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# CONETORI OF HIGH GENERA

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Dedicated to Professor Sorin Mager, on his 75 years,
for his bright contribution to the Stereochemistry.

**ABSTRACT.** Nanocones are taken as starting structures for designing various 3D nanostructures. Toroidal objects of genera from one to five are built up by using conical zones and appropriate nanotubes. In the same sense, units derived by opening the Platonic solids operated by various map operations are used. The topology of the resulting objects is discussed in connection with the strain estimated at the POAV1 level of theory.

## 1. Introduction

A map *M* is a combinatorial representation of a closed surface.[1] Several transformations (*i.e.*, operations) on maps are known and used for various purposes.[2,3]

Let us denote in a map: *v* - number of vertices, *e* - number of edges, *f* - number of faces and *d* - vertex degree.

Recall some basic relations in a map:[4]

$$\sum d\, v_d = 2e \qquad (2)$$

$$\sum s\, f_s = 2e \qquad (3)$$

where $v_d$ and $f_s$ are the number of vertices of degree *d* and number of *s*-gonal faces, respectively. The two relations are joined in the famous Euler[5] formula:

$$v - e + f = \chi(M) = 2(1-g) \qquad (4)$$

with $\chi$ being the Euler *characteristic* and *g* the genus[6] of a graph (*i.e.*, the number of handles attached to the sphere to make it homeomorphic to the surface on which the given graph is embedded; *g* = 0 for a planar graph and 1 for a toroidal graph). Positive/negative $\chi$ values indicate positive/negative curvature of a lattice.

If a graphene sheet is divided into six sectors, each with an angle of 60º (Figure 1), and if *m* of these sectors (with *m* varying from 1 to 5) are

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selected sequentially with the dangling bonds being fused together (see below), a series of five single-walled nanocones is obtained, with a linear angle α at the cone apex equal to 112.9º, 83.6º, 60.0º, 38.9º, and 19.2º. These values correspond to the formula:[7]

$$\alpha = 2\arcsin(m/6) \qquad (1)$$

One can add two extreme cases: (i) the graphene sheet, with all *m* = 6 sectors being involved, corresponding to a "cone" with an angle of 180º; and (ii) when *m* = 6, one obtains a "cone angle" equal to zero, corresponding to a nanotube capped at one end with any combination of hexagons and six pentagons, *e.g.*, a "half-buckminsterfullerene". Thus *nanotubes capped at one end can be considered to be a particular case of nanocones,* and indeed Ebbesen has observed by transmission electron microscopy how a blunt nanocone with *m* = 5 on adding a sixth 60º sector becomes converted into a nanotube.[8,9]

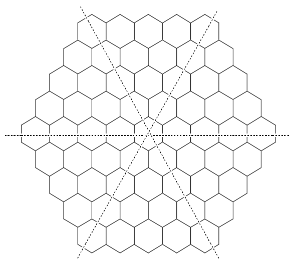


**Figure 1.**
The six sectors on a honeycomb lattice

In the hereafter text we will consider only cones ending in polygons of s = 3 to 5 with no other polygonal defect of the graphite sheet. The name of such objects includes: [tip polygon]CN_length of the cone body, in number of hexagon rows (Figure 2).


**Figure 2.**
A nanocone ending in a trigon

## 2. Single Conetori

Conical zones may be involved in the construction of the so-called "distinct-walled tori" DWT, proposed by Nagy *et al*.[10] to appear by sealing a double-walled carbon nanotube DWNT in two distinct position, by an electron beam. Proposals of toroidal structures bearing polygonal defects are known since the pioneering times of nanoscience.[11-13]

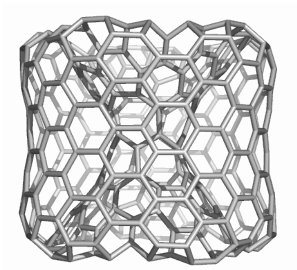
Such structures, of genus 1, called hereafter conetori, are built up, in general, by two conical zones joined by two tubes, one internal and the other external, having corresponding distinct diameters. Their name includes: [cone tip polygon]CT_cone length_type and length of internal tube(tiling)_type and length of external tube(tiling), the length being given in number of hexagon rows. The tube is either an H (zig-zag) or V (armchair) one.[14]

Function of the composing parts the conetori are classified as follows.

### *2.2.1. Conetori with Internal H-tube, External V-tube*

Even the small conetori (Figure 5) of this type are strained structures, it could be imagined that by increasing the number of atoms, they could become more relaxed molecules, as suggested in Figure 6. This huge object can be covered by disjoint coronenes (by the generalized map operation (2,2)[15]); it appears the opportunity to address the question of aromaticity of such total resonant molecular systems and consequently the possible increase of molecule stability.

[5]CT_2_H0(7)_V4(5,7,5)
v =360; S=5.44



[5]CT_2_H1(7)_V5(5,7,5)
v =370; S=5.05

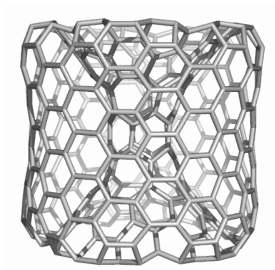


**Figure 3.**
Conetori with internal H-tube, external V-tube

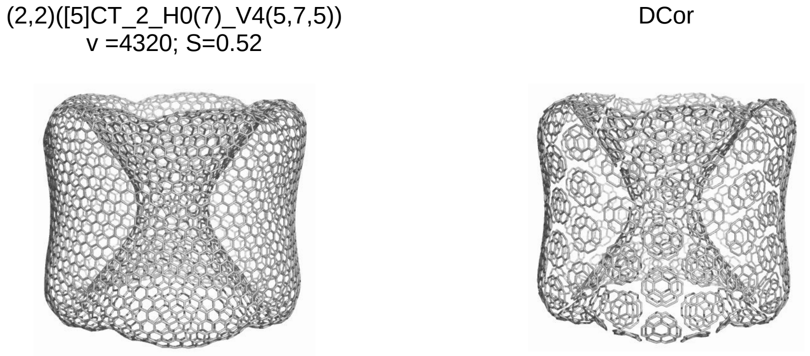



**Figure 4**.
Conetorus with disjoint coronenic units

***2.2.2. Conetori with Internal V-tube, External V-tube***

Cones of this type show (5,8,5) tiling at the junction with the inner tube while (5,7,5) at that with the outer tube (Figure 5a). The octagons can be eliminated by a Stone-Wales operation (*i.e*., edge rotation, specified by RO in Figure 5b). Systematic search on the stability of tori belonging to this type has been reported in ref.[10]

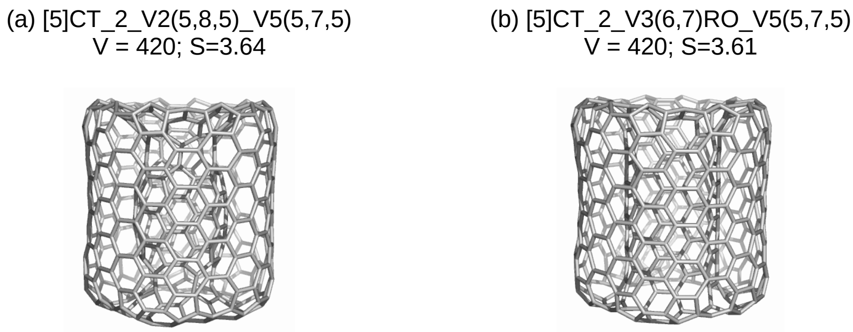



**Figure 5.**
Conetori with internal V-tube, external V- tube

**3. Multi Tori**

The torus of $g = 1$ is the simplest one in the series of objects of high genera. Such structures can be generated by opening the Platonic solids, operated by some map operations. In the following some of the most interesting classes of multi tori are illustrated and characterized from the topological point of view.

### ***3.1. Tori of g =2 and g =3***

By intersecting two simple tori in one or two points, multi tori of *g*=2 and *g*=3, respectively, can be constructed (Figure 6).
Systematic construction of such multi tori is based on the Platonic solids: they are operated by some map operations, *e.g.*, quadrupling *Q*, capra *Ca*, etc., and next every original face opened. In this way, repeat units in possible infinite lattices or finite multi tori, by joining every pair of open faces by an appropriate nanotube segment, can be constructed. The objects in Figure 7 originate in the tetrahedron T while those in Figures 8 to 11 in the cube C.

DT; $v$=936; $e$=1404; $f_7$=12; $f_6$=454; $g$=2; S=5.81

TT; $v$=984; $e$=1476; $f_7$=24; $f_6$=464; $g$=3=2x2-1; S=6.77

**Figure 6.**
Multi tori of genera g=2 and g=3

DT(T); $v$ = 124; $e$ = 186 $f_7$=12; $f_6$=48; $g$ = 2; S = 14.44

Op(Ca(T)) ; $v$ = 40; $e$ = 54; $f_7$= 12; $g$ = 2; S = 10.432

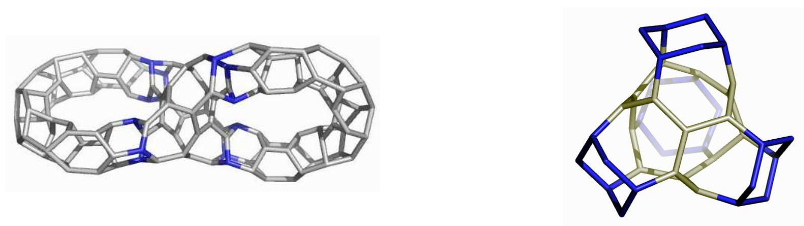


**Figure 7**.
*Double torus of g=2*, and its core derived from the tetrahedron T

Observe the objects in Figure 8 are isomers having the open faces of the cube ended as the “armchair” - V - tube (a) and “zig-zag” - H - tube (b). Clearly, the attached tubes have to have the same open ends. Also note the very low strain in the (b) object, which is further observed in the derived triple torus (Figure 9b, compared with Figure 9a). The both objects in Figure 8 were inferred in the molecular realization of the celebrate Dyck graph,[16-18] on 32 vertices of valence 3, 48 edges, 12 octagons, girth 6, diameter 5, and chromatic number 2. It is non-planar and has the genus $g$ = 1 (*i.e.*, there exists an embedding of the graph on the torus).[17] Cycle counting revealed 12 octagons and 16 hexagons.

(a) $E_{2a}(Q(C))$; $v$ = 56; $e$ = 72; $f_8$ = 12; $g$ = 3 ; S =2.05

(b) $E_1(Q(C))$; $v$ = 56; $e$ = 72; $f_8$ = 12; $g$ = 3 ; S = 0.50

**Figure 8.**
Core units for m*ulti tori of high genera*, derived from the cube C

TT(C)_264V_CCA12A; $v$ = 264; $e$ = 396; $f_8$=12; $f_6$=116; $g$ = 3; S = 13.86

TT(C)_296H_CQSI7; $v$ = 296; $e$ = 444; $f_8$=12; $f_6$=132; $g$ = 3; S = 10.01

**Figure 9**.
*Triple tori*, $g$=3 with the core derived from the cube C

The strain S, in terms of the POAV1 theory,[19-22] of such objects of high genera[18] is relaxed as the number of atoms increases. It is evident, when compare the structures in Figures 10 (320 atoms) and 11 (2240 atoms), with a clear drop in their strain.

TT_320H_CA; $v$ = 320;
$e$ = 480; $f_7$=24; $f_6$=132; $g$ = 3
S = 9.29

(b) $Op(Ca(C))$; S = 2.171
$v$ = 80; $e$ = 108; $f_7$ = 24; $g$ = 3

**Figure 10.**
*Triple torus*, $g$=3 and its core derived from the cube C

$Ca_S(TTH\_CA_R)$; $v$ =2240; $e$ = 3360; $f_7$=24; $f_6$=1092; $g$ = 3; S = 2.54

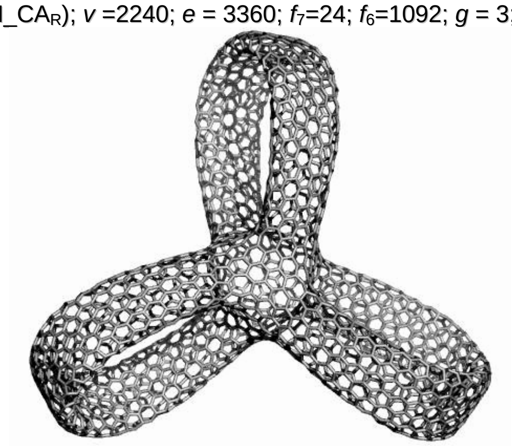


**Figure 11.**
A more relaxed t*riple torus*, $g$=3, by Capra operation

### *3.2. Structures of High Genera*

Structures of high genera can be generated, as above mentioned, by opening the Platonic solids, operated by some map operations. Units derived as above may form either infinite lattices of negative curvature[23-26] or closed cages, showing porous structure. Spongy carbons have been recently synthesized.[27] Objects like those in Figure 12, of genus 5, can be built up, on the unit derived by opening the chamfering/quadrupling transform of cube (see Figure 8), by closing together six cones emerging from the open faces. They are isomers comprising either a V or an H tubular inner unit.

| (a) PTCV; $v$ = 248; $e$ = 372; $f_8$=24; $f_6$=92; $g$ =5; S=5.47 | (b) PTCH; $v$ = 248; $e$ = 372; $f_7$=24; $f_8$=12; $f_6$=80; $g$ =5; S= 5.65<br>HF=17.74; Gap=4.56; $D_{2h}$ |
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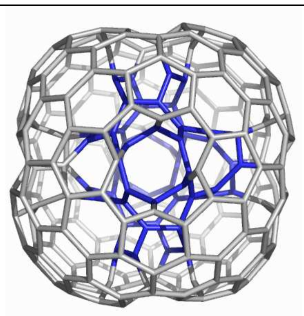
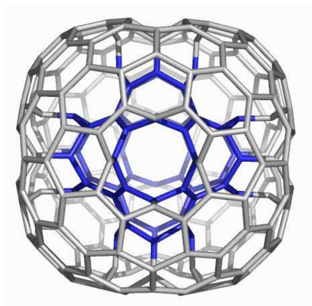
|  |  |

**Figure 12.**
*Multi tori, g*=5, with the core derived from the cube C

Objects of high genera have also been modeled by Lenosky et al.,[23,24] Terrones *et al*.[25,26] and more recently by Lijnen and Ceulemans.[18]

Structures have been optimized at the Amber MM HyperChem level (Polak-Ribiere conjugate gradient, at RMS = 0.005) and the strain computed by the JSChem software program.[28]

**Conclusions**

Conical zones are involved in several nanostructures, starting from the intersecting units of nanotubes to finite or infinite structures. Multi tori appear in zeolites or in spongy (carbon) structures, as parts of the infinite P- or FRD-type negatively curved surfaces. The toroidal objects including conical zones could appear as real molecular structures, as the nanotubes filled by spherical fullerenes turn in double walled nanotubes, the sealing of which enabling (elongated) toroidal structures with distinct walls.

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