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NANORING ENCODING REVISITED

The rules for encoding carbon nanorings have been revised as to values of corresponding code parameters. It has been shown that encoding Z-nanorings enables to distinguish their chirality that results either from initial nanotubes chirality or arises owing to twisting achiral nanotubes when closure into nanorings.

The practical application of the universal code for nanotubes and nanorings described by us earlier [1] showed that this code does not work properly in two cases [2]. This concerns:

a) chiral nanorings resulting from achiral nanotubes;

b) special case of nanorings which have zigzag arrangement of C-C bonds in the cross-section (so-called Z-nanorings).

Let us remind that a universal **nanoring** code (p, *q, w*, χ, *t, α,* β) gives an information about:

1) the structure of the nanotube rolling-up of which results this nanoring;

2) a way of connecting opposite nanotube ends.

A nanoring results formally from closing the ends of a nanotube. That's why encoding the latter does not differ in principle from encoding the nanoring formed by it. Really, a structure of any **nanotube** is determined by the universal code *(p, q, w,* χ, *t)* which has been defined earlier [1] and has the same parameters as a code of a nanoring. Parameters *p, q, w* describe the structure of an invariant unit (a macrocycle resembling a necklace) repeating *t* times in a nanotube cross-section. A literal parameter χ is an index for chirality (R, S) or its absence (RS).

A nanotube can closure in a nanoring without mutual twisting of its ends (a = β = 0) as well as with a circumrotation about a large nanoring ring axis (parameter β) or partial twisting about it (parameter a). In the case of twisting at least one of these two parameters does not equal zero and a nanoring becomes *chiral.* Thus, the case α = β = 0 means that the corresponding nanoring is *achiral.*

A detailed analysis of nanotube a- and β-twisting when nanorings closure (Fig. 1) has shown that α and β parameters can take on values of real integers, i.e. they can be both positive and negative (in the previous

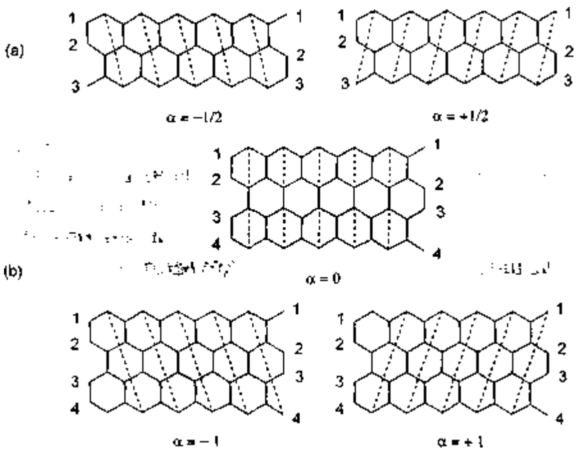

Figure 1. Evolvents of Z-nanoring fragments containing an odd (a, $t = 3$) and even (b, $t = 4$) number of invariant units (necklaces). Figures show the atoms that are connected at the nanotubes formation. "Zigzag" atom connections when nanorings closure are dotted. The arrow indicates a direction of a nanotube derivative and a large nanoring axis

report [1] the α value was supposed to be only positive). Plus sign means a clockwise twist, minus sign means an anticlockwise twist.

We have also stated that the result of Z-nanotubes closure (i.e. closure of nanotubes with parameters $\rho = 1$, $q = 0$) depends on if a t parameter is even or **odd,** namely:

- in the case of an **even** t parameter and zero α and β parameters an *achiral* nanoring is formed. This is due to the fact that atoms in the vertices of a necklace zigzag that are connected at the formation of the nanoring are lying on its derivatives;
- in the case of an **odd** t parameter a *chiral* nanoring is always formed. The atoms in the vertices of the necklace zigzag that is connected at the formation of the nanoring when $\beta = 0$ are not lying on its derivatives (Fig. 1) but they are shifted either clockwise or anticlockwise by a half of a necklace "tooth" (by one "tooth" and a half, two "teeth" and a half and so on) and thus it corresponds to a twist which can be defined by $\alpha = \pm 1/2, \pm 3/2, \pm 5/2$ and so on.

A note should be taken here that α value is defined by a w number of base units *(p* and *q* parameters) that are constituents of an invariant unit (necklace). If a nanoring consists of an *even* number of necklaces then, for example, $\alpha = +1$ means twisting by one "tooth" of a zigzag clockwise, $\alpha = -2$ corresponds to twisting by two "teeth" anticlockwise etc. In the case of nanorings with an *odd* number of necklaces α parameter can take on *only half-integer* values as it was described above.

Furthermore, for both even and odd Z-nanorings a χ chirality parameter depending on the structure of an initial Z-nanotube is the same and equals RS while on the whole a nanoring can be chiral because of nanotube α-twisting when a nanoring closures.

Therefore we have the following revisions to the rules of nanoring encoding given in our previous article [1]:

- α and β parameters which determine nanotube twisting when nanorings closure can take on values, that can be positive and negative;
- encoding Z-nanorings *(p = I, q = 0)* enables to differentiate a chirality (1) resulting from chirality of corresponding nanotubes (parameter/? > 1) and (2) arising because of nanotube twisting when nanorings closure (a * • 0, β Φ0);
- Z-nanorings with *odd* numbers t of invariant units (necklaces) have half-integer values of an α parameter ($\pm 1/2, \pm 3/2, \ldots$); these nanorings are **always chiral;**
- Z-nanorings with *even* numbers t of invariant units (necklaces) can have achiral structure in the case of $\alpha = \beta = 0$.

1. *Komilov M.Yu., Plakhotnyk V. V., Mykhailenko O. V., Ljubchuk T. V., Reutov D. V., Isaev S. D.* New approach to nanotube and 6-nanoring encoding *II* Acta NaUKMA, Academia, Kiev.- 2002.- Part II,- № 20,- P. 509-511.

2. *Mykhailenko O. V.* Fullerenes, nanotubes and nanorings: stereochemistry and encoding (nomenclature). Complexes of fullerenes with calixarenes *II* Diss. ... cand. chem. sci.: 02.00.03.- Kiev National Taras Shevchenko University.-K., 2005.- 138 p.

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ЩОДО КОДУВАННЯ НАНОКІЛЕЦЬ

Повторно переглянуто правила кодування карбонових нанокілець стосовно значень відповідних параметрів коду. Показано, іцо кодування Z-нанокілець дозволяє розрізняти їхню хіральність, яка є наслідком хіральності вихідних нанотрубок або виникає внаслідок скруту ахіральних нанотрубок при замиканні нанокілець.