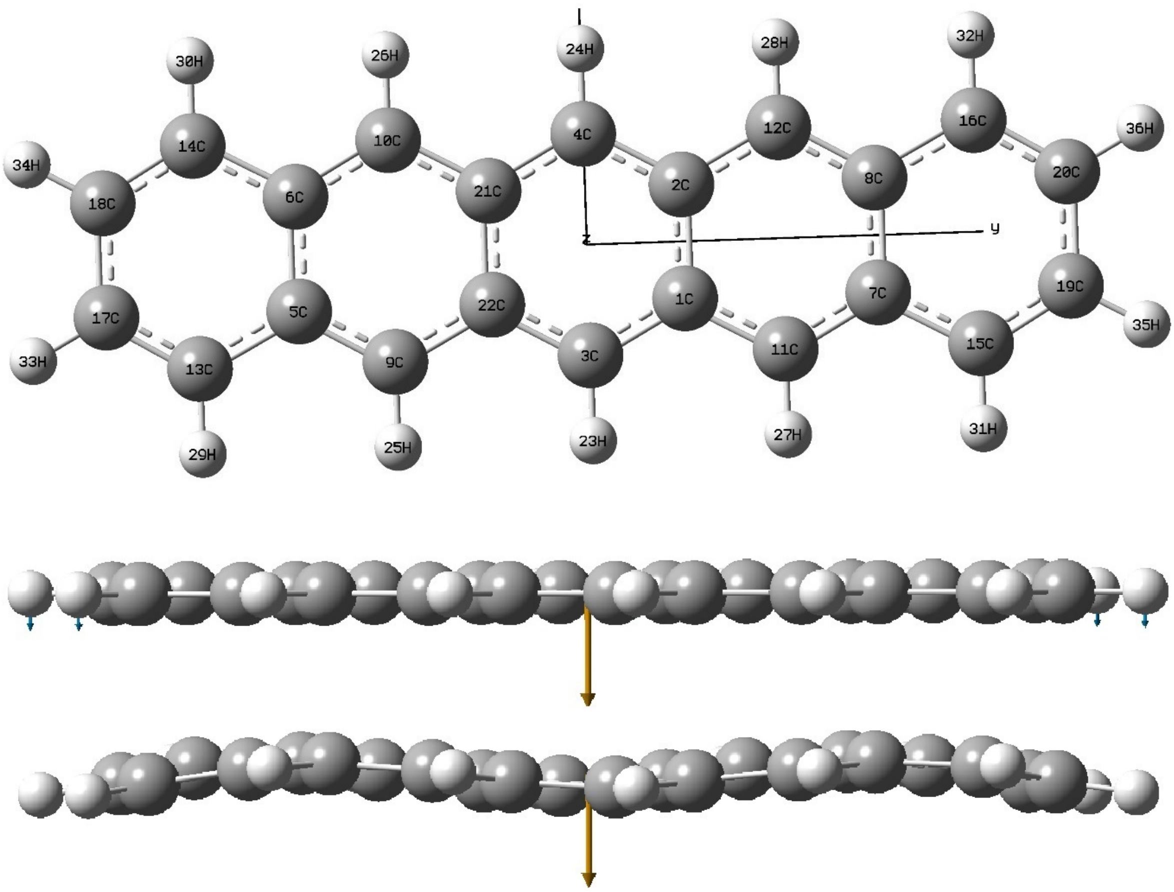

Fig. 9. The pentacene $C_{22}H_{14}$ molecule leaf with the sine-like soliton sections.

6. Zigzag or meander soliton behaviour of a twisted structure of pentagons in a pentacene leaf. The sine-like case

In this case again, the distance between the consecutive leaves of the modified pentacene (leaves being six carbon-atomic pentagons) $C_\xi H_\eta$, in our case $C_{22}H_{16}$ (Figs 3 and 9) amounts at d=1.6 nm. We suppose that the leaves of pentacene are far from being co-planar; they meet optimal energetic conditions when they form solitary zigzags and meanders.

If we concentrate on the sine-like case (Figs 11 and 12) we get:

Theorem 2. A section of the pentacene $C_{22}H_{16}$ *leaf orthogonal to the silicone* SiO_2 *substrate, in the sine-like case is a sine-like soliton curve with maxima at* $h \in (0.139$ nm, 0.140 nm) (cf. Figs 3, 9, 10, 11, and 12).

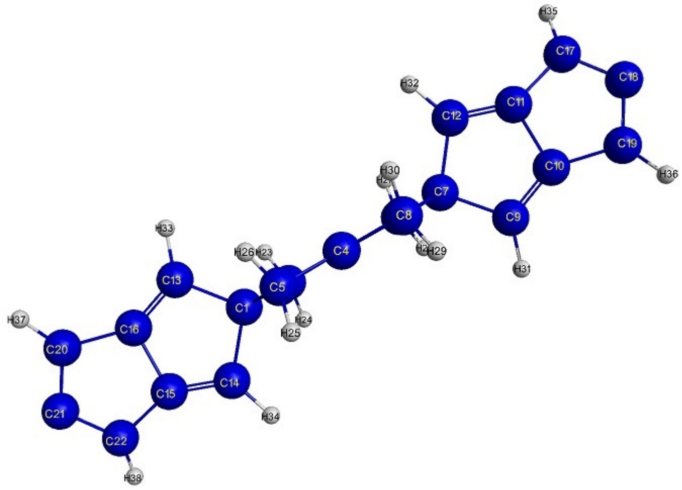

Fig. 10. Some candidate $C_{22}H_{16}$ for a pentacene molecule in the form of six pentagons. A twisted sine-like soliton structure.

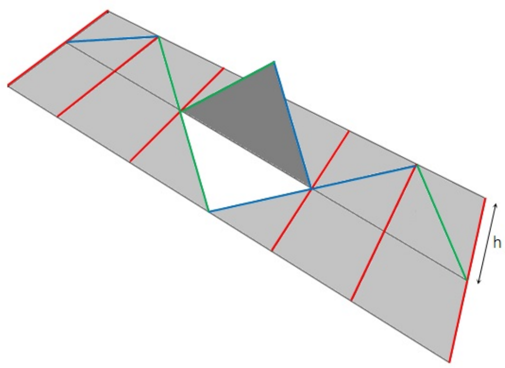

Fig. 11. The pentacene molecule structure in the form of six pentagons. Form in the sine case. The right screw-twisted structure.

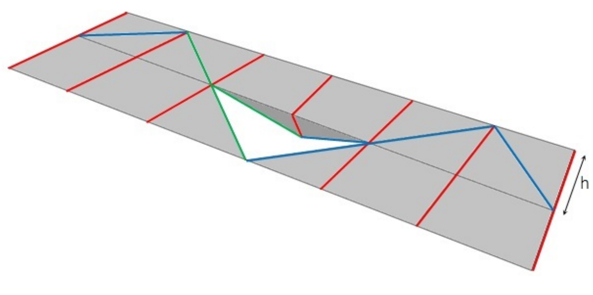

Fig. 12. The pentacene molecule structure, the left cosine twisted case.

7. Zigzag or meander soliton behaviour of a twisted structure of pentagons in a pentacene leaf. The cosine-like case

In this case again, the distance between the consecutive leaves of the modified pentacene (leaves being carbon atomic pentagons) $C_\xi H_\eta$, in our case $C_{22}H_{16}$ (Figs 3 and 10) amounts at d≈1.6 nm. It appears that the leaves on the pentacene are far from being co-planar: they have optimal global energetic conditions having the form of soliton zigzags or meanders. We are concentrated on the cosine-like case (Figs 14 nad 15) and arrive at:

Theorem 3. *A section of the pentacene* $C_{22}H_{16}$ leaf *orthogonal to the silicone* SiO_2 *substrate, in the cosine-like case is a cosine-like soliton curve with maxima at* $h \in (0.139 \text{ nm},\ 0.140 \text{ nm})$ (cf. Figs 3, 11, 14 and 15).

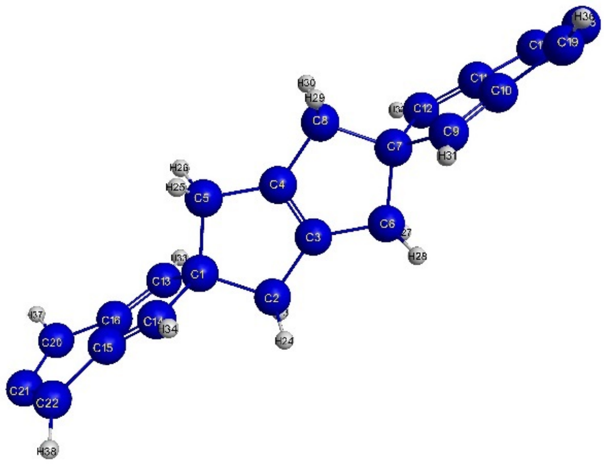

Fig. 13. Some candidate $C_{22}H_{16}$ for a pentacene molecule in the form of six pentagons. Another twisted cosine-like structure.

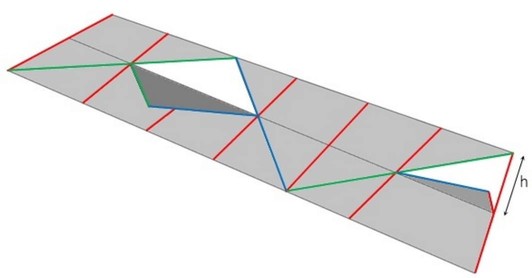

Fig. 14. The pentacene structure in the right-cosine twisted case.

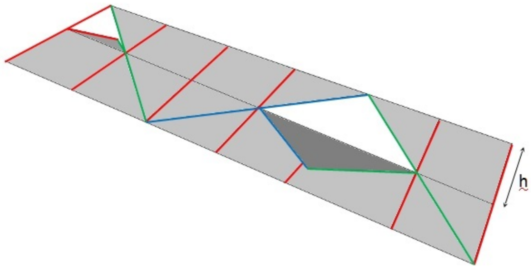

Fig. 15. The pentacene structure in the left-cosine twisted case.

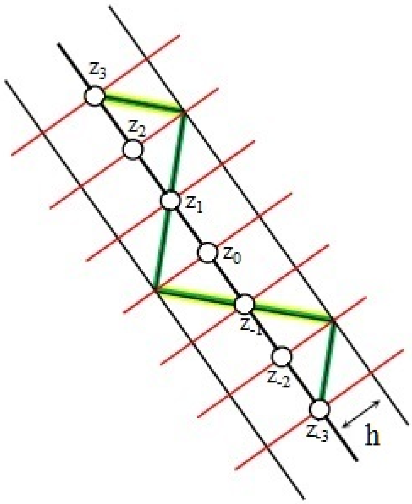

Fig. 16. A section of the pentacene $C_{22}H_{16}$ leaf orthogonal to the silicone SiO_2 substrate, in the sine-like twisted case.

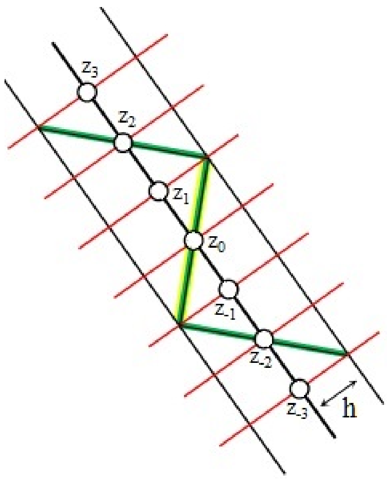

Fig. 17. A section of the pentacene $C_{22}H_{16}$ leaf orthogonal to the silicone SiO_2 substrate, in the cosine-like twisted case.

8. Conclusions. Pentacene as a foliated manifold with a soliton behaviour of leaves

Summing up we may consider pentacene, both in the form $C_{22}H_{14}$ and $C_{22}H_{16}$ as a foliated manifold with a soliton behaviour. In the senary case the system is quite close to a system of parallel planes because of considerable difference between distance d≈1.6nm and the maximal deviation δ=0.013nm of surfaces forming the system of leaves.

The whole configuration may have several mathematical and physical properties worth further investigation.

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GEOMETRYCZNE ASPEKTY BINARNYCH, TERNARNYCH, KWATERNARNYCH I SENARNYCH STRUKTUR W FIZYCE

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

Obserwujemy, że struktury kwinarne i senarne, zarówno w przypadku pentacenu, jak i innych polimerów, można utworzyć ze struktur binarnych i senarnych w sensie równań różniczkowych i opisu geometrycznego. Liście pentacenu umieszczone na silikonowym podłożu mają postać pięciu połączonych węglowo-wodorowych sześciokątów; w całości nie tworzą dokładnie struktury planarnej lecz lekko falującą, która minimalizuje energię całkowitą. W przypadku struktury kwinarnej liście tworzą odosobnione, niemal periodyczne zygzaki i meandry.

Słowa kluczowe: algebry skończenie wymiarowe, pierścienie i algebry łączne, binarne struktury fizyczne, ternarne struktury fizyczne, kwinarne struktury fizyczne, senarne struktury fizyczne, pentacen, polimer