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Topology Counting in Nanostructures

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ABSTRACT. Tubulenes are capped nanotubes built up from two caps and a distancing nanotube/neck of diverse decoration. Ways of "in silico" construction of several finite nanostructures, classified by their neck and/or caps, are presented. Topological periodicity is presented as constitutive typing enumeration. Semiempirical calculations support the idea that new, relatively stable molecules may appear in the soot of vaporized graphite.

1. INTRODUCTION

Fullerenes and nanotubes represent 0D and 1D novel carbon allotropes that have non-preceding physico-chemical properties [1-4]. They are promising candidates for the development of nanodevices and super strong composites [5-11].

Apart from the well-known C_{60} and C_{70}, other cages have been isolated in the solid state. Recently, the small cages C_{36} and C_{20} have been reported [12-14] and their halves used for modelling capped narrow nanotubes [15].

A fullerene is, according to a classical definition, an all-carbon molecule C_N consisting entirely of pentagons (exactly 12) and hexagons (N/2-10) [16]. Non-classical fullerene extensions to include rings of other sizes have been considered [17,18].

Some basic relations in polyhedral graphs come out from the Euler's results [19]:

$$N - E + F = 2 \tag{1}$$

where N, E, and F are the number of vertices, edges and faces, respectively. Relation (1) is given here for a graph embedded on the sphere. Other basic relations are:

$$\sum_d d \cdot v_d = 2E \tag{2}$$

$$\sum_s s \cdot f_s = 2E \tag{3}$$

where v_d and f_s denote vertices of degree d and s-sized faces, respectively.

In view of calculating the strain energy appearing due to diverse polygonal angles, we use the POAV1 theory [20-23], which defines the π-orbital axis vector is as the vector making equal angles $\theta_{\sigma\pi}$ to the three σ-bonds of the sp^2 carbon atom and a *pyramidalization* angle as:

$$\theta_p = \theta_{\sigma\pi} - 90^o \tag{4}$$

This angle is used for estimating the strain energy, induced by a pyramidalized carbon atom, by:

$$SE = 200 \cdot (\theta_p)^2 \tag{5}$$

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with θ_p being measured in radians. The difference $120 - (1/3) \cdot \sum \theta_{ij}$ gives the deviation to planarity.

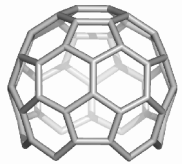
This paper is organised as follows: several caps are designed and named in Section 2, Capping Nanotubes. The next Section 3, *z*-Tubulenes, presents tubulenes constructed with zigzag distancing nanotubes, peanut-shaped, periodic fulleroids and some topology counting theorems. Section 4 draws conclusions. The paper is ended by references.

2. CAPPING NANOTUBES

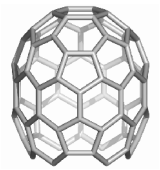
Covering transformation is one of the ways in understanding chemical reactions occurring in fullerenes [38-41]. A capped nanotube we call here a tubulene. Covering is different for the caps and for the nanotube/neck distancing the two caps. A constructive enumeration of nanotube caps the reader can find in ref. 24. Within this paper we limit at the *kfz*-caps, obtainable by cutting off the polar ring (of size *k*) and suitable to Z nanotubes (Figure 1). The parent cages are easily deducible from the name of caps, which includes the number of atoms *N*, the *a*-spiral code [25] and the fitting tube specification, *e.g.*, Z[*c*,*n*], *c* being the number of atoms in the cross-section while *n* is the number of such sections along the tube. The number of atoms in the neck is $c \times n$. Note the value $n = 0$ for the tube length in the cap name (see below). When no ambiguity exists, the specification of the polyhex (6,3) covering for tubes is omitted. Also note that, in two integer parameter (*k*,*l*), notation [26], the armchair (single walled) nanotube SWNT is (*c*/2, *c*/2) while the zigzag one is (*c*/2,0).

(a) Cap $C_{11k(k\,6^k(56)^k(65)^k-Z[2k,0])}$ $k = 5$

(b) Cap $C_{9k(k\,(56)^{k/2}(665)^{k/2}(656)^{k/2}-Z[2k,0])}$ $k = 6$



(c) Cap $C_{12k(k\,(56)^{k/2}(665)^{k/2}6^k(656)^{k/2}-Z[2k,0])}$ $k = 6$



(d) Cap $C_{11k(k\,5^k7^k5^{2k}7^k-Z[2k,0])}$ $k = 7$

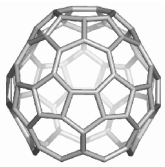


Figure 1: The types of *kfz*-caps herein used for capping nanotubes.

Various caps and various junction zones could be used to construct tubulenes [27-30]. Both the cap and nanotube covering can be changed by appropriate operations.

3. *kfz*-TUBULENES

The cap shown in Figure 1a fit to Z-nanotubes (possibly having various covering). Figure 2 illustrates two peanut-shaped *kfz*-tubulenes of the $C_{66(6\,6^6(56)^6(6\,5)^{6-Z[12,0]})}$ cap with different distancing nanotubes (observe the complete description of covering).

$C_{168(6\,6^6(56)^6(65)^6 7^6 6^6 6^6 7^6)}$ (D_{6d}) $C_{168(6\,6^6(56)^6(65)^6 7^6(57)^3(75)^3 7^6)}$ (S_6)

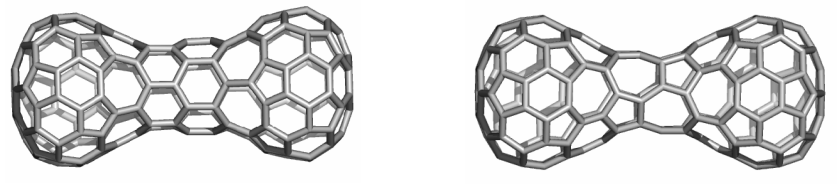


Figure 2: Peanut-shaped *kfz* -tubulenes.

The cages in Figure 3 have the shorter distancing tube (one atom and zero atom rows, respectively) between the two caps (Figure 1a and 1b, respectively). The name of such tubulenes includes the code for the cap and distancing zone up to the second cap, if the two caps are identical, or full description, if they are different.

(a) $C_{120(56^5(56)^5(65)^5 7^5 7^5-Z[10,1])}$ (b) $C_{108(6(56)^3(665)^3(656)^3 7^6-Z[12,0])}$

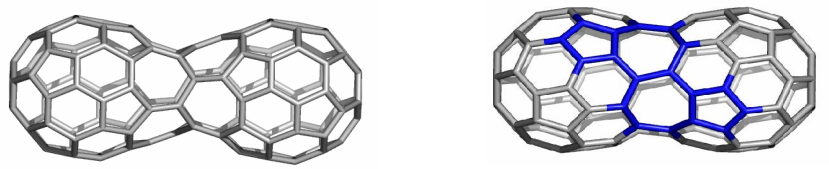


Figure 3: Peanut-shaped *kfz*-tubulenes with the shortest distancing tube

Peanut tubulenes show negative curvature, induced by the presence of rings larger than hexagons. Cages such those in Figure 3 have been observed, by transmission electron microscopy TEM, in the coalescence reactions occurring in C_{60} peapods [31]. Their energetic and topology are shown in the following sections.

3.1. PERIODIC FULLEROIDS

At moderate temperature and pressure spherical fullerenes arrange in one dimensional assemblies [32]. The primary sp^3 [2+2] adduct rearranges, either by Stone-Wales edge rotations [33] and/or atom exclusion [34], to give "dimers", oligomers or just corrugated tubules (*e. g.*, having repeat units of peanut-shape, like the objects in Figure 3), as observed in fullerene peapods by thermal annealing or by electron irradiation [31]. Fullerene coalescence, the main molecular transformation occurring in such processes, is presented in detail elsewhere [35].

Let consider the $C_{11k(k\,6^k(56)^k(65)^k-Z[2k,0])}$ cap (Figure 1a) and the Z-tube having length n = 1; a repeat "dimerization" leads to periodic *kfz*-tubulenes of corrugated shape, of general formula $C_{N(k\,6^k(56)^k(65)^k\,7^k-Z[2k,1]-r)}$, just observed in annealed fullerene peapods [31]. The last subscript r in the above formula means the number of sphere-like repeat moieties. N is calculable by formula: $N = 12kr$ (see Table 1). Figure 4 illustrates such a periodic "fulleroid" [29].

$C_{N(k\,6^k(56)^k(65)^k\,7^k-Z[2k,1]-r)}$; $k = 5$; $r = 4$

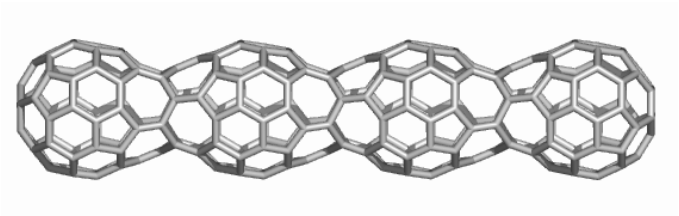


Figure 4: A periodic kfz-tubulene.

We were interested in topological characterization of such all sp^2 periodic objects. The following theorem [29] states the counting formulas (*i.e.*, number of faces of size s, f_s, edges shared by faces of given size , $e_{s1,s2}$ and vertices shared by corresponding faces, $v_{s1,s2,s3}$) for objects with k = 4 to 7.

Table 1: Tiling counting formulas for periodic fulleroids of general formula $C_{N(k\,6^k(56)^k(65)^k\,7^k-Z[2k,1]-r)}$

k = 4, 5, 6, 7	
Faces	Vertices
$f_{4k} = 2t_4$*	$v_{4,6,6k} = 2kt_4$
$f_{5k} = 2kr + 2t_5$	$v_{5,6,6k} = 2k(2r + 3 + t_5)$
$f_{6k} = 2k(r+1) + 2t_6$	$v_{5,6,7k} = 4k(r-1)$
$f_{7k} = 2k(r-1) + 2t_7$	$v_{5,7,7k} = 2k(r-1)$
Edges	$v_{6,6,6k} = 2kt_6$
$e_{4,6k} = 2kt_4$	$v_{6,6,7k} = 2kt_7$
$e_{5,6k} = 2k(3r + 2 + t_5)$	$v_{7,7,7k} = 2k(r-1)$
$e_{5,7k} = 4k(r-1)$	Total No. atoms
$e_{6,6k} = 2k(r + 2 + t_6)$	$N_k = 12kr$
$e_{6,7k} = 2k(r - 1 + t_7)$	
$e_{7,7k} = 4k(r-1)$	

* $t_s = 1$ if $s = k$, and *zero* otherwise

THEOREM 1. *For a periodic fulleroid, of general formula* $C_{N(k\,6^k(56)^k(65)^k\,7^k-Z[2k,1]-r)}$, *the number of faces, edges, and vertices of various types*

composing its associate graph, can be counted function of the repeat parameter r and polar ring size k (Table 1).

The theorem is demonstrated by construction.

Semiempirical calculations in the series $C_{N(k\ 6^k\ (56)^k (65)^k\ 7^k - Z[2k,1]-r)}$, k = 5, for the first four terms (parent fullerene, with r = 1, included) show HF values in the range of C_{60}, and large enough gaps (Table 2).

Table 2: Semiempirical PM3 data for periodic fulleroids of the series $C_{N(k\ 6^k\ (56)^k (65)^k\ 7^k - Z[2k,1]-r)}$

	Cage (k; r)	N	Sym.	HF/atom	Gap
1	5; 1	60	I_h	13.512	6.593
2	5; 2	120	D_{5d}	12.547	6.204
3	5; 3	180	D_{5d}	12.224	5.917
4	5; 4	240	D_{5d}	12.062	5.819

3.2. ((5,6,7)3) *kfz*-TUBULENES

Tubulenes capped with *kfz*-caps, like $C_{9k(k\ (56)^{k/2}(665)^{k/2}(656)^{k/2} - Z[2k,0])}$ (Figure 1b), derived from C_{60}, and those cut off from C_{78} (an example is given in Figure 1c), are ((5,6,7)3) *kfz*-tubulenes with the shortest distancing tube. They have the general formulas:

- $C_{N(k\ (56)^{k/2}(665)^{k/2}(656)^{k/2}\ 7^k - Z[2k,0])}$ (Figure 3b) [36],
- $C_{N(k\ (56)^{k/2}(665)^{k/2}\ 6^k\ (566)^{k/2}\ 7^k - Z[2k,0])}$ (Figure 5a),
- $C_{N(k\ (56)^{k/2}(665)^{k/2}\ 6^k\ (656)^{k/2}\ 7^k - Z[2k,0])}$

and combinations of the three types (see Figure 5b). HF values, calculated with the PM3 Hamiltonian, are listed in Table 3 (entries 1 to 5). These values are in the range of that for C_{60}, lower for the peanuts derived from C_{78}. The strain energy per atom S, by POAV1 (see above), is lower than that calculated for C_{60} (comparison made with the [2+2] adduct sp^3 dimer). The gaps are, however, with about 2 eV lower to that for C_{60}, suggesting a relative kinetic instability.

(a) $C_{144(6(56)^3(665)^3 6^9(566)^3 7^6 - Z[12,0])}$ (b) $C_{126(6(56)^3(665)^3(656)^3 7^6\ (656)^3 6^9(665)^3(65)^3 6)}$

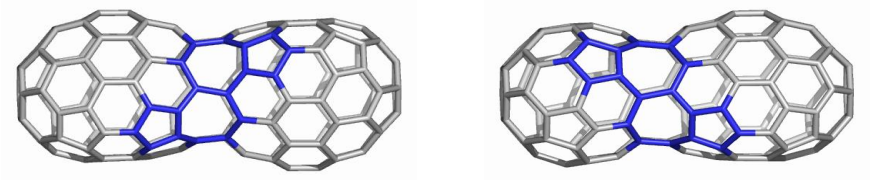


Figure 5. Peanut-shaped *kf* z–tubulenes with the shortest distancing tube

Periodic tubulenes of corrugated shape, like the *kfz*–tubulene in Figure 6, were observed in C_{60} peapods submitted to prolonged thermal annealing (the inner tube) [49]. Oligomers with r = 2 to 4 show pretty low HF values (Table 3, entries 5 to 7). The corresponding of the k = 5 peanut dimer $C_{120(56^5(56)^5(65)^5 7^5 7^5 - Z[10,1])}$ (Figure 3a) [36], namely the k = 6 dimer, $C_{120(6(56)^3(665)^3(656)^3 7^6 - Z[12,1])}$, was also inferred in the coalescence of C_{60} [37].

$$C_{204(6(56)^3(665)^3(656)^3 7^6 - Z[12,0]-r)}\ ;\ r = 4$$

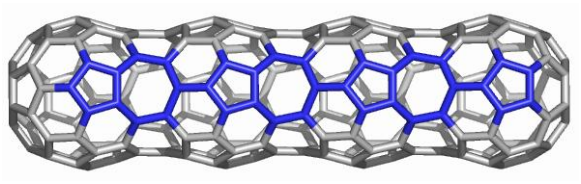


Figure 6: Periodic tubulene with the repeat spherical moiety derived from C_{60} by cutting off the polar hexagons.

The ((5,6,7)3) covering pattern is easily derived, by Stone-Wales edge flipping, in polyhex (6,3) nanotubes [38,39]. It can also be embedded in the torus (Figure 7).

$$T_{N((566)^{k/2}(665)^{k/2}7^k - Z[2k,0]-r)}\ ;\ \mathrm{k} = 6;\ r = 30;\ N = 8kr$$

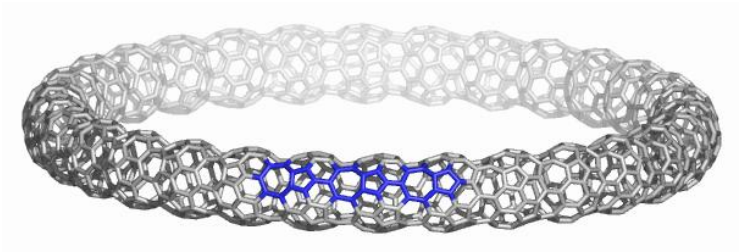


Figure 7: A toroidal embedding of the ((5,6,7)3) pattern.

The topology of ((5,6,7)3) decorated structures is calculable as stated by the following [36]:

THEOREM 2. *For a periodic* ((5,6,7)3) *covering, of local signature:* $t_{5j}(0, 4, 1)$; $t_{6j}(2, 2, 2)$; and $t_{7j}(1, 4, 2)$, j = 5, 6, 7, *the number of faces, edges, and vertices of various types composing its associate graph, embedded in the torus, can be counted function of the repeat parameter r and ring size k of the* (*equivalent*) *tube cross section* (Table 4).
The theorem is demonstrated by construction.

Table 3. Semiempirical PM3 data for periodic peanut cages (Figure 13) and their relatives; for comparison, C_{60} is included.

	Cage	Sym.	HF/atom (kcal/mol)	Gap (eV)	*S*/atom (kcal/mol)
1	$C_{144(6(56)^3(665)^3 6^k (566)^3 7^6 - Z[12,0])}$	D_{3d}	11.911	4.729	5.530
2	$C_{144(k\ (56)^{k/2}(665)^{k/2} 6^k (656)^{k/2} 7^k - Z[2k,0])}$	S_6	11.666	4.049	5.343
3	$C_{144(6(56)^3(665)^3 6^k (566)^3 7^6 (665)^3 6^6 (665)^3 (65)^3 6)}$	C_3	11.789	4.266	5.436
4	$C_{126(6(56)^3(665)^3(656)^3 7^6\ (656)^3(566)^3(65)^3 6)}$	C_{3v}	12.349	4.796	5.848
5	$C_{108(6(56)^3(665)^3(656)^3 7^6 - Z[12,0]-2)}$	D_{3d}	12.953	4.870	6.493
6	$C_{108(6(56)^3(665)^3(656)^3 7^6 - Z[12,0]-3)}$	D_{3d}	12.878	4.502	5.687
7	$C_{108(6(56)^3(665)^3(656)^3 7^6 - Z[12,0]-4)}$	D_{3d}	12.681	4.484	5.321
8	C_{60}	I_h	13.512	6.593	8.257

Table 4: Tiling counting formulas for toroids, of periodic ((5,6,7)3) covering, with general formula $T_{N((566)^{k/2}(665)^{k/2}7^k - Z[2k,0]-r)}$.

$k = 4, 6, \ldots$	
Faces	Vertices
$f_5 = kr$	$v_{5,6,6} = 3kr$
$f_6 = 2kr$	$v_{5,6,7} = 2kr$
$f_7 = kr$	$v_{6,6,7} = kr$
Edges	$v_{6,7,7} = 2kr$
$e_{5,6} = 4kr$	Total no. atoms
$e_{5,7} = kr$	$N = 8kr$
$e_{6,6} = 2kr$	
$e_{6,7} = 4kr$	
$e_{7,7} = kr$	

A torus T((5,6,7)3)VA[*p*,*q*] derived, from an equivalent (6,3)Z[*c*,*n*] torus, by SW edge rotations, has the parameters: (*p*; *q*) = (*c*/4; *n*/4), with $c = 2f_7$ and the repeat unit parameter $r = q$ (see Table 4).

3.3. ((5,7)3) z-TUBULENES

The *tz*-Cap $C_{3k(k5^k-Z[2k,0])}$ fits to a suitable phenylenic ((4,6)3)H tube [40] (Figure 5), to give a cage $C_{N(k5^k7^k(46)^k7^k5^k k)}$, which further rearranges to a cage $C_{N(k5^k7^k5^{2k}7^k5^k k)}$, k = 5,7, decorated with only pentagons and heptagons (see below).

The *kfz*-cap $C_{11k(k5^k7^k5^{2k}7^k-Z[2k,0])}$, derived from the above cage, leads, by identifying the *z*-boundary, to a "dimer" (Figure 8, k = 7).

$2(C_{11k(k5^k7^k5^{2k}7^k-Z[2k,0])} - k)$; $k = 7$ $\qquad$ $C_{20k(k5^k(7^k5^{2k}7^k)^2 5^k k)}$; $k = 7$

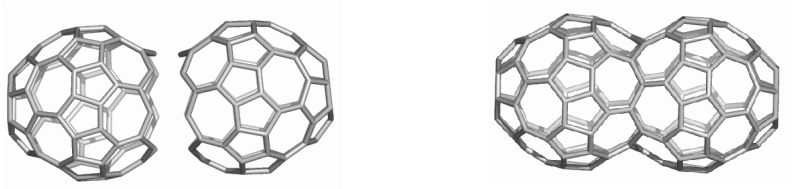


Figure 8: An *in silico* "dimerization" process.

The coupling process can continue to give periodic cages of formula $C_{N(k5^k(7^k5^{2k}7^k)^r 5^k k)}$, with $N = 4k(2r+1)$ (see Table 5). In the above formula, r counts the spheroidal repeat units, r = 2, 3,...

An example of such periodic cages is given in (Figure 9). It is a third cage having 260 points and ((5,7)3) decoration ($f_5 = f_7 + 12$; $f_7 = 60$), in addition to the phantasmagoric fullerenes designed by Fowler and Dress, respectively [41].

$$C_{260(k5^k(7^k5^{2k}7^k)^r 5^k k)};\quad k=5;\quad r=6$$

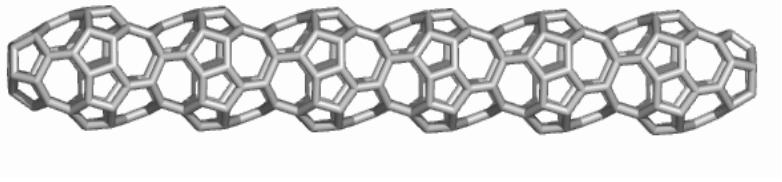


Figure 9: Diudea's C_{260} cage with ((5,7)3) decoration.

The topology of ((5,7)3) decorated structures is calculable as shown in the following [36]:

THEOREM 3. *For a periodic cage with* ((5,7)3) *decoration, the number of faces, edges, and vertices of the various types can be counted function of the repeat unit r and polar ring size k* (Table 5).

The theorem is demonstrated by construction.

Table 5: Periodic cages with ((5,7)3) decoration - net counting.

Formulas for k = 5; 7	
$f_{5k} = 2k(r+1) + 2t_5$	(1)
$f_{7k} = 2kr + 2t_7$	(2)
$e_{5,5k} = 2k(r+1+t_5)$	(3)
$e_{5,7k} = 2k(3r+2+t_7)$	(4)
$e_{7,7k} = 2k(2r-1)$	(5)
$v_{5,5,5k} = 2kt_5$	(6)
$v_{5,5,7k} = 2k(2r+1+t_7)$	(7)
$v_{5,7,7k} = 2k(r+1)$	(8)
$v_{7,7,7k} = 2k(r-1)$	(9)
$N_k = 4k(2r+1)$	(10)

* $t_s = 1$ if $s = k$, and *zero* otherwise

$T_{N(7^k5^{2k}7^k-Z[2k,0]-r)}$; k = 6; r = 30; $N = 8kr$

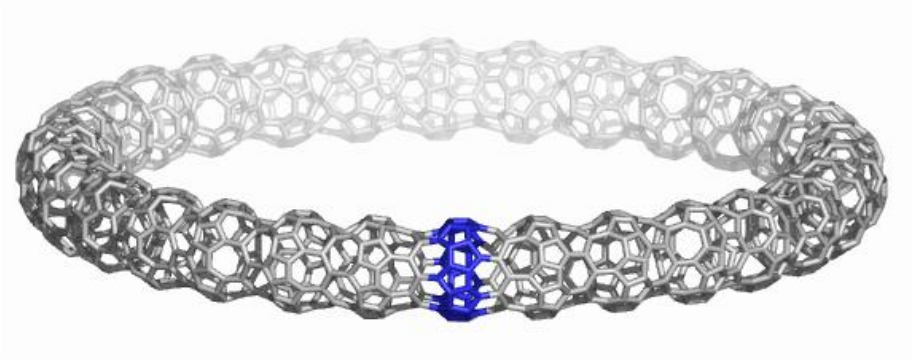


Figure 10: A toroidal embedding of the ((5,7)3) pattern.

A toroidal embedding of the ((5,7)3) pattern is shown in Figure 10.

PM3 calculations for some all ((5,7)3) periodic cages are given in Table 6. Only the dimeric tubulene $C_{140(7 5^7 (7^7 5^{17} 7^7)^2 5^7 7-Z(14,1))}$ (entry 4) appears to have the HF closer to C_{60} (entry 5), while the π-electronic structure is pseudo-closed or open.

Table 6: PM3 data for data for some all ((5,7)3) periodic cages of general formula $C_{N(k 5^k (7^k 5^{2k} 7^k)^r 5^k k-Z[2k,1])}$

	Cage *N*, *k*, *r*	Sym.	HF/at.	Gap
	tube Z[10,1]			
1	60, 5, 1	C_i	21.158	5.623
2	100, 5, 2	C_i	18.906	5.592
	tube Z[14,1]			
3	84, 7, 1	C_i	16.249	4.538
4	140,7, 2	C_i	15.828	5.114
5	C_{60}	C_i	13.512	6.596

As a consequence, the all ((5, 7)3) tubulenes tend to isomerize to the more stable *fa*-tubulenes [36].

Semiempirical calculations have been performed on a 2×1GHz Pentium III PC by using the PM3 Hamiltonians, in standard parametrization supplied by HyperChem (version 4.5, Hypercube, Inc.) [42] software. Structures were optimized by using the Polak-Ribier conjugate-gradient method, the energy minimization was terminated at an RMS gradient <0.01 kcal/(Å·mol) for all structures.

Spectral data (see Discussion) were calculated by TOPOCLUJ 2.0 Software Package [43]. Stone-Wales rearrangements were performed by the CageVersatile 1.1 software package [44].

4. CONCLUSIONS

Construction of tubulenes, by various capping of armchair and zigzag nanotubes, was presented. Periodicity of their constitutive topology was evidenced by typing enumerations.

Semiempirical and strain energy calculations support the idea that new, relatively stable molecules, with various tessellation, may candidate to the status of real molecules.

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